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International Nuclear Energy Research Initiative

2005 Annual Report

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Foreword

The International Nuclear Energy Research Initiative (I-NERI) was established by the U.S. Department of Energy (DOE) in fiscal year (FY) 2001 as a mechanism for conducting collaborative research and development (R&D) with international partners in advanced nuclear energy systems development. I-NERI was created in response to recommendations of the President's Committee of Advisors on Science and Technology (PCAST) in the Committee's 1999 report entitled *Powerful Partnerships: The Federal Role in International Cooperation on Energy Innovation.*

The international collaborative research of I-NERI allows DOE to better leverage its economic resources, expand its knowledge base on nuclear science and engineering, and establish valuable intellectual relationships with researchers from other countries. Current collaborating countries and international organizations include: Brazil, Canada, the European Union, France, Japan, the Republic of Korea, and the Organization for Economic Cooperation and Development/Nuclear Energy Agency.

I-NERI R&D directly supports the goals and objectives of DOE's Generation IV Nuclear Energy Systems Initiative, the Advanced Fuel Cycle Initiative, and the Nuclear Hydrogen Initiative. In FY 2005, a new Implementing Arrangement was signed with Japan, and new projects were initiated with Brazil, Japan, and the Republic of Korea.

The I-NERI Program also promotes the education of our future nuclear scientists and engineers. In 2005, 85 students from undergraduate, graduate, and doctoral programs participated in I-NERI research projects at 12 U.S. universities.

This annual report describes the FY 2005 programmatic accomplishments and summarizes progress on I-NERI research projects initiated in FY 2002 through FY 2005 based on information submitted by the principal investigators.

Dennis R. Spurgeon, Assistant Secretary
for Nuclear Energy
U.S. Department of Energy

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International Nuclear Energy Research Initiative

1.0 Introduction

The International Nuclear Energy Research Initiative (I-NERI) supports the *National Energy Policy* by conducting research to advance the state of nuclear science and technology in the United States (U.S.). I-NERI sponsors innovative scientific and engineering research and development (R&D) in cooperation with participating countries. The research performed under the I-NERI umbrella addresses the key issues affecting the future of nuclear energy and its global deployment. I-NERI research is directed towards improving cost performance, increasing proliferation resistance, enhancing safety, and improving the waste management of future nuclear energy systems. A link to the program website can be found at http://www.nuclear.gov/programoffices.html.

This *I-NERI 2005 Annual Report* serves to inform interested parties about the program's organization, progress of the collaborative research projects, and future plans for the program. It covers I-NERI activity since FY 2002.

Section 2 of this report discusses background information on the series of events that led to the creation of the I-NERI program. The participating countries in current I-NERI collaborative agreements are also presented.

Section 3 presents an overview of program goals and objectives, a work scope summary for the three constituent program areas, a description of the I-NERI organization, and an overview of funding since the program's inception.

A summary of programmatic accomplishments is presented in Section 4 highlighting key activities for each year of the program, areas of research under each bilateral agreement, and a profile of participating organizations. This section also identifies the ten projects completed in FY 2005.

Details of the R&D work scope for current I-NERI collaborative projects with Brazil, Canada, the European Union, France, Japan, the Republic of Korea, and the Organization for Economic Cooperation and Development (OECD) are presented in Sections 5 through 11, respectively. For each participating country, the report presents an index of projects and collaborating organizations, along with a summary of technical accomplishments achieved by each project in FY 2005.

2.0 Background

In January 1997, President Clinton requested that his Committee of Advisors on Science and Technology (PCAST) review the current national energy 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 responding to this request, the PCAST Energy R&D Panel determined that ensuring a viable nuclear energy option to help meet the U.S. future energy needs was of great importance. The panel thereby recommended that a properly focused R&D effort should be implemented by the U.S. Department of Energy (DOE) to address the principal obstacles to achieving the nuclear energy option. The DOE R&D effort was also to focus on improving cost performance, increasing proliferation resistance, enhancing safety, and improving the waste management of nuclear energy systems.

In response to the PCAST recommendations, DOE established the Nuclear Energy Research Initiative (NERI) in 1999. Information and annual reports on the NERI program are available at the NERI website: http://neri.ne.doe.gov.

Recognizing the need for an international component of the NERI program, PCAST issued a subsequent report in June of 1999 entitled *Powerful Partnerships: The Federal Role in International Cooperation on Energy Innovation*, which promotes "bilateral and multilateral research focused on advanced technologies for improving the cost, safety, waste management, and proliferation resistance of nuclear fission energy systems." The report further states, "The costs of exploring new technological approaches that might deal effectively with the multiple challenges posed by conventional nuclear power are too great for the United States or any other single country to bear, so that a pooling of international resources is needed..."

The I-NERI component of NERI was established in FY 2001 in response to PCAST recommendations. The I-NERI activity is designed to enhance DOE's ability to leverage its limited research funding for nuclear technology research with additional funding from other countries.

To date, seven I-NERI collaborative agreements have been fully implemented between DOE and the following international partners:

- Commissariat à l'Energie Atomique (CEA) of France
- Republic of Korea Ministry of Science and Technology (MOST)
- Organization for Economic Cooperation and Development (OECD)/Nuclear Energy Agency (NEA). (The U.S. Nuclear Regulatory Commission (NRC) is the primary U.S. client, with DOE as a contributing partner.)
- European Atomic Energy Community (EURATOM)
- Department of Natural Resources Canada
- Brazilian Ministry of Science and Technology (MST)
- Agency of Natural Resources and Energy of Japan (ANRE) and the Ministry of Education, Culture, Sports, Science, and Technology of Japan (MEXT)

Since the program's inception, a total of 58 projects have been initiated: 16 with France, 21 with the Republic of Korea, 10 with the European Union, 7 with Canada, 2 with Brazil, and 2 with Japan. DOE is engaged in discussions with the Republic of South Africa (agreement expected in FY 2006), the United Kingdom, and Argentina, with the intent of establishing additional I-NERI collaborations.

3.0 I-NERI Program Description

3.1 Mission

The I-NERI program has the mission of sponsoring innovative scientific and engineering R&D in cooperation with participating countries. The I-NERI mission includes the directive to address key issues affecting the future use of nuclear energy and its global deployment by improving cost performance, increasing proliferation resistance, enhancing safety, and improving the waste management of future nuclear energy systems.

3.2 Goals and Objectives

Through its mission, the I-NERI program is designed to foster closer collaboration with international researchers, improve communications, and expand the sharing of nuclear research information. In order to accomplish its assigned mission, the I-NERI program has established the following overall objectives:

- Develop advanced concepts and scientific breakthroughs in nuclear energy and reactor technology in order to address and overcome the principal technical and scientific obstacles to the expanded use of worldwide nuclear energy
- Promote collaboration with international agencies and research organizations in order to improve the development of nuclear energy
- Promote and maintain a nuclear science and engineering infrastructure in order to resolve future technical challenges

Since the I-NERI program's inception, the Office of Nuclear Energy (NE) has coordinated wide-ranging activities among governments, industry, and the worldwide research community regarding the development of advanced nuclear energy systems.

3.3 International Agreements

In order to initiate an international collaboration, a government-to-government agreement must be in place. I-NERI agreements were established to allow international bilateral R&D collaborations in the area of nuclear technology. These agreements are the vehicle to conduct Generation IV, AFCI, and NHI R&D with member countries of the Generation IV International Forum (GIF). There are currently 11 GIF members: Argentina, Brazil, Canada, European Union, France, Japan, Republic of Korea, Republic of South Africa, Switzerland, the United Kingdom, and the United States. The United States has established I-NERI bilateral agreements with six of these members (Brazil, Canada, European Union, France, Japan, and the Republic of Korea) plus the OECD. The GIF partners are in the process of establishing agreements to conduct multilateral R&D among GIF countries. In the meantime, I-NERI, through the implementation of these bilateral agreements, enables R&D collaborations to begin developing next generation energy systems.

3.4 Program Organization and Control

NE manages I-NERI, with advice from the Nuclear Energy Research Advisory Committee (NERAC). NE's Office of International Nuclear Affairs negotiates and establishes the I-NERI bilateral agreements. After agreements are established, the office of Advanced Nuclear Research manages the R&D work under these agreements. The I-NERI Program Manager manages the overall implementation of the agreements and administers all international collaborations under these agreements. The Idaho Operations Office (ID) negotiates and monitors the cooperation agreements with U.S. entities.

The U.S. appoints a DOE Country Coordinator for each I-NERI collaboration who represents the United States in bilateral meetings and negotiates areas of collaboration, selects new projects, and evaluates existing projects. The collaborating country establishes a similar function.

The U.S. also appoints technical coordinators for each of the R&D areas of the agreement. These are the National Technical Directors (NTDs), who are assisted by System Integration Managers (SIMs). There are seven NTDs to represent the seven technology areas of the Generation IV and the Advanced Fuel Cycle Initiatives: 1) systems analysis, 2) fuels, 3) materials, 4) energy conversion, 5) chemical separations, 6) transmutations, and 7) system design and evaluation. The SIMs manage the technologies for each of the six Generation IV reactor concepts. The NHI program also has Technical Directors (TDs) for its major research areas of thermochemical cycles, high temperature electrolysis, and systems interface.

The NTDs, SIMs, and TDs assist the Country Coordinators in identifying cooperative research areas and defining specific work scopes. They review periodic progress reports and advise the Country Coordinator. They also participate on a panel of technical experts to formally evaluate the projects during annual project reviews.

Figure 1 illustrates the DOE organizational structure for control and administration of the I-NERI program during FY 2005.

3.5 Funding

Currently, I-NERI is the only vehicle for cost-shared international R&D collaboration in Generation IV, AFCI, and NHI technology. In addition, I-NERI enables collaboration with the GIF countries on a bilateral basis until multilateral agreements are established.

The I-NERI program provides an effective means for international collaboration on a leveraged, cost-shared basis. Each country in an I-NERI collaboration provides funding for their respective project participants. Actual cost-share amounts are determined for each jointly selected project. The program has a goal to achieve approximately 50-50 matching contributions from each partner country.

I-NERI projects have resulted in total leveraged U.S. contributions of $76.3 million and international contributions of $75.3 million, of which $14.0 million is from Canada, $26.4 million is from France, $18.5 million is from the Republic of Korea, $0.9 million is from Japan, $11.7 million is from the European Union, and $3.8 million is from Brazil.

Funding provided by the U.S. may only be spent by U.S. participants. I-NERI projects are typically for a duration of three years and are funded annually by the Generation IV, AFCI, and NHI programs.

3.6 Work Scope

In FY 2004, DOE restructured the I-NERI program to support scientific and engineering research and development (R&D) with participating countries whose R&D work scopes closely link to the principal NE R&D programs: Generation IV Nuclear Energy Systems Initiative, Advanced Fuel Cycle Initiative (AFCI), and Nuclear Hydrogen Initiative (NHI). The work scopes of the FY 2005 I-NERI projects were defined so that they supported the R&D needs of these programs as well.

Candidate project work scopes are jointly developed by the U.S. and the collaborating country. The U.S. contribution to the work scope is based upon current-year budgets and a review of the technical quality and budget of the proposed joint projects in order to make recommendations to the Country Coordinators.

The Country Coordinators select R&D projects based on conformance with the bilateral agreement and current

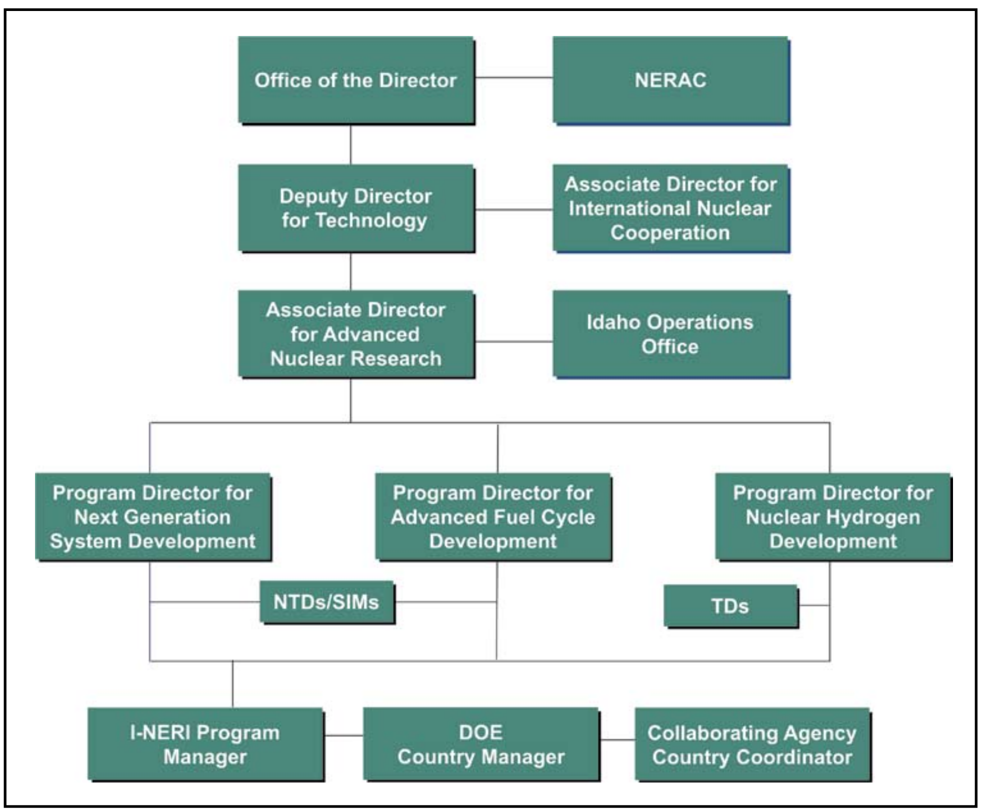

Figure 1. Office of Nuclear Energy I-NERI organizational chart in FY 2005.

Generation IV, AFCI, and NHI programmatic needs.

Following is an overview of the individual work scopes for the three programs:

Generation IV Nuclear Energy Systems Initiative. The Generation IV program is developing next-generation nuclear energy systems that offer advantages in the areas of economics, safety, reliability, and sustainability, with a goal of commercial deployment by 2030. Using a technology roadmap that was created by member countries in the Generation IV International Forum (GIF), this program was assigned six reactor system and fuel cycle concepts that were deemed most promising for achieving the aforementioned advantages. These designs are the: Gas-Cooled Fast Reactor (GFR), Lead-Cooled Fast Reactor (LFR), Molten Salt Reactor (MSR), Sodium-Cooled Fast Reactor (SFR), Super-Critical Water-Cooled Reactor (SCWR), and the Very-High Temperature Reactor (VHTR). The program has eight technology goals:

1) Provide sustainable energy generation that meets clean air objectives and promotes long-term availability of systems and effective fuel utilization for worldwide energy production
2) Minimize and manage nuclear waste, notably reducing the long-term stewardship burden in the future and thereby improving protection for the public health and the environment
3) Increase assurances against diversion or theft of weapons-usable materials
4) Ensure high safety and reliability
5) Design systems with very low likelihood and degree of reactor core damage
6) Create reactor designs that eliminate the need for offsite emergency response
7) Ensure that systems have a clear life-cycle cost advantage over other energy sources
8) Create systems that have a level of financial risk that is comparable to other energy projects

Advanced Fuel Cycle Initiative. This initiative responds to the 2001 *National Energy Policy* recommendation that the United States "… develop reprocessing and fuel treatment technologies that are cleaner, more efficient, less waste-intensive, and more proliferation-resistant." These technologies are key components of the fuel cycles that are required for Generation IV nuclear energy systems. Each of the six advanced reactor designs will use fuel cycles that are significantly different from those used by existing U.S. reactors. For this initiative, research must focus on recycling, fuel treatment, and conditioning technologies that have the potential to dramatically reduce the quantity and toxicity of spent nuclear fuel, thus decreasing the need for geological disposal. The AFCI mission is to develop proliferation-resistant spent nuclear fuel treatment and transmutation technologies in order to enable a transition from the current once-through nuclear fuel cycle to a future sustainable closed nuclear fuel cycle.

Nuclear Hydrogen Initiative. The NHI program supports the President's Hydrogen Fuel Initiative. The goal of this initiative is to develop the technologies and infrastructure to economically produce, store, and distribute hydrogen for use in fuel cell vehicles and electricity generation. Hydrogen can be produced using a variety of technologies, each of which has its advantages and limitations. The primary advantage of nuclear energy production technologies is the ability to produce hydrogen in large quantities, at a relatively low cost, without the emission of any greenhouse gases. The goal of the NHI is to demonstrate the commercial-scale, economically feasible production of hydrogen using nuclear energy by the year 2020. The NHI will conduct R&D on enabling technologies, demonstrate nuclear-based hydrogen producing technologies, study potential hydrogen production schemes, and develop deployment alternatives to meet future needs for increased hydrogen consumption.

4.0 I-NERI Program Accomplishments

The I-NERI program began in the second quarter of FY 2001 with an initial focus on developing international collaborations, program planning, and project procurements. Awards for the first set of I-NERI collaborative research projects with France were made at the end of FY 2001. The I-NERI program's progress for FY 2001 through 2005 is summarized in Section 4.1.

4.1 Programmatic Accomplishments

The primary programmatic accomplishments during each year of the I-NERI program's lifetime, along with planned accomplishments for the upcoming fiscal year, are briefly described below.

FY 2001-2004 Accomplishments. In FY 2001, the first year of the I-NERI program, DOE signed collaborative agreements with the Republic of Korea and France. By the end of FY 2001, the U.S./France collaboration was initiated with the award of four projects. A competitive procurement was conducted for the U.S./Republic of Korea collaboration.

In FY 2002, the U.S. and the Republic of Korea (ROK) awarded the first six projects. OECD signed on with a new collaboration agreement, under which one new project was awarded. One new project was also initiated under the U.S./France collaboration.

In FY 2003, five new awards were initiated under the U.S./Republic of Korea collaboration. DOE also signed I-NERI cooperative agreements with the European Commission, Canada, and Brazil.

In FY 2004, I-NERI researchers completed two U.S./France projects that were awarded in FY 2001. Seven new projects were initiated with Canada, eleven with France, six with Korea, and eight with the European Union. Japan became an I-NERI participant during Fiscal Year 2004, signing a new cooperative agreement.

FY 2005 Accomplishments. During FY 2005, four new projects were initiated with the Republic of Korea, two with the European Union, one with Brazil, and one with Japan. U.S. contributions for FY 2005 totaled $17.0 million, plus another $18.7 million of international contributions that includes $3.8 million from Canada, $5.0 million from the European Union, $5.4 million from France, $3.5 million from the Republic of Korea, $0.7 million from Japan, and $0.4 million from Brazil.

During this fiscal year, researchers completed work on eight cooperative projects that began in FY 2001 through 2003. Final activities are ongoing for the remaining two FY 2003 projects. Following is a summary of noteworthy accomplishments achieved during FY 2005:

- Initiated the first research project under the U.S. bilateral agreement with Brazil
- Initiated the first research project under the U.S. bilateral agreement with Japan
- Added four new projects to the U.S. Korea collaboration
- Completed FY 2004 annual project performance review for the U.S./Canada, European Union, France, and Republic of Korea collaborations

Planned FY 2006 Activities. Following is a list of activities that are planned for FY 2006:

- Initiate a new research project under the agreement with Japan in March 2006
- Initiate a new research project under the agreement with Brazil in April 2006
- Initiate new cooperative projects under other existing agreements
- Sign a new cooperative research agreement with South Africa
- Continue pursuing cooperative agreements with the United Kingdom, Argentina, and other prospective partner countries

4.2 Current I-NERI Collaborations

In FY 2005, there were 40 ongoing I-NERI projects. Brief descriptions of these I-NERI collaborations are provided in the sections that follow. Descriptions of the work scopes, listings of funded projects, and brief project status reports are provided in Sections 5 through 11 for the joint nuclear research that the U.S. has undertaken with each foreign partner.

Table 1 presents a breakdown of the number of project awards for each country by fiscal year. Figure 2 shows the distribution of projects by each of the three major program areas since the program's inception. It should be noted that prior to FY 2004 all of the projects were related strictly to the Generation IV initiative.

Brazil. Cooperative research projects with the Brazilian Ministry of Science and Technology (MST) will take place primarily in the areas of advanced nuclear fuels and materials, based on a bilateral agreement signed June 20,

Collaborating Country	FY 01	FY 02	FY 03	FY 04	FY 05	FY 06	Total
France	4	1		11			16
Korea		6	5	6	4		21
EURATOM				8	2		10
Canada				7			7
Brazil					1	1	2
Japan					1	1	2
Total	4	7	5	32	8	2	58

Table 1. Number of projects awarded.

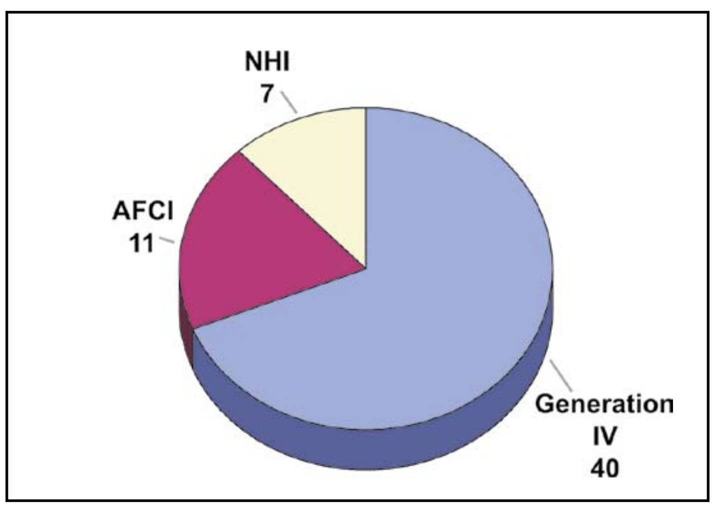

Figure 2. Project distribution by program area.

2003. Research with Brazil will entail instrumentation, operations and control, and human interaction of the Integral Primary System Reactor (IPSR), along with an investigation into shared resources for multiple modular reactor designs.

Canada. The collaborating agency in Canada is Atomic Energy of Canada Limited (AECL). The U.S./Canada collaboration includes R&D proposals in the Generation IV, AFCI, and NHI areas under a June 17, 2003 bilateral agreement. Coooperative research will focus on nuclear hydrogen production, sustainable and advanced fuel cycles, and supercritical water reactors.

European Union. The collaborating agency for the European Union (EU) is the European Commission. The U.S./EU collaboration includes R&D proposals in the Generation IV, AFCI, and NHI areas under a March 6, 2003 bilateral agreement. Cooperative research will be undertaken in the areas of reactor fuels and materials, advanced reactor design, and transmutation of high-level waste.

France. The collaborating agency in France is the Commissariat à l'Énergie Atomique (CEA). The U.S./France collaboration focuses on developing Generation IV advanced nuclear system technologies that will enable the U.S. and France to move forward with cutting-edge R&D that will benefit the range of anticipated future reactor and fuel cycle designs. Specific R&D topical areas, under the July 9, 2001 bilateral agreement, include advanced gas-cooled reactors, fuel and materials development, simulation of radiation damage, and nuclear hydrogen production.

Japan. An agreement was signed with the Agency of Natural Resources and Energy (ANRE) of Japan on May 26, 2004. The areas of collaboration under this agreement are innovative light water technologies, innovative processing technologies of reactor fuel for light water reactors, innovative fuel technologies using solvent extraction, and radioactive waste management. On February 8, 2005, DOE and Japan's Ministry of Education, Culture and Sports, Science and Technology (MEXT) signed the Implementing Arrangement concerning cooperation in the field of research and development of innovative nuclear energy technologies including reactor design, processing technologies, and solvent extraction.

Republic of Korea. The participating agency in the Republic of Korea is the Ministry of Science and Technology (MOST). The U.S./Republic of Korea collaboration focuses on advanced technologies for improving the cost, safety, and proliferation resistance of nuclear energy systems, based on a May 16, 2001 bilateral agreement. Research areas include next-generation reactor and fuel cycle design, innovative plant design, advanced fuels/materials, gas-cooled fast reactors, supercritical water reactors, and nuclear hydrogen prouction. Within these areas of collaboration, I-NERI projects were selected competitively from researcher-initiated proposals based upon the results of independent peer-evaluation processes.

OECD. The U.S. teamed with a number of the 30 member states of OECD NEA to conduct reactor materials experiments and associated analyses. The U.S. funding team consists of the NRC, the Electric Power Research Institute (EPRI), and DOE. DOE funded the first three years of this research. The bilateral agreement signed March 2002 addresses research to resolve ex-vessel debris coolability issues and molten core-concrete interaction.

4.3 Program Participants

This subsection provides an organizational profile for the seven bilateral agreements and a complete list of the I-NERI program participants. In addition, it presents the level of U.S. university student participation in active I-NERI projects during 2005.

Award Profiles. Figure 3 illustrates the number of current I-NERI collaborators by type of organization. Table 3 provides a detailed breakdown of the participating organizations.

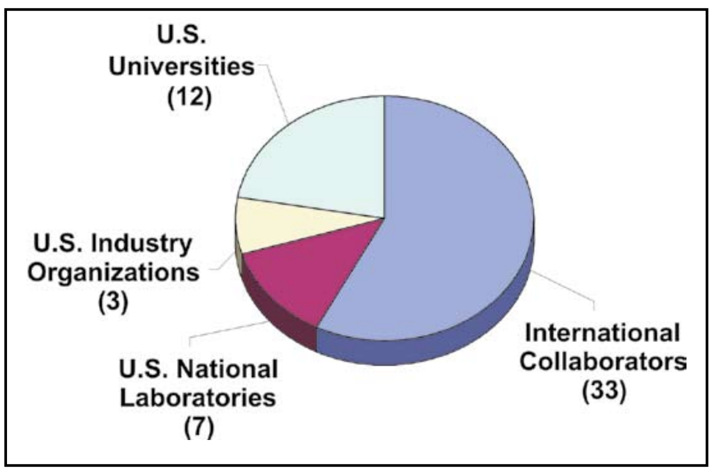

Figure 3. I-NERI organizational profile.

U.S. Student Participation. As noted in Figure 3, a total of 12 U.S. universities and colleges participated in I-NERI research projects in 2005. Approximately 85 students from these institutions worked on active I-NERI research projects during the year. Their distribution by university degree level is noted in Figure 4.

Table 3: Organizations participating in I-NERI research projects.

U.S. National Laboratories

Argonne National Laboratory
Brookhaven National Laboratory
Idaho National Laboratory
Los Alamos National Laboratory
Oak Ridge National Laboratory
Pacific Northwest National Laboratory
Sandia National Laboratories

U.S. Industry Organizations

Gamma Engineering
General Atomics
Westinghouse Electric

U.S. Universities

Iowa State University
Massachusetts Institute of Technology
Ohio State University
Pennsylvania State University
Purdue University
University of California-Santa Barbara
University of Florida
University of Illinois at Chicago
University of Maryland
University of Michigan
University of Notre Dame
University of Wisconsin

International Collaborators

Industry Organizations

Atomic Energy of Canada Limited
Electronuclear
Framatome-ANP, Lyon
Gass Technology Institute
Hitachi Works
Hitachi, LTD
Korea Hydro and Nuclear Power Company
Toshiba Corporation

Universities

Cheju University
Chosun University
Chungnam National University
École Polytechnique de Montréal
Hanyang University
Korean Maritime University
Pusan National University
Seoul National University
Tohoku University
University of Manchester
University of Manitoba
University of Sherbrooke
University of Tokyo
University of Bordeaux

Governmental Organizations

Brazilian Ministry of Science and Technology
Chalk River Laboratories
Commissariat à l'Energie Atomique (CEA)
Instituto de Pesquisas Energéticas e Nuclearares (IPEN)
Japan Atomic Energy Research Institute (JAERI)
Joint Research Center Institute for Transuranium Elements (ITU)
Japan Atomic Energy Agency (JAEA)
Korea Advanced Institute of Science and Technology (KAIST)
Korea Atomic Energy Research Institute (KAERI)
Korean Electric Power Research Institute (KEPRI)
Organization for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA)

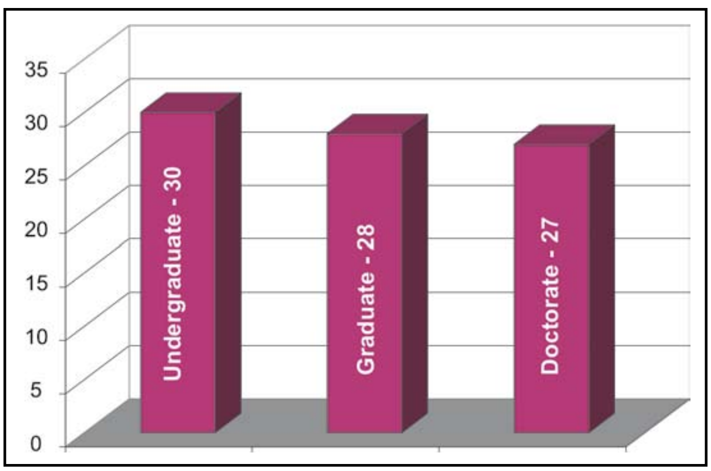

Figure 4. 2005 I-NERI U.S. student participation profile.

4.4 Completed I-NERI Projects

This year marked the completion of five FY 2003 I-NERI projects, three projects from FY 2002 and two projects carried over from FY 2001. Note that research on two FY 2003 projects is being carried into the following fiscal year through no-cost extensions.

Based on the documented accomplishments, it is apparent that the I-NERI program's stated goals and objectives continue to be satisfied. Collaborative efforts between the public and private sectors in both the U.S. and partnering foreign countries have resulted in significant scientific and technological enhancements in the global nuclear power arena. The international collaborations have forged lasting ties that will continue promoting the strong infrastructure necessary to overcome future challenges to the expanded use of this vital source of clean and reliable power. In conjunction with parallel efforts undertaken by the NERI program, Generation IV, AFCI, and NHI, this program has helped to revive the Nation's leadership role in international nuclear R&D. The resulting technological and scientific advances will ensure that the U.S. remains competitive in both the global and domestic nuclear energy marketplaces.

Table 4 notes the ten projects completed in 2005. More detailed information on each can be found in the corresponding project summaries in Sections 5 through 11 of this report.

Project Number	Title	Lead Organization
2001-007-F	Nano-Composited Steels for Nuclear Applications	Oak Ridge National Laboratory
2001-002-F	Development of Generation IV Advanced Gas-Cooled Reactors with Hardened/Fast Neutron Spectrum	Argonne National Laboratory
2002-001-F	High-Efficiency Hydrogen Production from Nuclear Energy: Laboratory Demonstration of S-I Water Splitting	Sandia National Laboratories
2002-001-N	Melt Coolability and Concrete Interaction (MCCI) Program	Argonne National Laboratory
2002-016-K	Advanced Computational Thermal Fluid Physics (CTFP) and its Assessment for Light Water Reactors and Supercritical Reactors	Idaho National Laboratory
2003-002-K	Passive Safety Optimization in Liquid Sodium-Cooled Reactors	Argonne National Laboratory
2003-008-K	Developing and Evaluating Candidate Materials for Generation IV Supercritical Water Reactors	Idaho National Laboratory
2003-013-K	Development of Safety Analysis Codes and Experimental Validation for a Very-High-Temperature Gas-Cooled Reactor	Idaho National Laboratory
2003-020-K	Advanced Corrosion-Resistent Zirconium Alloys for High Burnup and Generation IV Applications	The Pennsylvania State University
2003-024-K	Development of Structural Materials to Enable the Electrochemical Reduction of Spent Oxide Nuclear Fuel in a Molten Salt Electrolyte	Argonne National Laboratory

Table 4. I-NERI projects completed in 2005.

5.0 U.S./Brazil Collaboration

The U.S. Department of Energy (DOE) and the Brazilian Ministry of Science and Technology (MST) signed a bilateral agreement on June 20, 2003. The U.S. Secretary of Energy, Spencer Abraham, signed the agreement with Brazilian Minister of Science and Technology, Roberto Amaral. The first collaborative project under this agreement was awarded in FY 2005.

5.1 Work Scope Areas

R&D topical areas for the U.S./Brazil collaboration include:

- Advanced reactor developments for future-generation nuclear energy systems
- Advanced reactor fuel and reactor fuel cycle integration
- Life management and upgrading of current operating reactors
- Advanced fuel and material irradiation and use of experimental facilities
- Environmental and safety issues related to new reactor and fuel cycle technologies
- Fundamental areas of nuclear engineering and science

5.2 Project Summaries

One new project was awarded during FY 2005. An abstract of this project follows.

Directory of Project Summaries

Development of Advanced Instrumentation and Control for an Integral Primary System Reactor

PI (U.S.): D. Holcomb, Oak Ridge National Laboratory

PI (Brazil): Antonio Barroso, Instituto de Pesquisas Energéticas e Nucleares (IPEN)

Collaborator: Westinghouse Electric Company

Project Number: 2005-001-B

Project Start Date: March 2005

Project End Date: September 2008

Project Abstract

The Integral Primary System Reactor (IPSR), one of the International Near-Term Deployment (INTD) concepts, has gained considerable attention and interest as a viable Generation IV design. Among the technical issues to be addressed for IPSR deployment are the lack of a systematic assessment of unique instrumentation requirements, the need for innovative approaches to plant operation and control, and interaction of the human operator with plant systems.

A significant instrumentation challenge for the International Reactor Innovative and Secure (IRIS) design, a leading IPSR candidate, is obtaining accurate in-vessel water level measurements due to the irregular internal geometry. The research team will investigate two measurement systems: an ultrasonic, torsional waveguide-based technique and a cooled-fluid-based lance type probe with advanced signal processing algorithms. The researchers propose to overcome the technological limitations of ultrasonic in-vessel water level measurement—signal transmission and complex analysis—by enclosing the entire transduction system within the reactor vessel so only electrical signals are transmitted through the pressure boundary. The cooled-fluid based probe is a new device that makes use of fluid flow and the difference in heat-transfer coefficients in the vapor and liquid regions, applying modern digital signal processing and finite element techniques to determine water level and density.

This study will also assess approaches to IPSR plant operation and control. In support of this objective, the IRIS consortium will make plant models available, and researchers will address specific areas that require further consideration. For example, co-generation (i.e., desalination, heating/steam, hydrogen production, etc.) is an attractive option for modular reactors, but optimization requires reconfiguration of the balance-of-plant as electrical load varies. This entails development of a hierarchical supervisory control system.

The final area of the proposed research is the interaction of the operator with the plant control and protection systems. Most IPSR concepts, unlike current light water reactors, can respond to transients or accidents without operator action because transients evolve very slowly due to the plant's large thermal inertia. This project will study emergency procedure guidelines, human-machine interfaces, and control room architecture, taking into account the possibility of controlling multiple modules from a single control room. Researchers will investigate self-organized maps, a special class of artificial neural networks, to support operator actions and decision-making.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

6.0 U.S./Canada Collaboration

The Director of NE, William D. Magwood IV, signed a bilateral agreement on June 17, 2003, with the Assistant Deputy Minister of the Department of Natural Resources Canada, Ric Cameron, and the Senior Vice President Technology of Atomic Energy of Canada Limited, David F. Torgerson. The first U.S./Canada collaborative research projects were awarded in FY 2004.

6.1 Work Scope Areas

R&D topical areas for the U.S./Canada collaboration include:

- Hydrogen production by nuclear systems
- Sustainable and advanced fuel cycles
- Supercritical water-cooled reactor concepts

6.2 Project Summaries

In FY 2004, the initial year of the collaboration, seven research projects were initiated. These projects continued into FY 2005. A listing of the I-NERI U.S./Canada projects that are currently underway follows, along with summaries of the accomplishments achieved in FY 2005.

Directory of Project Summaries

High-Temperature Electrolyzer Optimization

PI (U.S.): Richard D. Doctor, Argonne National Laboratory

PI (Canada): Atomic Energy of Canada Limited (AECL)

Collaborators: Chalk River Laboratories, Idaho National Laboratory (INL)

Project Number: 2004-001-C

Project Start Date: May 2004

Project End Date: December 2006

Research Objectives

The objective of this project is to thermally optimize the High Temperature Electrolysis-Very High Temperature Gas Reactor (HTE-VHTR) combined plant. The primary tasks are to perform computational fluid dynamics (CFD) analysis of individual flow channels in the HTE cells and carry out plant flowsheet analysis. Researchers are focusing on the electrolysis-fuel cell CFD and process design, i.e., "flowsheet" analysis.

For the particular cells being investigated, the stack can operate either as a solid-oxide fuel cell (SOFC) or a solid-oxide electrolysis cell (SOEC). Heat transfer and electrochemical efficiencies will degrade depending upon the extent of flow field deviations from uniformity inside and outside each cell of the stack. To achieve the highest net efficiency and the lowest net cost, it is necessary to completely understand the thermal and flow processes inside and outside of the cell.

Two basic cell configurations have been proposed in the literature: planar (also termed "bipolar" or "flat plate") and tubular. The planar solid-oxide fuel cell (PSOFC) can be either electrolyte or electrode (usually anode) supported. In this research, the CFD and electrochemical modeling will be initially limited to the flow pattern analysis within the fuel cell cavities of a single planar SOFC fuel cell. As the SOEC computational fluid dynamic model is completed, the results will be used in the Aspen electrolyzer model. Integrating the CFD model and the process simulation will facilitate a workflow for overall plant design optimization. This will also enable researchers to fully evaluate the required energy transfers, resulting temperatures, and overall system efficiency of different system designs.

Researchers will focus on two primary tasks. First, they will perform CFD analysis of individual flow channels in the HTE cells. Second, they will concentrate on plant flowsheet analysis to thermally optimize the HTE-VHTR plant combination based on process design and economic trade-offs.

Research Progress

In the first task, researchers investigated the CFD models using COMSOL and pursued multi-physics finite-element modeling for the HTE-cells for a configuration of 38 boundaries. A high-temperature steam electrolysis cell operates at 700-900°C. Water and air (for oxygen stripping) are supplied continuously to the cell. A solid oxide electrolysis cell works on the principle that at these elevated temperatures, the yttria-stabilized zirconia (YSZ) electrolyte becomes an oxygen ion conductor. The YSZ electrolyte is sandwiched between two porous electrodes. The porous electrode and electrolyte facilitate the formation of a three-phase boundary, an interface between the electrolyte phase, electrode phase, and gas phase, where the reaction is to take place. Water must diffuse through the porous electrode and come into the vicinity of this three-phase boundary. The electrodes must be porous enough to allow the gas to diffuse easily through them, but not so porous as to become a poor electrical conductor. The oxygen atom is then liberated from the H_2O molecule and picks up two electrons from the cathode to become an oxygen ion. This oxygen ion is then transported through the electrolyte by means of oxygen ion vacancies in the crystal lattice of the electrolyte. The oxygen ion moves from vacancy to vacancy, driven by the electric field produced by the potential applied to the electrodes. When the oxygen ion reaches the three-phase boundary at the anode-electrolyte interface, it transfers its charge to the anode material, combines with another oxygen atom to form O_2, and diffuses out of the anode.

During electrolysis, the voltage is continuously recorded to determine the losses due to overpotentials. Figure 1 shows the results for convergence of a CFD and multi-physics HTE-cell model that links CFD, heat transfer, electrolysis, chemical diffusivity, and changes in electrical resistivity for case with no radiative heat transfer. The model moves seamlessly between the fuel cell and electrolysis modes while being completely predictive of voltage and current, which are manual inputs in other models.

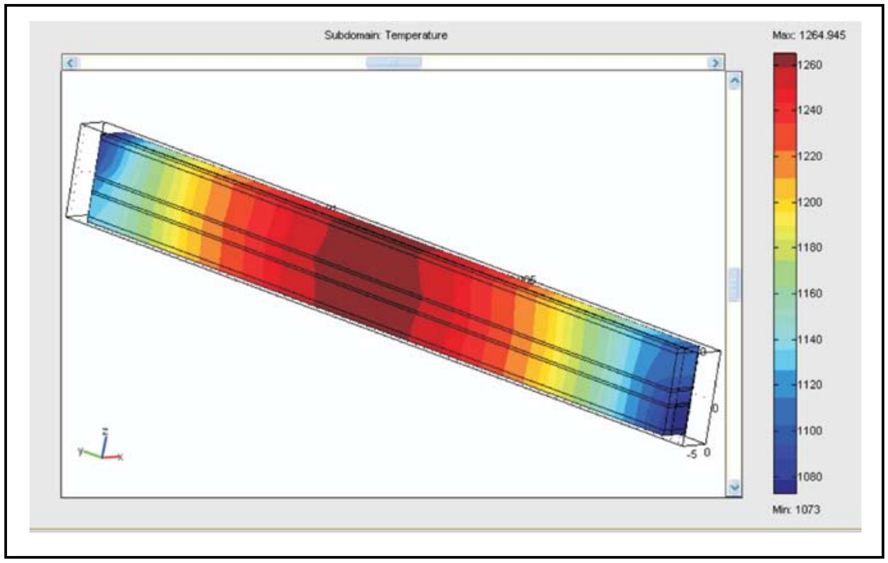

Figure 1. SOEC at 0.9 V with 9:1 H_2:H_2O and no radiative heating included.

The results were not calibrated against actual stack parameters for validation, hence are typical rather than actual values for the 1.5 mm slice through the HTE-cell. Convergence across the entire cell slice-by-slice would then need to fit into an overall stack model. While the feasibility of pursuing this approach to CFD modeling is very encouraging, at present no further work is planned.

To satisfy a second line of inquiry, researchers developed a CFD model to simulate a planar three-dimensional SOEC by using a finite element approach. This model combined an electrochemical (EC) module developed in-house and the commercially available CFD code STAR-CD. It calculates the local electrochemical kinetics of the SOEC coupled to the mass- and heat-balances of the gaseous flow and the solid medium. The main coupling between the EC and CFD modules is due to the mutual use of the temperature profile. The CFD module provides the temperature field for the EC module to generate the current density distribution by using the temperature-dependent electrochemical parameters. The EC module provides the species and heat generation rates, based on the current density that it calculates, for the CFD module to generate the consistent temperature profile. The model of the representative SOEC, as shown in Figure 2, uses 12 layers of elements: 4 layers in each flow mesh, 1 layer in each oxygen electrode (anode), and 2 layers in each hydrogen electrode (cathode). The planar area of the cell layers is divided into 40x40 elements, thus the complete cell in the finite element model is comprised of 19,200 elements.

The sensitivity of results with respect to further fineness in the discretization of the cell is negligible with the given number of elements per cell. Researchers investigated the influence of several parameters using a sensitivity analysis on efficiency, temperature, and current density profiles. The following parameters were varied for this analysis: the electrochemical properties (oxygen electrode exchange current density and hydrogen electrode limiting

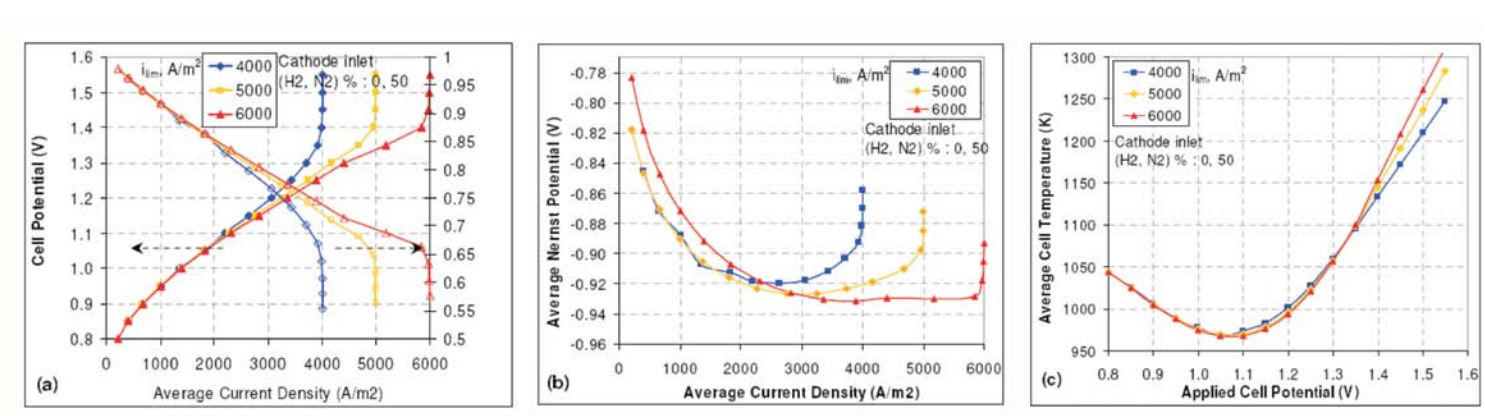

Figure 2. Effect of the hydrogen electrode limiting current density on the (a) polarization & voltage efficiency, (b) average Nernst potential, and (c) average temperature in the SOEC.

current density), hydrogen mass fraction at the cathode inlet, nitrogen mass fraction at the cathode inlet, and flow configuration (cross-flow and parallel-flow). For each case, the polarization behavior of the simulated cell was studied within the applied cell potential of 0.8–1.6 V. These promising results have been reviewed in some detail with INL. The next step is to obtain as much information as possible respecting the SOEC materials of construction and operating conditions currently being used at INL; vary the model inputs accordingly; and compare these data against experimental results for polarization, temperature, and flow before expanding further.

To achieve the highest net efficiency and the lowest net cost, a detailed understanding of the thermal and flow processes outside of the SOEC is required. The balance-of-plant process design or "flowsheet" analysis for the high-temperature electrolysis was performed using the ASPEN-Plus software package. The project team settled on a production target of 9 tonnes H_2/hr where hot hydrogen product from the SOEC was directly quenched with feed water that undergoes a phase change to steam. It is believed that this may prove to be a practical route to maximize heat recovery from the hydrogen product.

The researchers performed the following process design case studies:

- Production rate 9 tonnes H_2/hr
- Steam-reagent-grade liquid feed water at ambient conditions of temperature and pressure was assumed (i.e., the water is deareated, decarbonated, and demineralized)
- Moderate pressure operation with three bar at SOEC for inlet feeds of:
  - o 50% H_2O: 50% H_2
  - o 66.66% H_2O: 33.33% H_2
  - o 75% H_2O: 25% H_2
  - o 90% H_2O: 10% H_2
- High pressure operation with 15 bar at SOEC for inlet feeds of 75% H_2O: 25% H_2
- Conversion rate in SOEC of 50% for steam to H_2
- Hot H_2 goes to a direct quench with steam-reagent-grade liquid feed water that undergoes a phase change to steam to maximize heat recovery from hydrogen
- Air-stripping of hot O_2 product at 6:1 volume ratio with heat recovery with no O_2 product
- Delivery pressure of dry H_2 at plant boundary, or "fence" of 413.7 bar (~6,000 psig)

In each of these case studies, the researchers included a schematic of the solid oxide electrolysis cells as they would appear in the balance-of-plant configuration. They also included the major stream compositions, temperatures, pressures, and thermodynamic properties. The team is currently evaluating the overall system configuration and connectivity options, including various recycle stream options and options for heat exchangers.

Planned Activities

Planned activities will examine the case of a NorskHydro conventional electrolyzer and compare the economics for this case against economics as based on ASPEN process design studies for the SOEC following the lead of an oil industry-based project scoping approach. A major issue of concern is maintaining coordination with the overall NHI efforts to develop the balance-of-plant case design and economics. For example, it is clear that the costs of nuclear heat and electricity from Generation IV reactors are not independent variables, and having even a relative ratio of costs will greatly assist optimization efforts.

A summary of initial results using this spreadsheet program are shown in Figure 3 for the NorskHydro system. The cost of hydrogen comes to $3.09/kg using company-supplied capital costs, maintenance, and availabilities for a 15 percent rate of return and electric power at $34/MWh.

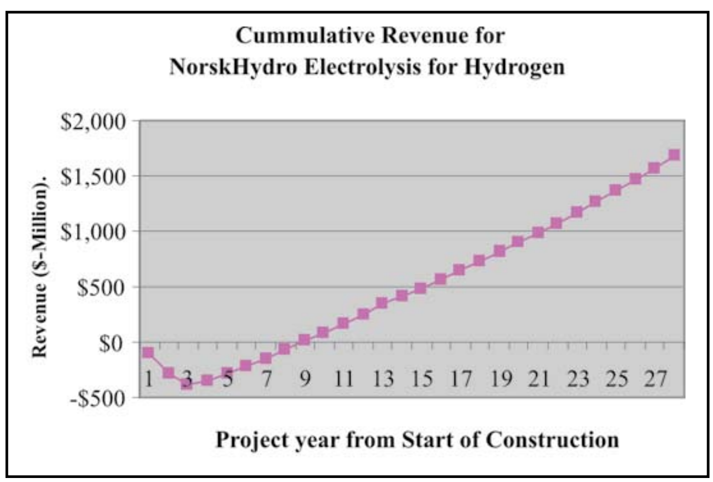

Figure 3. Projected revenue for NorskHydro H_2 electrolysis system.

Development of Inert Matrix Fuels for Plutonium and Minor Actinide Management in Power Reactors

PI (U.S.): J. Carmack, Idaho National Laboratory (INL)

PI (Canada): P. Boczar, Atomic Energy Canada Ltd. (AECL)

Collaborators: University of Florida, Los Alamos National Laboratory, Brookhaven National Laboratory

Project Number: 2004-002-C

Project Start Date: October 2004

Project End Date: September 2008

Research Objectives

There is interest in the investigation of inert matrix fuels (IMFs) for scenarios involving stabilization or burn down of plutonium for existing commercial power reactors. IMFs offer the potential advantage of more efficient destruction of plutonium and minor actinides (MA) relative to mixed oxide (MOX) fuel. Greater efficiency of plutonium reduction results in greater flexibility in managing plutonium inventories and in developing strategies for disposition of MA, as well as potential fuel cycle cost savings. Because fabrication of plutonium-bearing (and MA-bearing) fuel is expensive relative to UO^2 in terms of both capital and production, a cost benefit can be realized by reducing the number of plutonium-bearing elements required for a given burn rate. The choice of matrix material may also be manipulated either to facilitate fuel recycling or to improve proliferation resistance by making plutonium recovery extremely difficult.

In addition to improving plutonium/actinide management, an inert matrix fuel (IMF) having high thermal conductivity may provide operational and safety benefits. Lower fuel temperatures could be used either to increase operating and safety margins, to uprate reactor power, or a combination of both. The Canada Deuterium Uranium (CANDU) reactor offers flexibility in plutonium management and MA burning by virtue of on-line refueling, a simple bundle design, and good neutron economy. A full core of inert matrix fuel containing either plutonium or a plutonium-actinide mix can be utilized, with plutonium destruction efficiencies greater than 90 percent and high actinide destruction efficiencies exceeding 60 percent.

The Advanced CANDU Reactor (ACR) could allow additional possibilities in the design of an IMF bundle, since the tighter lattice pitch and light-water coolant reduce or eliminate the need to suppress coolant void reactivity, allowing the center region of the bundle to include additional fissile material and to improve actinide burning. The ACR would provide flexibility for managing both plutonium and MA from the existing light water reactor (LWR) fleet, and would be complementary to the Advanced Fuel Cycle Initiative (AFCI) in the U.S. Many of the fundamental principles concerning the use of IMF are nearly identical in the ACR and other types of LWRs, including fuel/coolant compatibility, fuel fabrication, and fuel irradiation behavior. In addition, the U.S. and Canada both have interest in developing Generation IV Super-Critical Water-Cooled Reactor (SCWR) technology, to which this fuel type would be applicable for plutonium and MA management. An inert matrix fuel with high thermal conductivity would be particularly beneficial to any SCWR concept.

Research Progress

Fuel Selection. The researchers have established goals for IMF development, assessed IMF candidates against this baseline, and selected several fuel materials for further study. Assessments have included analysis of neutronic behavior (Pu burn rate, reactivity swing), fuel thermal performance, fuel irradiation performance, and in-core corrosion resistance based on existing knowledge. They have issued a down-selection report.

Fabrication Development. Researchers have developed and qualified fabrication methods for inert-matrix fuels. They have identified fabrication methods for the various inert matrix fuels ($MgO-ZrO_2$, Zr-metal matrix) and performed test fabrication and characterization. Figure 1 is a photograph of a plutonium-bearing $MgO-ZrO_2$ matrix pellet. Figure 2 is a magnified photograph of a Zr-metal matrix fuel sample. Development of a candidate SiC inert matrix fuel composition has been initiated and preliminary fuel samples fabricated and characterized.

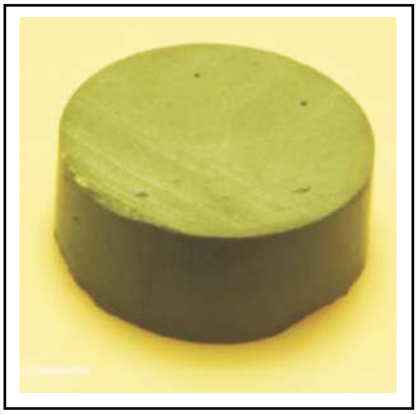

Figure 1. Photograph of dual-phase $MgO-ZrO_2-PuO_2$ pellet.

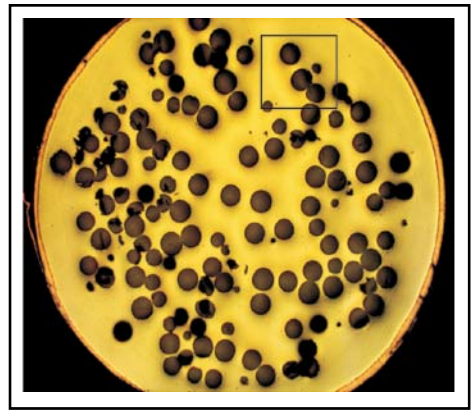

Figure 2. UO_2 particles extruded in a Zr-metal matrix.

Characterization. Experimental characterization of the candidate inert matrix fuels and matrix materials has been completed. Characterization included microstructure, thermal and mechanical properties, corrosion testing, and ion-beam irradiation in order to determine suitability for in-reactor irradiation testing and to provide a basis for fuel behavior modeling. Characterization activities will continue to further refine the fabrication processes for application to reactor test fabrication.

Fuel modeling. A finite element model has been constructed using the ABAQUS finite element analysis code to model the phase structure of both heterogeneous and homogenous inert matrices. This code allows estimation of key fuel properties, such as thermal conductivity and density, needed to support reactor irradiation experiment design and qualification. Simulations with a plutonium-only SiC-IMF and a plutonium-plus-actinides SiC-IMF were carried out. For both cases, the standard 37-element bundle was used. The plutonium or plutonium plus actinides were added to the outer two rings of elements while the central seven pins contained gadolinium. This burnable poison was added to suppress initial reactivity, reduce the refueling power ripple, and give the bundle a negative void reactivity.

With the plutonium-only case, each bundle would contain 250 g of Pu, and at the calculated refueling rate of 15 bundles per day, each CANDU unit could annihilate approximately one metric ton of plutonium per year. At an 80 percent capacity factor, 94 percent of fissile Pu is destroyed. Bundle and channel power remain within current licensing limits.

In the plutonium-plus-actinides simulation, 356 g of Pu, plus a 44 g mixture of neptunium, americium, and curium are present in the fresh fuel. Sixty percent of the actinides and 90 percent of the plutonium are destroyed in this simulated process, amounting to approximately 70 kg of actinides and 860 kg of Pu per CANDU unit per year.

Reactor physics, safety, and licensing analysis. Four-bundle, neutronic, thermal-hydraulic, and transient analyses of proposed inert matrix materials has been performed and compared with the results of similar analyses for reference uranium oxide fuel bundles. The results of this work are to be used for screening purposes to identify the general feasibility of utilizing specific inert matrix fuel compositions in existing and future light water reactors. Compositions identified as feasible using the results of these analyses still require further detailed neutronic, thermal-hydraulic, and transient analysis study coupled with rigorous experimental testing and qualification.

Irradiation Testing and Post-irradiation Examination. The design of a screening irradiation test, designated LWR-2, is currently in the design and planning stages. The LWR-2 test will include a variety of candidate inert matrix fuel compositions fabricated by the U.S. and the European Comission's Institute for Transuranium Elements (ITU). A preliminary irradiation test (LWR-1a) has been removed from the ATR and is currently undergoing post irradiation examination (PIE) at the INL. The results of PIE on an advanced-MOX composition from LWR-1a that incorporates approximately 4,000 ppm neptunium oxide will

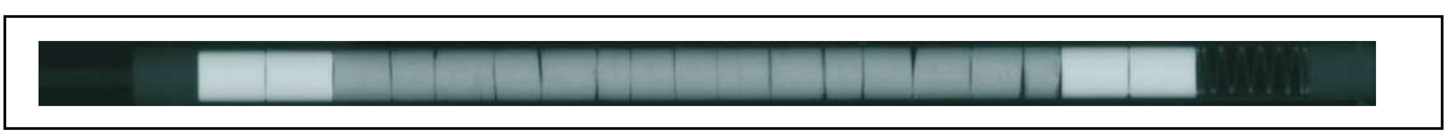

Figure 3. Neutron radiograph of 94 percent dUO_2 – 6 percent $RGPuO_2$ - <1 percent NpO_2 sample PROF-3 irradiated to ~9 GWd/tU burnup.

be reported in the next year. Figure 3 is a neutron radiograph of the LWR-1a MOX rodlet following exposure in the Advanced Test Reactor.

Project personnel have participated in the planning and design efforts for the LWR-2 irradiation test. AECL personnel have visited the Idaho National Laboratory and participated in the LWR-2 coordination meeting. SiC is expected to have adequate resistance to structural damage due to neutrons but another route via which damage can occur is fission fragments. In order to simulate fission-fragment damage, the SiC-IMF along with several other potential IMF candidate materials were bombarded with high-energy (72 MeV) iodine ions. Polished specimens were exposed to a 3 mm diameter beam produced by an accelerator at temperatures ranging between room and 1,200°C. The maximum dose applied was equivalent to typical CANDU 6 burnups. Following exposure, profilometry was performed to detect any relief in the polished surface. Only Zirconia, SiC, and UO_2 showed no sign of relief under all of the test conditions. This result supports, but does not prove, that the SiC-IMF will be stable in reactor.

Table 1 provides a summary of the MOX and Inert Matrix Fuel compositions planned for inclusion in the LWR-2 experiment.

Designation	Description	Composition	Fabricator
LWR-2-A	RG-MOX at high burnup (LWR-1a)	$(U,Pu)O_2$	INL
LWR-2-B	Advanced MOX (Np, Am additions)	$(U,Pu,Np,Am)O_2$	INL
LWR-2-C	IMF replacement to reference MOX	$(Pu)O_2$ - MgO-ZrO_2	INL
LWR-2-D	IMF (Np addition)	$(Pu,Np)O_2$, MgO-ZrO_2	INL
LWR-2-E	IMF replacement to Advanced MOX	$(Pu,Np,Am)O_2$, MgO-ZrO_2	INL
LWR-2-F	Sphere Pac target (low fertile matrix)	UO_2 - AmO_2	ORNL
LWR-2-G	Sphere Pac target (inert matrix)	PuO_2 or ZrO_2 - AmO_2	ORNL
LWR-2-H	PuO_2 Cercer - Cermet	PuO_2, YSZ or Mo (if feasible)	Euratom
LWR-2-I	Pu - FeCr Ferritic (ITU fabrication)	Pu, Fe/Cr	Euratom
LWR-2-J	SiC Inert Matrix	UO_2-SiC IMF	AECL
LWR-2-K	Advanced IMF (Univ. of Florida)	PuO_2 - MgO-ZrO_2-Nd or Yb	UF/INL
LWR-2-L	Zr metal inert matrix	(PuO_2, Zr)	INL
LWR-2-M	WG-MOX at high burnup (LWR-1a)	(U, Pu)O_2	INL

Table 1. Summary of IMF compositions for LWR-2.

Planned Activities

Efforts in the U.S. and Canada will be focused on fabricating fuel test specimens to be included in an irradiation test planned for the Idaho National Laboratory Advanced Test Reactor. Fuel specimens will be fabricated for both out-of-pile characterization and in-reactor irradiation tests. Figure 4 shows a schematic diagram of a LWR-2 test assembly rodlet that will contain one of the individual fuel compositions listed in Table 1. The LWR-2 test assembly is currently planned to be installed into the Advanced Test Reactor in the spring of 2007.

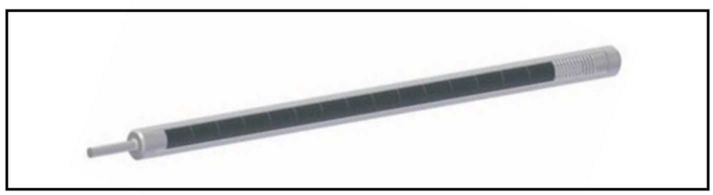

Figure 4. 3-D representation of an LWR-2 fuel irradiation test pin.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Evaluation of Materials for Supercritical Water-Cooled Reactors

PI (U.S.): D. Wilson, Oak Ridge National Laboratory

PI (Canada): H. Khartabil, Atomic Energy Canada Ltd. (AECL)

Collaborators: University of Wisconsin, University of Michigan, University of Notre Dame, University of Sherbrooke

Project Number: 2004-003-C

Project Start Date: October 2004

Project End Date: September 2007

Research Objectives

To meet the goals of the Generation IV Nuclear Energy Systems Initiative, it is essential to establish international collaborations to share resources and expertise. Both Canada and the United States have a shared interest in developing advanced reactor systems that employ supercritical water (SCW) as a coolant. The goal of this project is to establish candidate materials for supercritical water reactor (SCWR) designs and to evaluate the mechanical properties, dimensional stability, and corrosion resistance. This project will address critical issues related to radiation stability, corrosion, and stress corrosion cracking performance in candidate materials for SCWR.

Research Progress

In FY 2005, researchers completed a corrosion exposure test at 500°C with a dissolved oxygen content of 25 ppb for 1,026 hours. They conducted a detailed analysis of samples from this exposure, as well as samples previously exposed in FY 2004 at 500°C with a dissolved oxygen content of 2 ppm for 576 hours.

As shown in Figure 1, weight gains increased from the nickel based alloy 625, to the austenitic alloy D9, to the ferritic-martensitic (F/M) alloy HCM12A. Similarly, the morphology of the scales indicates an increasing coarsening structure, as shown in Figure 1. For austenitic alloys, the weight gain due to oxidation in supercritical water is typically smaller and less predictable than for ferritic-martensitic (F/M) alloys. This may be caused by oxide layer spalling, a tendency exhibited by most austenitic steels with increasing exposure time. Such spallation may be related to fine-scale porosity that develops in the spinel layer. To improve the oxide scale adherence, alloy 800H samples were thermo-mechanically processed to reduce the fraction of high-energy grain boundaries. Such a modification may reduce the anisotropy in the oxide layers and mitigate the effect of differential thermal expansion between hematite and

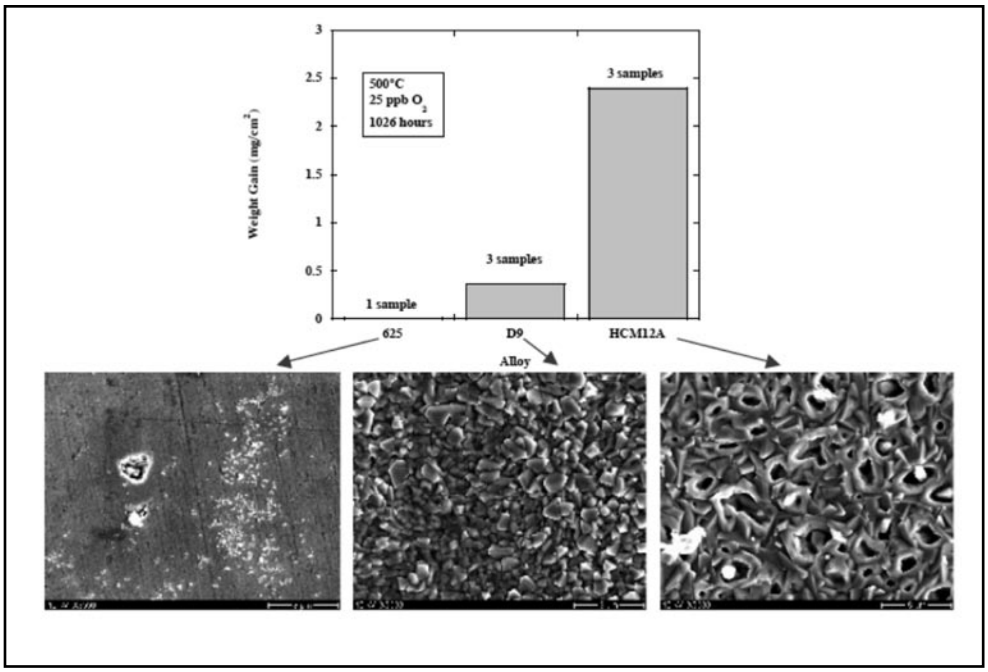

Figure 1. Typical weight gain of a nickel-based alloy (625), an austenitic steel (D9), and a ferritic-martensitic steel (HCM12A).

magnetite by increasing the fraction of hematite, which would improve the oxide adherence.

All the tested F/M steels showed a typical dual layer after exposure to 500°C supercritical water at 25 ppb dissolved oxygen concentration, composed of an outer Fe-O magnetite layer and an inner Fe-Cr-O spinel layer. As illustrated in Figure 2, among the tested F/M alloys, the 9Cr oxide dispersion strengthened (ODS) alloy showed the lowest weight gain due to oxidation, even though it has less bulk chromium (9 weight percent Cr) than HCM12A (12 weight percent Cr). Researchers also tested three nickel-based alloys C22, INCONEL 625, and 718. All the samples showed fairly good corrosion resistance in the SCW environment. However, pitting was observed in all these Ni-base alloys.

Plasma source surface modification to implant oxygen was performed on several F/M steels (T91, HT9, and HCM12A). The experimental results showed a significant improvement in both corrosion resistance and oxide scale adhesion. This improvement is likely due to the formation of nanometer-sized oxide particles on the surface of the implanted samples during the implantation process. These nanometer-sized oxide particles influence the behavior of the nucleation and growth of the oxide scale during the supercritical water exposure.

This phase of the study has provided information on growth kinetics and morphological characteristics of the oxide layer as well as microstructural changes in a wide range of candidate alloys. This information has provided an initial basis for determining the properties of alloys for the use in various components of a SCWR and a path forward for future focused studies of these alloys. Surface modification approaches, such as ion implantation and sputter deposition, as well as thermo-mechanical approaches, such as grain boundary engineering, provide useful directions for further improving specific alloys.

Researchers also completed a study of the temperature dependence of corrosion and the effect of temperature and dissolved oxygen on stress-corrosion cracking (SCC) of F/M steels T91, HCM12A, and HT-9. They conducted an experiment consisting of a constant extension rate tensile (CERT) test and an exposure test at 600°C for 191 hours.

As shown in Figure 3, oxidation at 600°C was extremely rapid, resulting in weight gains that were 4-5 times that at 500°C and almost 20 times that at 400°C. Weight gain followed an Arrhenius behavior, as shown in Figure 4. The calculated activation energies were 189.29 kJ/mol for T91, 177.14 kJ/mol for HCM12A, and 172.60 kJ/mol for HT-9. These values are consistent with either cation outward diffusion or inward diffusion of oxygen by a short circuit (e.g., grain boundary diffusion) process.

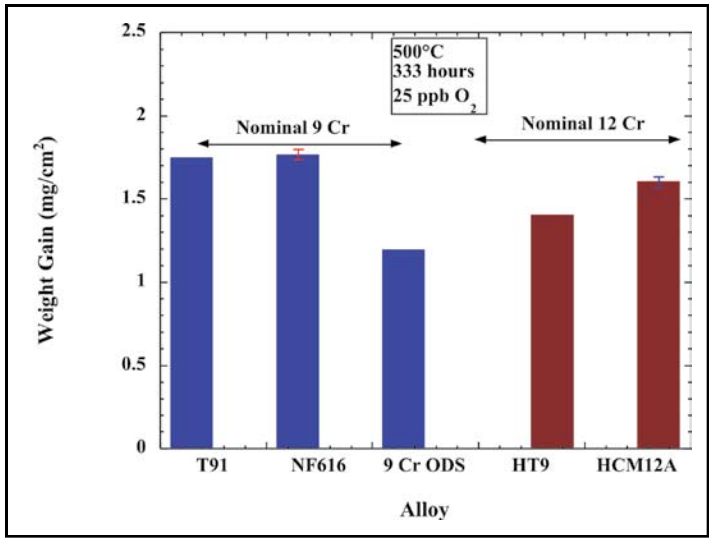

Figure 2. Superior corrosion resistance of the 9 Cr ODS material relative to other ferritic-martensitic steels.

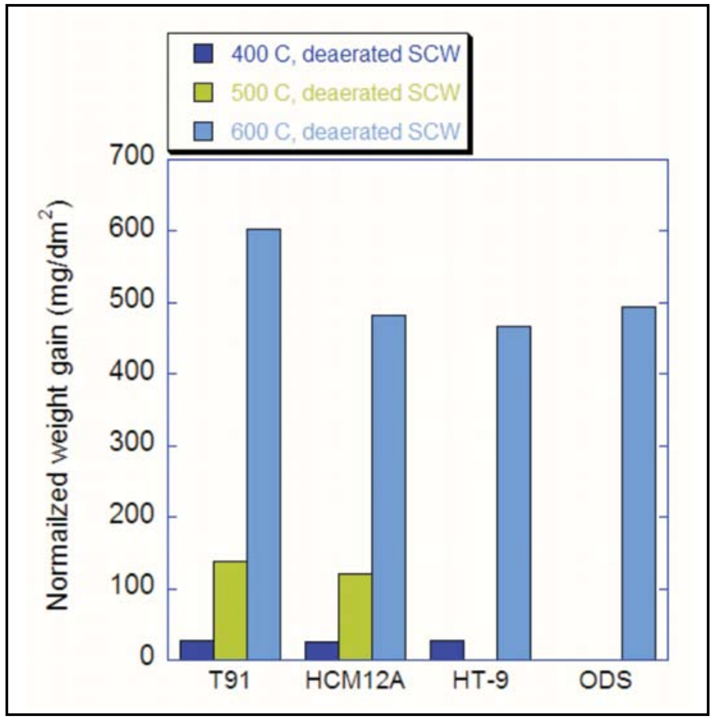

Figure 3. Oxide weight gain in F/M alloys and ODS at temperatures between 400 and 600°C following exposure in deaerated SCW, normalized to a 182-hour exposure time.

Analysis of the oxide surfaces revealed a rough and porous morphology. The oxide subgrains on 400°C specimens were equiaxed. At 500°C, both the subgrain size and porosity increased. At 600°C, the oxide grains were larger, with an average size of about five micrometers. Microcracks appeared on surface oxides for the first time at 600°C. X-ray diffraction (XRD) characterization identified these surface oxides as magnetite (Fe_3O_4) in all alloys and at all temperatures.

Oxide composition was determined on cross-section samples using energy dispersive spectrometry. The outer oxide has an oxygen-to-metal (O/M) ratio of approximately 1.3, which is consistent with an Fe_3O_4 structure and confirmed by XRD. The O/M ratio of the inner layer is approximately 1.1 to 1.3 and corresponds to a spinel oxide, $(Fe,Cr)_3O_4$. At 500°C, a transition region beneath the inner oxide emerged, where the metal content increased to bulk values and the oxygen content decreased to nearly zero. At 600°C, the transition region became more pronounced. In addition, a chromium-enriched layer was observed between the transition layer and the alloy substrate in some parts of the coupon.

The CERT test was conducted at a strain rate of 3 x 10^{-7} s^{-1}. The stress-strain behavior of the F/M alloys in this study very closely followed trends previously documented in the literature, with drops in yield strength and maximum strength between 400°C and 500°C, along with a decrease in uniform elongation and an increase in total elongation. At 600°C, the yield and maximum strengths dropped to less than half that at 400°C. In CERT tests in all environments, the yield strength and maximum stress for HT-9 was highest, followed by HCM12A and T91. All F/M alloys exhibited ductile failure at all temperatures in SCW. However, alloy HT-9 exhibited shallow intergranular (IG) cracks that increased in depth and number density with increasing temperature and dissolved oxygen content, as shown in Figure 5.

In summary, the latest results confirmed the Arrhenius behavior of oxidation of F/M alloys at temperatures to 600°C. The activation energy for oxidation is consistent with either cation outward diffusion or inward diffusion of oxygen by a short circuit process. The oxide is composed of between 2 and 4 layers, depending on the temperature. CERT results showed that all three of the F/M alloys failed by ductile rupture. However, alloy HT-9 exhibited shallow IG cracking that was more severe at higher temperature and higher dissolved oxygen content. Grain boundary engineering will be explored to determine if the intergranular stress corrosion cracking (IGSCC) susceptibility of this alloy can be addressed.

Several experiments have been performed to study the critical hydrogen concentration (CHC) under supercritical water pressures 3,600 psi (25 MPa) at various temperatures. The results indicated that the CHC is approximately 2E-5 molar hydrogen and is dependent on the temperature. As the temperature is increased toward the critical point, the evidence for the presence of a CHC

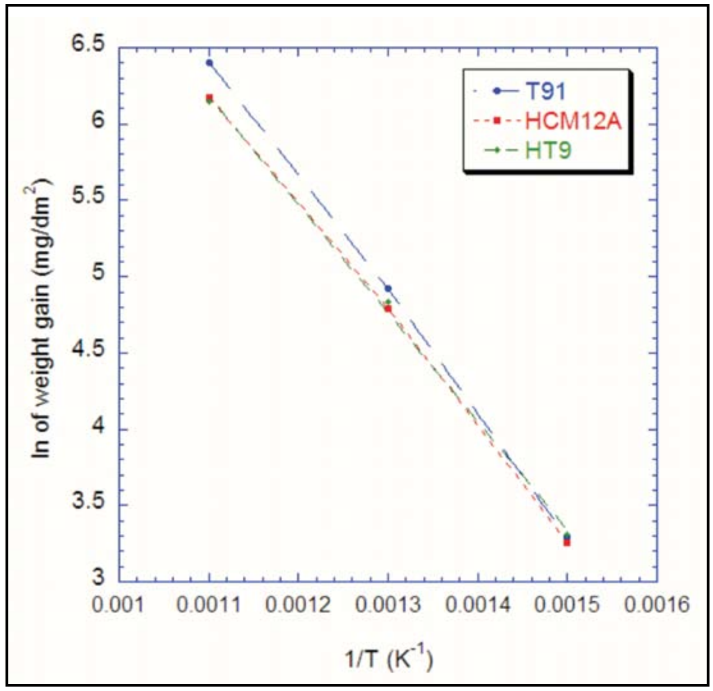

Figure 4. Log of weight gain vs. inverse temperature for T91, HCM12A, and HT-9, exhibiting Arrhenius behavior of oxidation and used to determine the activation energy for oxidation.

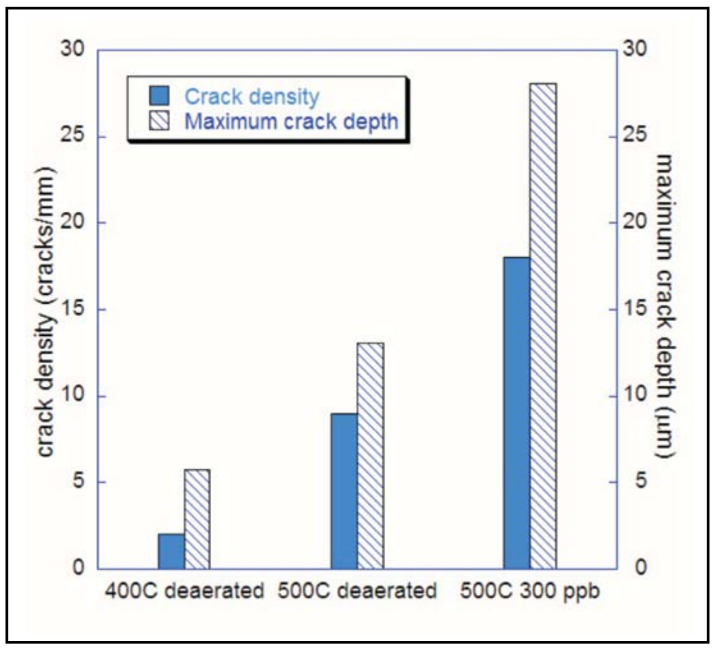

Figure 5. Crack depth and crack number density for HT-9 test in CERT mode at 3 x $10^{-7}s^{-1}$ in SCW.

is less obvious. At present, the reason for this is still unknown and further experiments are underway to help understand these observations. One hypothesis is that surface reactions between the metal tubing and the water in the presence of radiation are increasing near the critical point and interfering with the analysis method. This may suggest a highly increased corrosion rate in a radiation environment. Future tests will look at the effects of the CHC at different neutron-to-gamma ratios. Preliminary data indicate that at lower neutron-to-gamma ratios, the CHC is more evident.

In addition, researchers characterized the corrosion films formed on Inconel-690, Inconel-625 (Figure 6), Carpenter 20CB3, Nitronic-50, and AL6XN coupons after 483 hours exposure to supercritical water conditions. The corrosion rate for Inconel 690 is low, at 0.03 milligrams per square decimeter per day (mdd), while that of Carpenter 20 CB-3 was the highest at 0.48 mdd as determined by weight loss, or about 0.12 mdd as determined by corrosion film thickness. Raman spectra of the coupon surfaces exhibited bands indicating the presence of a spinel structure oxide. The systematic shift of the strongest Raman band to higher frequency with increasing Ni content in the alloy suggested that the films on the low Ni alloys are closest in composition to iron chromite ($FeCr_2O_4$), while the films on the high Ni alloys are closer to nickel ferrite ($NiFe_2O_4$) in composition.

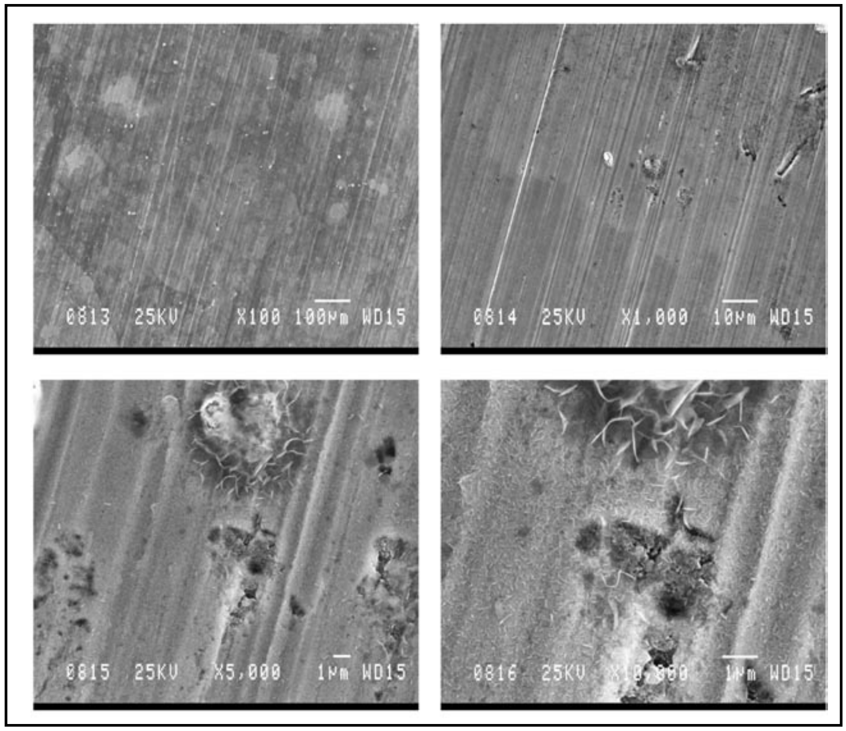

Figure 6. SEM images of Inconel 625 surface after 483 hours in static, neutral water at 450°C and >23 MPa, at magnifications of 100x, 1,000x, 5,000x, and 10,000x.

Researchers are also investigating the following three methods for applying an anti-corrosion coating:

- **Atmospheric Plasma-Jet**. Work continued on characterizing the plume species and initial tests were carried out on film deposition.
- **Sol-gel Dip Coating**. An extensive series of experiments were carried out to examine the effects of coupon preparation (composition, roughness), colloid preparation (Zr n-propoxide/water ratio, agglomeration time, aging/settling), dip-coating procedure (number of coats, drying time and temperature, coating speed), and sintering procedure (number of coats, sintering time and temperature) on the corrosion resistance of ZrO_2-coated steels in SCW. The surfaces of the coated coupons were examined using Auger, SEM, SIMS, AFM, and optical reflectance before and after exposure to SCW conditions in an autoclave at 450°C to characterize the thickness and composition of both the ZrO_2 films and the corrosion films formed on the coated coupons in SCW. Researchers found that the ZrO_2 films are approximately 100 nm in thickness and composed of particles approximately 100 nm in diameter. The ZrO_2 coatings were shown to reduce the general corrosion of carbon steel in SCW by approximately a factor of two. After exposure to SCW, the ZrO_2 coatings were thicker, non-continuous, and contained significant quantities of residual carbon.
- **Cubic Zirconia Coatings**. Stabilized cubic crystalline ZrO_2 layers were prepared on Zr alloys under contract by the National Research Council. The coatings are being characterized for their density, topography, morphology, bonding strength, and residual stress. Preparations are underway to carry out corrosion tests of several of these coupons in SCW.

The research team conducted a literature survey of radiolysis in SCW, and began modeling this with Monte-Carlo techniques. They also performed a preliminary assessment of options to build a SCW chemistry and materials test loop in the Chalk River Laboratories NRU reactor and developed design requirements.

Planned Activities

- Continue corrosion and stress corrosion cracking tests and surface analyses, including tests to higher temperatures
- Continue to investigate deposition of corrosion-resistant coatings using the plasma jet, surface modifications, and grain boundary engineering to improve corrosion resistance
- Continue reaction rate measurements to isolate and measure the relative neutron/beta gamma effects in the flux by comparison of in-reactor measurements to pure gamma measurements

- Evaluate possibility of in-situ measurement of chemical potential within SCW radiolysis loop
- Continue optimization of the sol-gel ZrO_2 coatings, focusing on reducing the amount of residual carbon in the films
- Test the samples with the Cubic Zirconia coatings
- Continue the work to extend the Monte Carlo model to SCW conditions
- Evaluate the effectiveness of grain boundary engineering in the SCC behavior in SCW

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

ACR Hydrogen Production for Heavy Oil Recovery

PI (U.S.): J. S. Herring, J. E. O'Brien, Idaho National Laboratory

PI (Canada): R. Sadhankar, Atomic Energy of Canada, Ltd. (AECL)

Collaborators: Chalk River Laboratories

Project Number: 2004-004-C

Project Start Date: June 2004

Project End Date: May 2007

Research Objectives

The objective of this project is to analyze the engineering feasibility of using the Advanced CANDU Reactor (ACR) as a source of steam and hydrogen for enhanced oil recovery, especially as needed by the Athabasca oil sands projects now under construction in Alberta. For hydrogen production, researchers are investigating the use of a high-temperature electrolysis (HTE) process coupled to the ACR, rather than conventional low-temperature electrolysis. Because of the lower operating temperatures of the reactor, some ohmic heating will be necessary to maintain the operating temperature of the HTE device. Results will be compared with the economics of low-temperature electrolysis and other means of hydrogen production. A preliminary conceptual design will be developed for the electrical/thermal integration of an ACR for hydrogen production and the production of steam for oil sands heating and mobilization. An economic analysis will be performed to assess the costs of hydrogen and steam production and compare these costs with the price of the petroleum recovered and the costs of producing hydrogen and steam in the Athabasca region using fossil fuels.

Research Progress

Researchers have developed a system simulation model of a high-temperature electrolysis plant coupled to an ACR using the HYSYS analysis code (see Figure 1). A detailed report on the results of this study, "Analysis of Commercial-Scale Implementation of HTE to Oil Sands Recovery," was completed in August 2005. The HYSYS model included a custom electrolyzer module developed specifically for this type of analysis. This engineering model enabled the evaluation of various system configurations and operating conditions in order to assess the ACR-HTE concept and perform some system optimization. Based on these results, the researchers have developed an ACR-HTE conceptual design and made performance comparisons to a baseline ACR-low-temperature electrolysis system.

High-temperature electrolysis has been proposed as an efficient hydrogen-production technology. This uses electrical power plus high-temperature process heat produced by an advanced high-temperature reactor. Researchers are also evaluating high-temperature thermochemical processes for nuclear hydrogen production. However, one advantage of high-temperature electrolysis over thermochemical processes is that the magnitude of the required high-temperature process heat is much smaller than for thermochemical processes. Consequently, a high-temperature electrolysis process could potentially be driven by the electrical power from a conventional nuclear plant, using lower temperature process heat from the reactor supplemented by electrical resistance heating, or possibly combustion-based heat input, to achieve the desired HTE operating temperature (800–900°C).

In order to perform a technical evaluation of this concept, researchers have considered the basic thermodynamics of HTE and developed a detailed system-level modeling capability. The system modeling activity assesses the feasibility of using HTE coupled with an ACR, plus develops a preliminary conceptual design of the overall process. The baseline process for comparison is conventional low-temperature electrolysis (LTE) coupled to an ACR. This HYSYS model included a custom one-dimensional electrolyzer module that was incorporated directly into the code. This electrolyzer model allows for the determination of the operating voltage, gas outlet temperatures, and electrolyzer efficiency for any specified

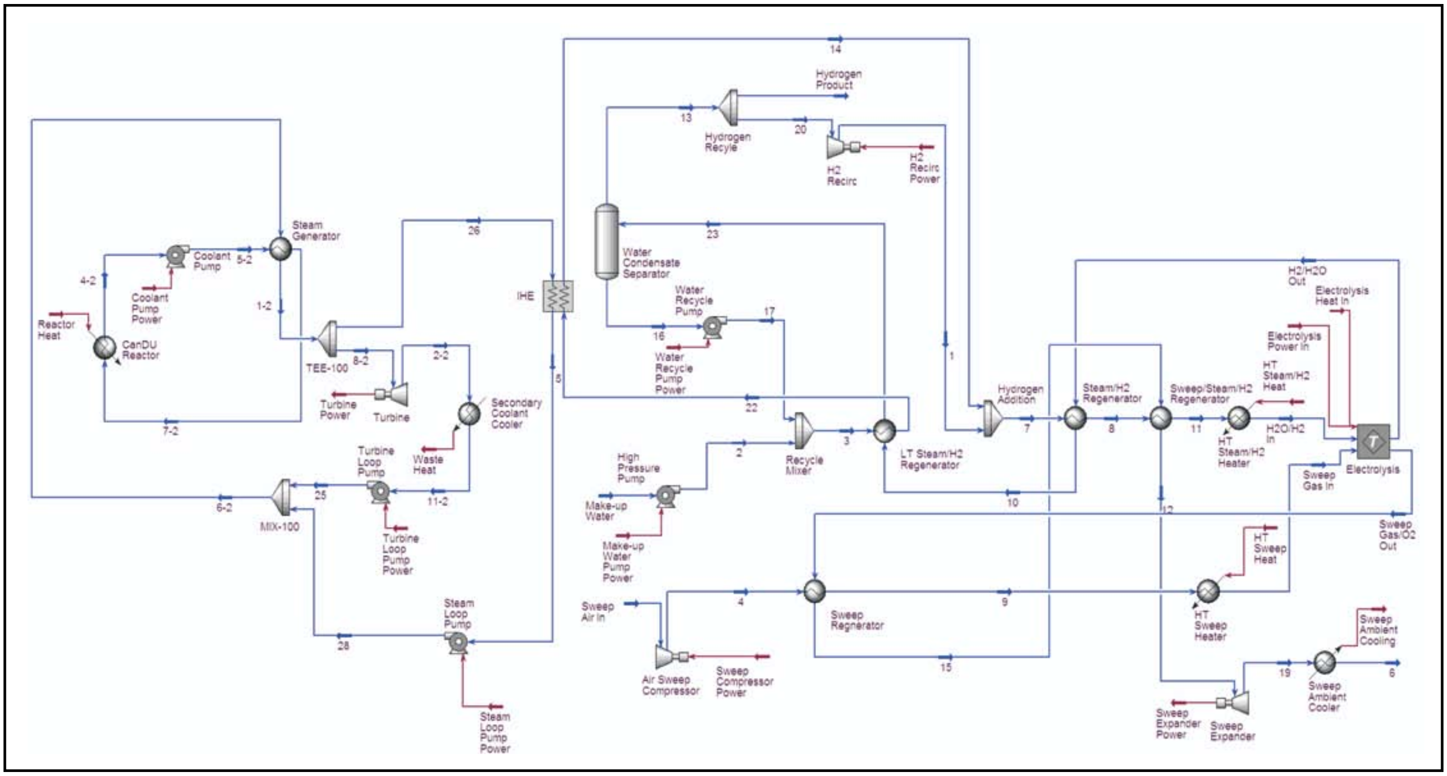

Figure 1. HYSYS process flow diagram for an ACR-700 HTE plant, with air sweep.

inlet gas flow rates, current density, cell active area, and external heat loss or gain. Results obtained with this system model indicated overall thermal-to-hydrogen efficiencies around 33–34 percent, with only a weak dependence on current density. These values compare favorably with corresponding overall thermal-to-hydrogen efficiencies achievable with low-temperature electrolysis.

Using HYSYS, a detailed process flow diagram (PFD) was defined that includes all of the components that would be present in an actual plant such as pumps, compressors, heat exchangers, turbines, and the electrolyzer. The one-dimensional electrolyzer model was validated by comparing results from this model with results obtained from a 3-D computational fluid dynamics (CFD) model developed using FLUENT. Results were reported in a paper entitled "Comparison of a One-Dimensional Model of a High-Temperature Solid-Oxide Electrolysis Stack with CFD and Experimental Results," which provides details on the one-dimensional electrolyzer model, the HYSYS process model for an ACR-700 HTE plant, and some representative results of parametric studies performed using the HYSYS process model.

Some preliminary economic analysis work has been carried out at AECL to assess the market for using hydrogen for oil sands development. It is clear that 1) the demand will be huge (upward of 6,000 tonne/d of hydrogen) and 2) the industry is searching for alternatives to steam reforming of natural gas. A contract study is being put in place to solidify our understanding of the distribution of the hydrogen market in northern Alberta and of the thinking of the oil sands industry on ways to produce it. A related economic analysis was prepared during this period, entitled "The Importance of Nuclear Energy in Reducing CO_2 Emissions and Fossil Fuel Imports."

Planned Activities

- Incorporate a 1-D integral electrolyzer model into a HYSYS ACR plant model coupled to a low-temperature electrolysis (LTE) plant
- Perform a scoping set of simulations to assess the effects of various operating conditions, pressure, gas flow rates, gas compositions (e.g., steam sweep vs. air sweep vs. no sweep), and stack area-specific resistance
- Evaluate various system configurations including pumps, compressors, turboexpanders, etc.
- Compare the hydrogen-production performance of the ACR-LTE system to the performance of an ACR-HTE system based on detailed modeling of both systems
- Finalize and issue a report on this task by September 16, 2006

The assessment of the market and opportunity for non-conventional hydrogen production will be completed in the next quarter. Additional economic analyses will be performed (by AECL) after the completion of the conceptual design study. The expected completion date is March 31, 2007.

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1. O'Brien, J. E., McKellar, M. G., Stoots, C. M., Hawkes, G. L., and Herring, J. S., "Analysis of Commercial-Scale Implementation of HTE to Oil Sands Recovery," August 2005.

2. O'Brien, J. E., Stoots, C. M., and Hawkes, G. L., "Comparison of a One-Dimensional Model of a High-Temperature Solid-Oxide Electrolysis Stack with CFD and Experimental Results," 2005 ASME International Mechanical Engineering Congress and Exposition, Nov. 5 – 11, 2005, Orlando.

3. Herring, J. S., "The Importance of Nuclear Energy in Reducing CO_2 Emissions and Fossil Fuel Imports."

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Supercritical Water-Cooled Reactor Stability Analysis

PI (U.S.): W.S. Yang, Argonne National Laboratory

PI (Canada): H. Khartabil, Atomic Energy of Canada Limited (AECL)

Collaborators: Massachusetts Institute of Technology, University of Manitoba, École Polytechnique de Montréal

Project Number: 2004-005-C

Project Start Date: October 2004

Project End Date: September 2007

Research Objectives

The objective of this project is to improve the understanding of potential instability problems of the Supercritical Water Cooled Reactor (SCWR) at supercritical conditions. The aim is twofold: to develop improved stability analysis tools and to define appropriate ranges for important design parameters that will ensure system stability. The project team will develop SCWR stability analysis codes and perform experimental studies. The researchers plan to develop two codes: 1) a frequency domain linear stability analysis code applicable to SCWR thermal-hydraulics and thermal-nuclear coupled stabilities and 2) a thermal-hydraulic stability analysis tool for studying the adequacy of SCWR sliding pressure startup and shutdown procedures. In parallel, researchers will assess the suitability of AECL codes, CATHENA and SPORTS, to perform flow stability analysis at supercritical conditions and implement needed modifications. Additionally, researchers will investigate coupled neutronic and thermal-hydraulic instabilities that can arise in a pressure tube reactor running at supercritical conditions using the neutron transport code, DRAGON, which has been developed at the Nuclear Engineering Institute at École Polytechnique de Montréal, together with a suitable thermal-hydraulics code to carry out the analyses. For the experimental study, researchers will investigate flow instability of supercritical fluids using an existing supercritical CO_2 loop at Argonne National Laboratory (ANL). The Canadian investigators will construct an experimental loop to study parallel-channel flow instabilities of water at supercritical conditions, using CO_2 and water as modeling fluids. They will also perform single and multi-channel flow instability tests.

Research Progress

Researchers have developed the frequency domain linear stability code, SCWRSA, for thermal-nuclear coupled stability analysis of SCWRs. In order to investigate the effects of water rods used in the current U.S. reference SCWR design, the research team employed single-channel thermal-hydraulics models for the coolant channel and water rod, along with point kinetics neutronics and one-dimensional fuel heat conduction models. The heat transfer between the coolant channel and water rod was modeled as one-dimensional conduction through the water rod wall, considering the effect of delayed reactivity feedback due to water rod density variation. Researchers also implemented the Jackson correlation for forced convection and the Dittus-Boelter correlation. For multi-channel analysis, the flow was distributed among parallel thermal-hydraulics channels. An iterative solution scheme was developed to determine the coolant and water-rod flow rates simultaneously by taking into account the heat transfer between coolant and water-rod. For linear stability analysis, researchers developed perturbation calculation models for flow redistribution among parallel channels, along with an efficient scheme to solve the resulting system of linear equations. Preliminary verification tests of the multi-channel analysis capability were performed using two-channel models derived from the U.S. Generation IV SCWR reference design. Although individual assemblies can be represented as separate channels, two-channel models were selected for these tests due to their simplicity and because of insufficient information on core power distribution, except for the target values of power peaking factors. The results showed that the iteration scheme for the steady state flow distribution converged on a solution after only a few iterations. It was observed that the heat transfer between coolant and water rod has a non-negligible effect on the steady state flow distribution. The decay ratios obtained with multi-channel models were smaller than those determined with single average-channel models, since the multi-channel model includes hot channel assemblies that introduce larger Doppler and coolant density feedback than average channel assemblies.

The researchers also developed a thermal-hydraulic stability analysis tool to study the adequacy of SCWR sliding pressure startup and shutdown procedures. Based on a single-channel thermal-hydraulics model, they developed stability boundary maps for density wave oscillations for both supercritical and subcritical pressure conditions, and applied them to the U.S. reference SCWR design. At supercritical pressures, a three-region model was used. This model consisted of a "heavy fluid" region, a mixed "heavy fluid" and "light fluid" region similar to the homogeneous-equilibrium two-phase mixture, and a "light fluid" region. Two important non-dimensional groups, i.e., a Pseudo-Subcooling number and an Expansion number, were defined as controlling the stability. Plotting the stability maps on a plane consisting of these two numbers, using a frequency domain analysis of the channel, shows that the U.S. reference SCWR design operates in the stable region with a large margin. Sensitivity studies produced results consistent with the trends of the earlier (subcritical pressure) two-phase flow models. During the sliding pressure start-up operation of the SCWR, a two-phase steam-water mixture at subcritical pressure will appear in the reactor core. Researchers applied a non-homogeneous (e. g., drift-flux) non-equilibrium two-phase flow model to this condition. The characteristic equation was numerically integrated, and the stability boundary maps were plotted on the traditional Subcooling number versus Phase Change number or Zuber number plane. These maps were used to modify the sliding pressure start-up strategies of the SCWR to avoid thermal-hydraulic flow instabilities.

The researchers completed their assessment of the CATHENA and SPORTS codes, and implemented the modifications needed to perform flow stability analysis at supercritical conditions. The thermo-physical properties at supercritical conditions were added to the CATHENA code using the National Institute of Standards and Technology (NIST) properties package. Because the SPORTS code has supercritical properties, the assessment compared a simple linear stability analysis for consistency. The results showed very good agreement between the linear model and the SPORTS code. It appeared that SPORTS is more suitable for performing stability analysis.

Using the preliminary CANDU-SCWR fuel design, input files were created for the DRAGON code. The water properties at supercritical condition were implemented into the DRAGON code to model the large density variations as the temperature increases beyond the critical point. Preliminary studies of the interaction between the thermal properties of the materials in the cell (water density and fuel temperature) and the effective multiplication constant of the cell were completed. In addition, a strategy to couple DRAGON with a thermal-hydraulic code was explored.

In a related NERI project, researchers performed natural circulation tests with horizontal heating and cooling sections at the existing supercritical CO_2 loop at ANL. No flow instabilities were observed with the loop, although previous numerical studies indicated the existence of such instability when the fluid is heated through the

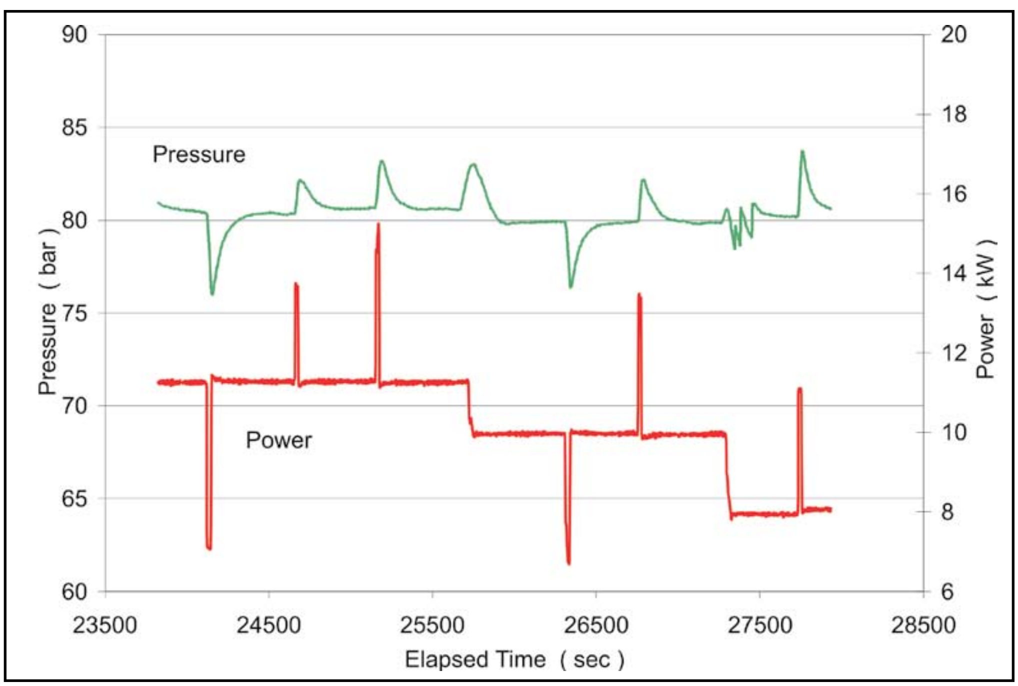

Figure 1. Input Power Perturbations and Pressure Responses.

pseudo-critical point. As shown in Figure 1 for the case of power input perturbation, the system remained stable for a variety of system perturbations. The effects of the pressurizer, which were not included in previous numerical studies, were investigated, and it was concluded that the pressurizer is not responsible for the discrepancy between experiment and calculations. Continued modeling work to identify the source of calculated instabilities is necessary.

Researchers completed construction of the parallel channel instability loop in Canada. The initial plan was to build the loop to withstand operation at supercritical conditions and then build two test sections: one for CO_2 (easier to build) and one for water to expedite the CO_2 tests. However, the plan was modified so that a single test section could accommodate both fluids, due to the complexity of the design option with interchangeable test sections. Commissioning and testing of the loop will begin following renewal of Gen IV funding for the Canadian effort.

Planned Activities

Researchers will conduct additional verification tests of the multi-channel analysis capability for continued development of the linear stability analysis code, SCWRSA. Additional geometry models and a time-dependent lower plenum model will also be implemented to extend the applicability to other SCWR design concepts different from the current U.S. reference design. A space-dependent kinetics model will not be implemented because of reduced funding level. Furthermore, the tasks to develop a thermal-hydraulic stability analysis tool for studying SCWR sliding pressure startup and shutdown procedures and to perform forced convection tests with an existing supercritical CO_2 loop at ANL have been stopped because of no available funding.

For the coupled neutronics and thermal-hydraulics simulations, researchers at École Polytechnique de Montréal will investigate the effect of density variations on neutron flux in parallel channels and assess the coupling of existing thermal-hydraulics codes (e.g., ASSERT and CATHENA) to DRAGON. Regarding the construction of the parallel channel instability loop, the team will perform pre-test simulations and complete construction of the dual CO_2 and water loops. Following the completion of construction, researchers will perform flow instability tests using supercritical CO_2 and water.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Thermal Hydraulic Benchmark Studies for SCWR Safety

PI (U.S.): J. R. Wolf, Idaho National Laboratory (INL)

PI (Canada): H. Khartabil, Atomic Energy Canada, Ltd. (AECL)

Collaborators: École Polytechnique de Montréal, University of Manitoba, Rensselaer Polytechnic Institute

Project Number: 2004-006-C

Project Start Date: October 2004

Project End Date: September 2007

Research Objectives

The objective of this project is twofold: 1) to address the critical issues associated with measuring heat transfer to supercritical water at prototypical conditions in a supercritical water reactor (SCWR) and 2) to develop tools to predict SCWR thermal transients. In addition to using supercritical water, researchers will also use surrogate fluids at supercritical conditions. These alternative fluids will provide valuable insight into physical phenomena that may be present and can significantly reduce the cost and time to complete an experimental program.

Research Progress

A primary objective of the U.S. effort is to design and construct a bundle test section for installation in the Benson facility supercritical water test loop in Erlangen, Germany.

The research team held a meeting with European and Korean researchers to identify requirements and interfaces for the test section. Participants agreed on the basic design concept for the test section. The test section design will include four heater rods simulating a section of SCWR fuel bundle along with channels for moderator flow. The design is flexible; thus, it will accept a solid moderator rod, such as planned for the Korean SCWR system. The test section for the Benson Loop supercritical loop is shown in Figure 1 and technical requirements are shown in Table 1.

In 2005, Rensselaer Polytechnic Institute joined the project as a U.S. collaborator. Their efforts over the next few years will focus on developing and applying their NPHASE computational fluid dynamics code to supercritical water analysis.

In the Canadian collaboration, the test loop designed to study parallel channel stability has been completed at the University of Manitoba. Tests will be initiated next year in both CO_2 and water.

The stability test facility is shown in Figure 2.

Planned Activities

Researchers will complete the final design of the Benson loop supercritical water heat transfer test section and then begin fabrication. Fabrication is not expected to be completed until fiscal year 2007. They will begin applying the NPHASE code for analyzing existing single tube supercritical water heat transfer experiments. Researchers will also begin a scaling study of analytical link test results from surrogate fluid experiments, such as the Canadians are performing to test data from actual supercritical water experiments. Finally, the team will continue with ongoing stability testing and initiate additional tests in a new facility specifically designed for testing passive safety features in an SCWR.

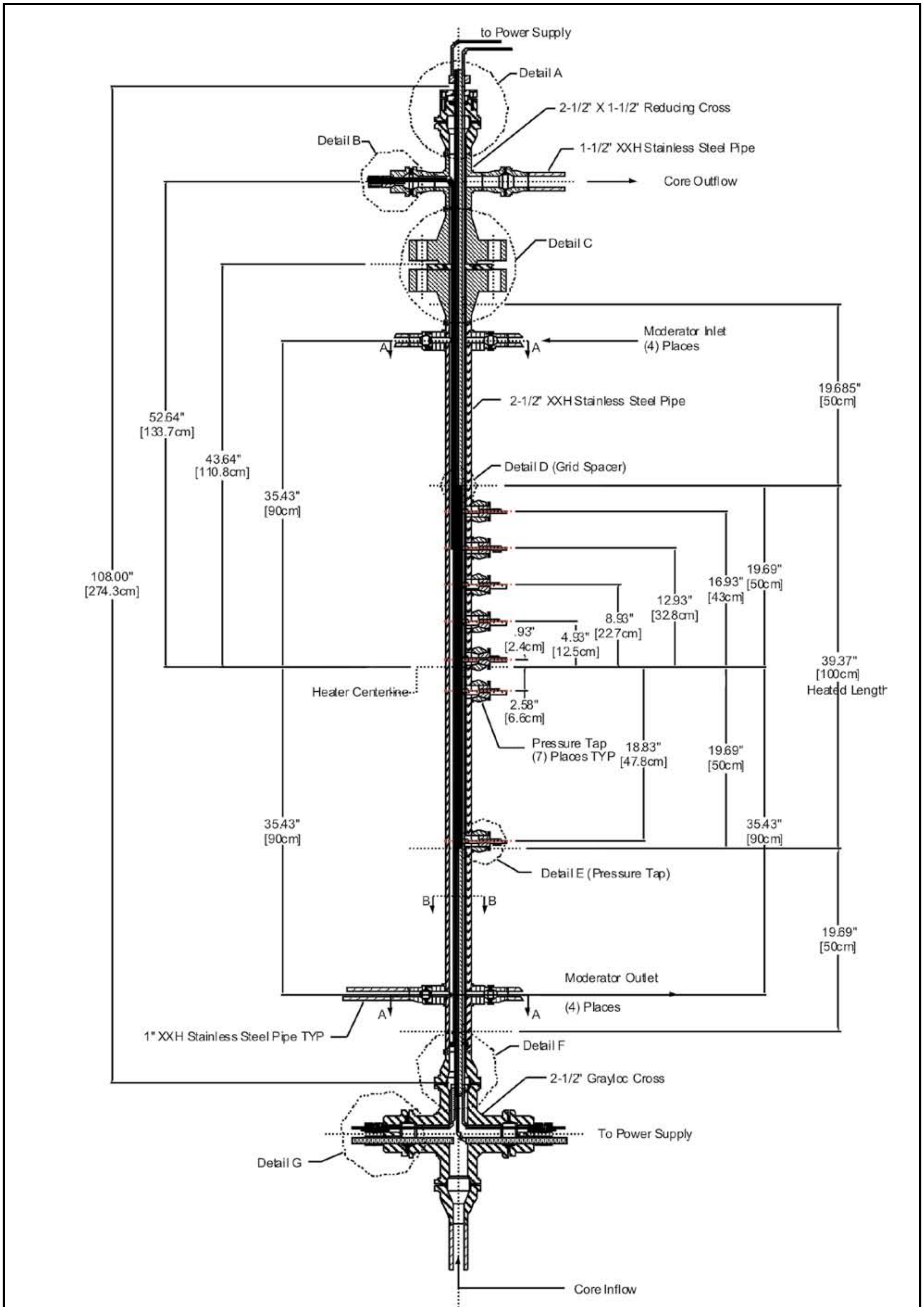

Figure 1. Benson loop supercritical water test section.

Bundle geometry	2x2, square tube insert
Maximum Pressure	25 MPa = 3,625 psia
Test section water inlet temperature (enthalpy window) both for coolant and moderator (individually chosen); two independent moderator flows	280 to 488°C
Maximum test section water outlet temperature	550°C
Maximum test section power flux	1,500 kW/m^2
Heater rod diameter	10 mm or equivalent
Heater rod heated length	1 m
Inlet length (unheated)	0.5m
Outlet length (unheated)	0.5m
Number of spacer grids	3 (at least)
Range of Coolant Mass flux	200 – 1,000 $kg/(m^2s)$
Number of heater rods	4 (one replaceable dummy rod (square))
Rod spacing to diameter ratio (pitch)	1.15
Direct or indirect heated rods	To be decided

Table 1. SCWR Benson loop test section requirements.

Figure 2. Canadian stability test facility.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Thermochemical Hydrogen Production Process Analysis

PI (U.S.): M. Lewis, Argonne National Laboratory

PIs (Canada): S. Suppiah and J. Li, Atomic Energy Canada Limited (AECL)

Collaborator: University of Nevada Las Vegas Research Foundation

Project Number: 2004-007-C

Project Start Date: June 2004

Project End Date: May 2007

Research Objectives

The goal of this I-NERI project is to evaluate the commercial viability of producing hydrogen using the copper-chlorine (Cu-Cl) cycle coupled to a nuclear reactor for process heat. The project has two primary objectives. The first objective is to conduct experimental work to enable a robust simulation of the Cu-Cl thermochemical cycle process. The second objective is to use this model to obtain preliminary cost estimates for producing hydrogen by the Cu-Cl cycle. The modeling work and the experimental research are being conducted iteratively.

Research Progress

Researchers have completed "proof of principle" experiments for all of the reactions within the cycle. The results showed that all of the reactions occurred as predicted and that the set of reactions could operate in a cyclic manner, i.e., the reaction yields were high and competing product formation was minimal.

Several Aspen simulations have been completed for the Cu-Cl cycle. The resulting efficiency from one simulation using equilibrium conditions was 42.4 percent based on the lower heating value (LHV). These results are promising and justify further work on the cycle.

The researchers completed a preliminary investigation of the various CANDU reactor concepts. Results indicated that the Mark 2 reactor meets the maximum temperature requirements of the Cu-Cl cycle and also has sufficient waste heat to assist with water removal.

The investigators agreed to change the scope of the work from that originally proposed; AECL accepted responsibility for designing an electrochemical cell and optimizing its operating parameters. ANL agreed to complete the simulation work and calculate cost estimates. ANL also provided the results of preliminary experimental work and the results of their literature surveys to AECL. The results of the literature survey further demonstrated proof of principle. For example, several papers and a patent [W. L. Chambers, and R. W. Chambers, U. S. Patent 3,692,647 (1972)] describe and demonstrate various aspects of electrochemical cells for disproportionating CuCl. ANL researchers also found solubility data for CuCl and $CuCl_2$ in aqueous hydrochloric acid solutions. CuCl is nearly insoluble in water but its solubility increases as the HCl concentration increases. $CuCl_2$, on the other hand, shows the opposite behavior, becoming less soluble as HCl concentration increases. These data will be used to optimize the performance of the electrochemical cell and to reduce the water content of the $CuCl_2$ solution, which impact the cycle's efficiency.

Planned Activities

Sensitivity studies in the current simulation showed a critical need for thermodynamic data that were not available in the literature. Plans have been made to measure unknown thermodynamic data for Cu_2OCl_2 and various hydrated species of $CuCl_2$ and CuCl in HCl solutions. These data will then be incorporated into the physical property database and the current Aspen simulation will be updated. Any new experimental results will be incorporated into the updated model as well. Sensitivity studies will be run for various operating conditions and the process design will be optimized. The ultimate objective is to determine hydrogen production costs from a robust model of the chemical process.

Further development of the electrochemical cell is pending the availability of funding. Researchers plan to investigate two options to produce hydrogen and cupric chloride as follows:

Option 1: $CuCl + 2HCl(aq) \rightarrow H_2(g) + CuCl_2$ or

Option 2: $2CuCl \rightarrow Cu + CuCl_2$

$CuCl_2 + H_2O \rightarrow 2HCl + CuCl_2$

As the experimental work proceeds to determine which option is better, simulations will be run concurrently to estimate efficiency and capital costs for both options. As the simulations become more robust, interactions with AECL will increase with the objective of optimizing cycle performance and investigating the coupling between the chemical facility and nuclear plant. Researchers also plan to conduct various simulations regarding heat management and coupling between the chemical plant and the nuclear reactor, depending on funding levels.

7.0 U.S./European Union Collaboration

The U.S. Department of Energy (DOE) and the European Atomic Energy Community (EURATOM) signed a bilateral agreement on March 6, 2003. Secretary of Energy Spencer Abraham signed the agreement for DOE and Commissioner for Research Phillipe Busquin signed on behalf of EURATOM. On February 24, 2004, the U.S. and EURATOM selected eight projects for collaboration.

7.1 Work Scope Areas

R&D topical areas for the U.S./EU collaboration include:

- Reactor fuels and materials research
- Advanced reactor design and engineering development
- Research and development related to the transmutation of high-level nuclear waste
- Transmutations-related system analyses

7.2 Project Summaries

Eight projects were approved in FY 2004. Researchers also began work on two additional projects last year that had been authorized in FY 2004. A listing of the I-NERI U.S./EU projects that are currently underway follows, along with summaries of the accomplishments achieved in FY 2005.

Directory of Project Summaries

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Development of Inert Matrix Fuels for Plutonium and Minor Actinide Management in LWRs

PI (US): J. Carmack, Idaho National Laboratory

PI (Europe): J. Somers, Joint Research Center Institute for Transuranium Elements (JRC-ITU)

Collaborators: Los Alamos National Laboratory, Oak Ridge National Laboratory

Project Number: 2004-001-E

Project Start Date: October 2004

Project End Date: September 2008

Research Objectives

Commercial power reactors are the only viable option for short- to mid-term (10-20 years) active management of plutonium and minor actinides. There is worldwide interest in using the existing fleet of commercial light water reactors (LWRs) for fuel cycle scenarios involving burn down of plutonium and stabilization of minor actinide (MA) inventories. The goal of this project is to develop feasibility data related to using inert matrix fuel (IMF) as fuels and minor actinide targets in the existing LWR fleet. IMF offers potential advantages when compared to conventional uranium matrix mixed oxide (MOX) fuel for plutonium management. For example, IMF allows for more efficient destruction of plutonium since the exclusion (or significant reduction) of ^{238}U from the fuel precludes the breeding of additional plutonium. Greater efficiency in reducing plutonium results in greater flexibility in managing plutonium inventories. The potential for fuel cycle cost savings also exists due to the reduced number of rods required to affect a given plutonium burn rate. In addition, IMF can be used to dispose of MA, particularly americium and neptunium. The choice of matrix material may be manipulated to facilitate either fuel recycling or direct disposal, while plutonium recovery can be made relatively straightforward or extremely difficult in order to control proliferation. In addition, inert matrix fuels having high thermal conductivity may also have operational and safety benefits. Ceramic-Metal (cermet) fuel, for example, operates at very low fuel temperatures, a fact that can be used to increase operating and safety margins or increase rated reactor power.

Because of interest in using existing water-cooled reactors for plutonium and MA management, all research and development concepts being analyzed in this project will be suitable for loading into present-day and near-term (Generation II and III) power reactor designs. This project will generate comparative data on the fabrication, properties, and irradiation behavior of several IMF fuel candidates. The data will provide valuable information on the feasibility of using IMF for the management of plutonium and MA in LWRs.

Research Progress

Fuel Selection. Researchers have established goals for IMF development, assessed IMF candidates against this baseline, and selected several materials for further study. Assessments have included analysis of neutronic behavior (Pu burn rate, reactivity swing), fuel thermal performance, fuel irradiation performance, and in-core corrosion resistance based on existing knowledge. A fuel selection report has been issued.

Fabrication Development. Researchers have developed and qualified fabrication methods for inert-matrix fuels. They have identified fabrication methods for $MgO\text{-}ZrO_2$ and Zr-metal matrix fuels and performed test fabrication and characterization. Figure 1 is a photograph of a plutonium-bearing $MgO\text{-}ZrO_2$ matrix pellet and Figure 2 is a magnified photograph of a Zr-metal matrix fuel sample.

The team developed a dust-free fabrication route permitting the routine achievement of high-density $(Zr,Y)O_2$ pellets, with a special view on the MILE irradiation test, which was subsequently cancelled. Two routes were chosen. In the first, cerium nitrate (a surrogate for the actinide) was infiltrated into $(Zr,Y)O_2$ sol gel beads. Following calcination, these beads were milled, then pressed and sintered. Due to the milling step, this process is not applicable to americium. In the second (Am-compatible) process, the $(Zr,Y)O_2$ beads were softened by adding carbon in the sol gel feed solution. This was later removed in the calcinations step by pyrolysis. The resulting "softer" beads permitted high actinide content infiltration and easier pressing. Both methods yielded pellets of similar quality and greater than 90 percent of the theoretical density.

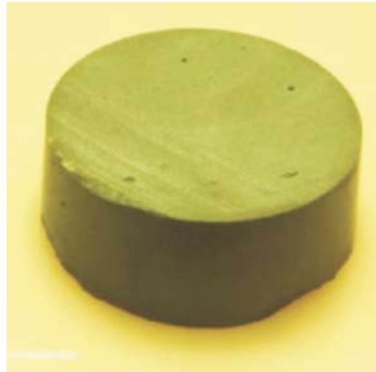

Figure 1. Photograph of dual-phase MgO-ZrO_2-PuO_2 pellet.

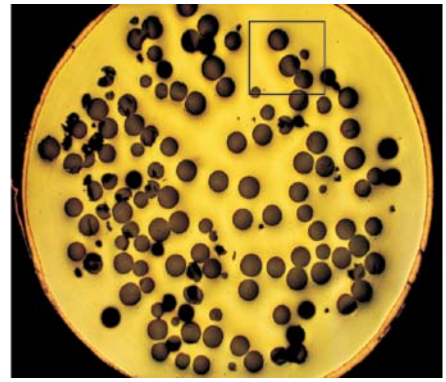

Figure 2. UO_2 particles extruded in a Zr-metal matrix.

Research on cermet fuels has been ongoing with molybdenum (Mo) as the metallic matrix. Although mainly associated with the FUTURIX irradiation tests in the Phénix reactor in France, cermet samples with $(Pu0.73Th0.23)O_2$/Mo have also been prepared. In this case, the ceramic $(Pu,Th)O_2$ phase was prepared from sol-gel-produced PuO_2 beads, which were infiltrated with Th nitrate and subsequently calcined to convert the nitrate to the oxide. The ceramic phase was diluted to 40 percent by volume by Mo addition and blending prior to pressing. Densities of 90 percent of the theoretical value were obtained. A photo of the surface of the pellet is shown in Figure 3.

Figure 3. Cermet $(Pu0.73Th0.23)O_2$/Mo (40:60 vol%) pellet end face.

Characterization. Experimental characterization of the candidate inert matrix fuels and matrix materials has been completed. Characterization including microstructure, thermal and mechanical properties, corrosion testing, and ion-beam irradiation, which has been carried out to determine suitability for in-reactor irradiation testing and to provide a basis for modeling fuel behavior. Characterization activities will continue to further refine the fabrication processes.

Fuel Modeling. A finite element model has been constructed using the ABAQUS finite element analysis code to model the phase structure of both heterogeneous and homogenous inert matrices. This code allows estimation of key fuel properties (such as thermal conductivity, density, etc.), needed to support reactor irradiation experiment design and qualification.

Reactor Physics, Safety, and Licensing Analysis. Four-bundle, neutronic, thermal-hydraulic, and transient analyses of proposed inert matrix materials has been performed and compared with the results of similar analyses for reference uranium oxide fuel bundles. The results of this work will be used for screening purposes to identify the general feasibility of utilizing specific inert matrix fuel compositions in existing and future light water reactors. Compositions identified as feasible using the results of these analyses still require further detailed neutronic, thermal-hydraulic, and transient analysis study coupled with rigorous experimental testing and qualification.

Irradiation Testing and PIE. The design of a screening irradiation test, designated LWR-2, is currently in the design and planning stages. The LWR-2 test will include a variety of candidate inert matrix fuel compositions fabricated by the U.S. and ITU team. A preliminary irradiation test sample of advanced MOX incorporating approximately 4,000 ppm neptunium oxide, which has been designated as "LWR-1a," has been removed from the Advanced Test Reactor (ATR) at the Idaho National Laboratory (INL), and is currently undergoing post-irradiation examination (PIE). The examination results

Figure 4. Neutron radiograph of 94% dUO_2 – 6% $RGPuO_2$ - <1% NpO_2 sample PROF-3 irradiated to ~9 GWd/tU burnup.

will be reported next year. Figure 4 is a neutron radiograph of the LWR-1a MOX rodlet following exposure in the Advanced Test Reactor.

Following an intensive discussion period, the MILE irradiation program in Beznau was finally abandoned. Discussions are ongoing regarding ITU's participation in an irradiation test (LWR-2) in the ATR. In parallel, a STREP proposal (LWR deputy) has been submitted to the European Commission, which, if accepted, will provide ITU an opportunity to irradiate fuels in two European reactors (BR2 in Belgium's Mol nuclear research center and the Borsele LWR in the Netherlands). Table 1 provides a summary of the MOX and Inert Matrix Fuel compositions planned for inclusion in the LWR-2 experiment.

Designation	Description	Composition	Fabricator
LWR-2-A	RG-MOX at high burnup (LWR-1a)	$(U,Pu)O_2$	INL
LWR-2-B	Advanced MOX (Np, Am additions)	$(U,Pu,Np,Am)O_2$	INL
LWR-2-C	IMF replacement to reference MOX	$(Pu)O_2$ - MgO-ZrO_2	INL
LWR-2-D	IMF (Np addition)	$(Pu,Np)O_2$, MgO-ZrO_2	INL
LWR-2-E	IMF replacement to Advanced MOX	$(Pu,Np,Am)O_2$, MgO-ZrO_2	INL
LWR-2-F	Sphere Pac target (low fertile matrix)	UO_2 - AmO_2	ORNL
LWR-2-G	Sphere Pac target (inert matrix)	PuO_2 or ZrO_2 - AmO_2	ORNL
LWR-2-H	PuO_2 Cercer - Cermet	PuO_2, YSZ or Mo (if feasible)	Euratom
LWR-2-I	Pu - FeCr Ferritic (ITU fabrication)	Pu, Fe/Cr	Euratom
LWR-2-J	SiC Inert Matrix	UO_2-SiC IMF	AECL
LWR-2-K	Advanced IMF (Univ. of Florida)	PuO_2 - MgO-ZrO_2-Nd or Yb	UF/INL
LWR-2-L	Zr metal inert matrix	(PuO_2, Zr)	INL
LWR-2-M	WG-MOX at high burnup (LWR-1a)	$(U, Pu)O_2$	INL

Table 1. Summary of IMF compositions for LWR-2.

Planned Activities

Efforts in the U.S. and at ITU will focus on fabricating fuel test specimens to be included in an irradiation test planned for the Idaho National Laboratory Advanced Test Reactor. Fuel specimens will be fabricated for both out-of-pile characterization and in-reactor irradiation tests. Figure 5 shows a schematic diagram of an LWR-2 test assembly rodlet that will contain one of the individual fuel compositions listed in Table 1. The LWR-2 test assembly is currently planned to be installed into the Advanced Test Reactor in the spring of 2007.

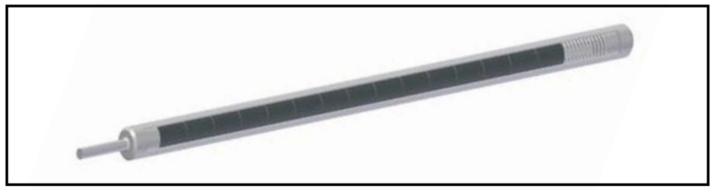

Figure 5. 3-D representation of an LWR-2 fuel irradiation test pin.

Development of Fuels for the Gas-Cooled Fast Reactor

PI (US): M. Meyer, Idaho National Laboratory

PI (Europe): J. Somers, Joint Research Center Institute for Transuranium Elements (JRC-ITU)

Collaborators: Oak Ridge National Laboratory, Los Alamos National Laboratory

Project Number: 2004-002-E

Project Start Date: October 2004

Project End Date: September 2007

Research Objectives

This project seeks to develop silicon carbide matrix, uranium carbide dispersion fuel in two forms: 1) a hexagonal block with coolant holes throughout and 2) a pin-type dispersion fuel utilizing silicon carbide and uranium carbide as the matrix and fuel phase respectively with an integral silicon carbide cladding suitable for gas-cooled fast reactor (GFR) service. Because fuel operating parameters and physical requirements for the GFR are outside of the current experimental nuclear fuel database, many basic viability issues will need to be addressed experimentally to demonstrate the feasibility of proposed GFR fuels. Two basic fuel types appear viable: refractory matrix dispersions and refractory metal or ceramic-clad pin-type fuels. Researchers will demonstrate the feasibility of these fuels by analyzing fuel requirements, simulating behavior using fuel performance models, fabricating fuel specimens, and characterizing microstructure and properties. They will conduct ion irradiation testing of materials to simulate material behavior at high irradiation doses in short times. The GFR-F1 test in the Advanced Test Reactor (ATR) at the Idaho National Laboratory (INL) and the FUTURIX-MI test in the French Phénix reactor also address basic issues regarding the irradiation behavior of the ”exotic” refractory materials required for GFR fuel service in a neutron-only environment. Ultimately, proof-of-concept for GFR fuel can only be demonstrated through irradiation testing of fissile-bearing specimens. The GFR-F2 fuel irradiation test in the ATR is planned as a fuel behavior test that will give the first true indication of fuel feasibility.

Research Progress

Current U.S. GFR fuel concepts are based on a dispersion of (U, Pu)C coated particles in a silicon carbide (SiC) matrix. The U.S. has two reference fuel forms— large hexagonal blocks with coolant holes drilled throughout or a refractory clad pin-type dispersion fuel. Both the block-type and the pin-type fuel will be fabricated through reaction bonding; however, the starting material preforms are fabricated in a slightly different fashion.

The method of reaction bonding used for the block-type fuel fabrication starts with a polymer-derived carbon preform. The polymer is produced with a specific amount of pore-forming agent that creates the appropriate porous microstructure. The polymer is cured and pyrolyzed to produce a porous carbon preform. The polymer can be cast in its final shape or the preform can easily be machined. The preform is then infiltrated with molten silicon which reacts with the carbon to form SiC. The microstructure of the preform must be tailored to produce a fully infiltrated sample with minimal residual silicon (5-15 volume percent). The microstructure is dependent upon the amount of pore former used in the original polymer mixture. The disadvantage of this process for fuel fabrication is that the sample will shrink on the order of 50 volume percent during pyrolyzation. If fuel spheres are incorporated at this point, the preform will crack due to the shrinkage of the matrix around the stable fuel particles. Therefore, a filler is added to control shrinkage. A ratio of filler powder to polymer of 80:20 is required to maintain the shrinkage to less than 5 percent.

The addition of filler materials affects the green, or pre-infiltrated, microstructure dramatically. If the microstructure is too coarse or too porous the final product may also be porous or may have a large amount of free silicon, which is detrimental to the high-temperature properties. There may also be residual carbon which will affect the irradiation properties. Adding filler materials makes the microstructure much finer, but if the microstructure is too fine the porous networks are closed off by SiC formation during infiltration, stopping the infiltration process before the interior volume of the sample is infiltrated. This has been seen with the required high filler loading. Another possible outcome of too fine of a microstructure or insufficient porosity is that as the SiC is formed and expansion takes place, the sample falls apart or cracks. By using a combination of particles sizes in the filler material, the microstructure is refined sufficiently for full conversion of carbon, yet maintains complete infiltration of the pellet. Samples made with 80 weight percent filler made up of 68 percent SiC platelets (-100 mesh +200 mesh), 12 percent SiC powder (-325 mesh), 15 percent graphite (-325 mesh), and 5 percent carbon black have produced a dense, fully infiltrated sample. Samples have also been successfully fabricated using only SiC powders as filler. The resulting pellets, however, have more residual silicon when compared to samples with a mixture of SiC and carbon fillers. Samples have also been fabricated using SiC-coated spheres as a surrogate fuel phase. These samples used filler powders of SiC, graphite, and carbon black powders. Samples containing 35 weight percent filler and a low volume of spheres (~25 percent) have been fully infiltrated, producing a dense sample with little porosity. However, excessive shrinkage occurred because the filler amount was low, which opened large gaps between the sphere and the matrix and cracks were formed. These gaps and cracks were subsequently filled with silicon, which led to an excess of free silicon. Figure 1 contrasts the effect of adding 35 weight percent filler powder to the same polymer precursor. Even though it has been found that 35 percent inadequately controls shrinkage, the dramatic effect on the microstructure can be seen.

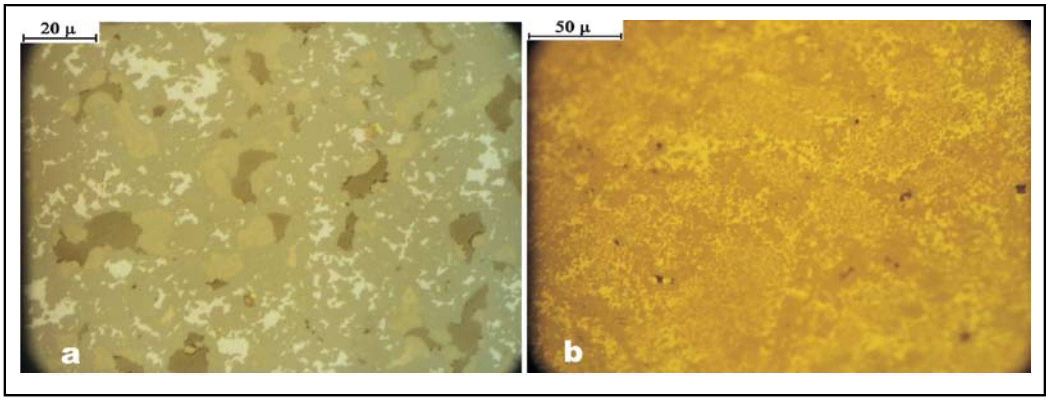

Figure 1a. Preform with no filler material, notice free carbon and large areas of residual silicon.

Figure 1b. Preform with filler material notice no free carbon and a finer distribution of residual silicon.

When sphere loading and amount of filler material are increased, porosity increases and the amount of material infiltrated and converted to SiC decreases. These effects are caused by the increased pressure needed to produce a pellet with the spherical particles fully surrounded by a consistent amount of matrix material. The increased pressure decreases the amount and size of open porosity. The porosity on the surface is closed off by SiC formation before the samples are fully infiltrated leaving a partially infiltrated sample. Samples have also been made using uranium carbide (UC) spheres. Further process development is required, however, to produce fully infiltrated dense samples. Because of the success seen in producing non- "fuel" loaded samples and the limited success seen in "fuel" loaded samples, this process is still a viable fuel fabrication route, but requires more process development.

Pin-type fuel fabrication by reaction bonding is also under development. In this fabrication process, the only carbon source is carbon powder added to SiC powder. Pin-type fuel fabrication starts by wet mixing fine powders of α-SiC and graphite along with surrogate fuel spheres. The mixture is dried and a binder (glycol) is added and pellets are made by uni-axial cold pressing. Debinding is done at 150°C in air, resulting in a material preform with interconnected porosity. Silicon infiltration is carried out by placing a preform in an argon atmosphere furnace along with silicon chips and heating to a temperature above 1,410°C. Parametric studies using various controlled precursor powder particle sizes, ratios of SiC and carbon powders, preform pressing pressure, and infiltration temperature have been performed to determine the optimum combination of material inputs and process variables. It was found that fine powders of α-SiC (70 percent of -100+200 mesh and 30 percent of -325 mesh) and graphite (-325 mesh) in a 75:25 ratio, mixed with 25 weight percent glycol, pressed at 9,000-18,000 psi, and infiltrated at 1,550°C yields well-infiltrated samples of matrix material, as shown in Figure 2. When spheres were added to the matrix, however, the infiltrated samples showed severe cracking, indicating that further optimization is required in order to incorporate fuel particles into the matrix.

In conjunction with fuel fabrication activities, researchers have also performed several material irradiation experiments. Heavy ion irradiation studies of ceramics (ZrN, TiC, TiN, and SiC) in FY 2005 continue following the work on ZrC in FY 2004. The irradiation conditions were 800°C and doses of 10 and 70 displacements per atom (dpa). All the irradiations were conducted with 1-MeV krypton ions using the IVEM-TANDEM facility at Argonne National Laboratory. The results showed that the irradiation performance of ZrC and ZrN under these conditions was poor, with these materials showing severe lattice expansion. In the case of TiC, TiN, and SiC, the irradiation performance was much improved, with lattice expansion of TiC and TiN reduced by a factor of about four compared to ZrC and ZrN at 70 dpa. Virtually no lattice expansion was observed in the SiC samples.

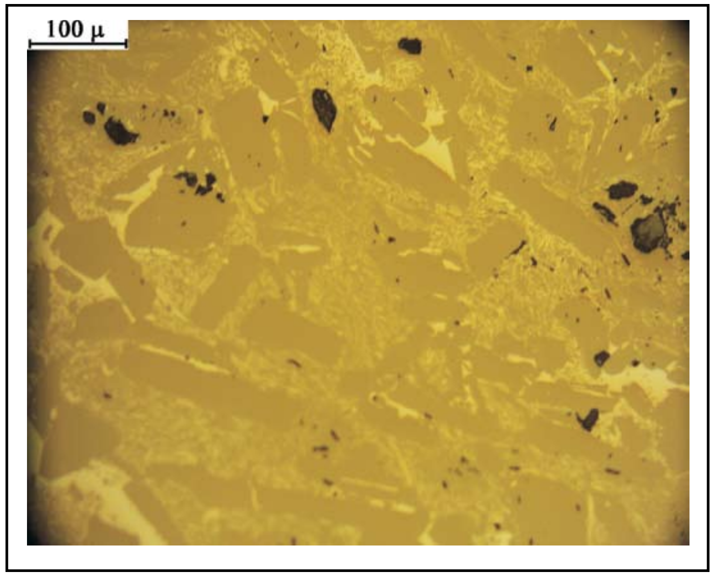

Figure 2. Microstructure of reaction bonded SiC using the proper ratio of particles sizes and compositions.

The GFR-F1 is a low-dose materials experiment that was irradiated in INL's Advanced Test Reactor. The experiment was not instrumented and the specimen temperature was not actively controlled. Various fill gas compositions were used to vary the heat transfer from the experiment capsules, so that specimen temperature is calculated to be approximately 1,000°C. The first experiment capsules are currently in the Hot Fuel Examination Facility (HFEF) at INL and have been examined by neutron radiography, which showed the samples were intact with no gross material failures.

Planned Activities

The FUTURIX-MI materials irradiation experiment will be inserted in the Phénix reactor in France in 2007. Samples of various high-temperature materials including refractory ceramics and alloys and appropriate documentation were prepared by three DOE labs and were delivered to the French Atomic Energy Commission (CEA) for insertion into Phénix.

Initial planning has started for the GFR-F2 fuel irradiation test, scheduled for fiscal year 2007. It is anticipated that the test configuration will mimic the existing AFCI hardware design and use a cadmium-filtered thermal neutron spectrum in the Advanced Test Reactor (ATR). The power, fuel loading, and target burnup will be prototypic of the reference GFR design. There will be two capsules destined for low (5 percent) and high (10 percent) burnup. The fuel samples will be representative of both block-type and pin-type fuel with two different fuel particle coatings. Fuel fabrication activities may carry into FY07.

Work on both fabrication and materials irradiation will continue through next year, resulting in samples being prepared for inclusion in GFR-F2. Work is planned to further optimize the microstructure of the SiC matrix material through a series of parametric studies involving filler powder particle size distribution and composition. Thus far into the project, reproducibility has been an issue due to limitations in the processing equipment control system, which will be upgraded in FY06. Work will continue in this area to ensure samples are reproducible. Also, sphere particle distribution and packing will be examined in a series of parametric experiments to optimize the fuel particle distribution. Work will also continue on uranium carbide sphere production through a rotating electrode atomization process with the subsequent particle characterization. Transmission electron microscopy characterization of the materials irradiated in the first GFR-F1 capsule will also take place.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Lead (Pb) Fast Reactor Engineering and Analysis

PI (U.S.): J. J. Sienicki, Argonne National Laboratory

PI (Europe): H. U. Wider, Joint Research Center of the European Commission, Institute for Energy (JRC-IE), Petten, the Netherlands

Collaborators: None

Project Number: 2004-003-E

Project Start Date: November 2004

Project End Date: November 2007

Research Objectives

Lead-Cooled Fast Reactors (LFRs) are ideally suited to meet the requirements of a future, sustainable world energy supply architecture that is optimized for nuclear rather than fossil energy. Those requirements include features that facilitate deployment in developing as well as developed nations such as proliferation resistance, sustainability with a closed fuel cycle, autonomous load following, passive safety, and a range of plant power levels compatible with varying extents of national nuclear infrastructure and electric grid development. Under the Generation IV Nuclear Energy Systems Initiative, research and development is in progress to determine the viability of a small, modular natural circulation LFR concept known as the Small Secure Transportable Autonomous Reactor (SSTAR). One mission of SSTAR is to provide electricity generation to match the needs of developing nations and remote communities or industrial operations (e.g., mining) that are off-grid, such as exist in the states of Alaska or Hawaii, island nations of the Pacific Basin (e.g., Indonesia), Ulung Island in the Republic of Korea, and elsewhere. In the European Union (EU), there is interest in a mid-size forced convection LFR called the European Lead System (ELSY). The objectives of this joint US/EC project are to advance the development of the SSTAR and ELSY concepts as well as the supporting analysis and experiment bases.

Research Progress

At the Argonne National Laboratory (ANL), researchers have carried out further development and investigation of the viability of the 20 MWe (45 MW_{th}) SSTAR. The research team has developed a new optimized core concept that incorporates transuranic (TRU) feed from spent light water reactor fuel. This core has a 30-year lifetime/refueling interval, which exceeds that of the previous 20-year core concepts. A new strategy for distributed deployment in the core of two separate groups of control and shutdown rods has also been developed. The compact core incorporates a lower fuel volume fraction of 0.45 and greater coolant volume fraction of 0.41, thereby decreasing the frictional pressure drop and enabling the height of the reactor vessel to be reduced. The new core has a burnup reactivity swing less than one dollar and achieves an average discharge burnup of 81 MWd/Kg of heavy metal (HM) and 131 MWd/Kg peak. The reactor vessel height has been reduced to about 14 meters from the previous 18 meters, while retaining single-phase natural circulation heat transport of the lead primary coolant at all power levels up to and exceeding nominal full power. The reduced height decreases the mass of the reactor system (mainly the Pb coolant) as well as the associated cost. It will also improve the reactor system's seismic response. Improvements have been made to the modeling of turbomachinery in the Supercritical Carbon Dioxide (S-CO_2) Brayton Cycle advanced energy converter which will enable researchers to better evaluate the conditions and efficiency of the S-CO_2 energy converter and optimize its coupling to SSTAR. The design analyses of the turbine and compressors have been improved based upon interactions with a manufacturer of custom-made turbines and compressors. Researchers have developed more realistic turbine and compressor designs and have carried out an improved evaluation of cycle and plant efficiencies for SSTAR. They have also further refined a concept for the in-reactor Pb-to-CO_2 heat exchangers (HXs). A plant efficiency of 44 percent was calculated for a peak cladding inner surface temperature limitation of 650°C, with core inlet and outlet temperatures of 420 and 564°C, respectively.

ANL carried out an updated assessment of thermal hydraulic experimental data needs for the LFR. This assessment provided a listing and discussion of experimental data needs and helped researchers identify needs for instrumentation and diagnostics for specific cases. A common thread is the need for additional experimental data that includes multidimensional effects with heavy liquid metal coolants. This data can only be obtained from a vessel filled with heavy liquid metal coolant and incorporating changeable models of the core and in-vessel structures. Development of diagnostics and instrumentation that can provide quality data is important to the successful operation of a multidimensional facility. A three-dimensional vessel capability to simulate the phenomena associated with CO_2 or steam blowdown following a heat exchanger tube rupture event and release of the working fluid into the Pb coolant is also needed.

At JRC-IE, experiments were performed under contract at the Forschungszentrum Karlsruhe (FzK) in Germany to evaluate whether radionuclides such as iodine, cesium-iodide, and cesium would be absorbed by lead-bismuth eutectic (LBE) such that the source term of an LBE-cooled reactor would only contain radioactive polonium. The FzK experiments showed that these three radionuclides were absorbed by LBE at 400 and 600°C. Iodine forms compounds with lead and bismuth; Cs forms an inter-metallic solution in LBE.

Preliminary work has started on experiments investigating the viability of disposing LBE and Pb in seawater following plant decommissioning. This is also relevant to potential cassette core shipping accidents at sea. Lead and LBE samples are ready for testing.

An evaluation was carried out of a new approach involving locating high-pressure heat exchangers in a simple flow path design diagonally above the core. This approach has advantages regarding the upward flow of the heavy liquid metal coolant in the heat exchanger and the possibility of including a passive check valve (e.g., a flapper) at the entrance to the heat exchanger. The latter would automatically close in case of a sudden pressurization in the heat exchanger caused by a steam generator or Pb-to-CO_2 heat exchanger tube rupture. An EU patent was granted for this invention. Extensive computational fluid dynamics calculations were performed using the STAR-CD computer code to show that this new approach does not significantly reduce the safety performance regarding emergency decay heat removal or unprotected loss-of-flow accidents in a pumped concept. Calculations were also carried out with STAR-CD investigating ex-vessel natural circulation air cooling for European LFR concepts. The ex-vessel air cooling approach was found to work well for LFRs up to 800 MW_{th} and for taller designs (e.g., 15 m). For a 1,440 MW_{th} LFR design, the ex-vessel air-cooling for the relatively low vessel (11 m) is not sufficiently effective. Regarding the safety parameters of the 1,440 MW_{th} LFR, it was found that oxide-fueled low-pressure drop cores have a sizeable positive coolant temperature reactivity coefficient due to the large mass of lead coolant involved. A reduction can be achieved through the insertion of thermalizing pins containing, for example, beryllium oxide. Unprotected Loss-of-Flow analyses of the 1,440 MW_{th} core showed that such an accident would be overcome by natural circulation alone — no negative feedback is required. This is due to the low-pressure drop of an LFR core and the simple flow-path design as proposed in the ANL SSTAR and STAR-LM concepts and the Ansaldo Accelerator-Driven System (ADS) design.

Experimental results were provided to ANL by JRC-IE including high-temperature uni-axial time-to-failure creep rupture experiments at a 70 MPa stress performed at JRC-IE. It was found that temperatures close to 900°C lead to times-to-failure of less than 30 minutes.

Planned Activities

ANL plans to continue development and evaluation of the SSTAR concept. Further identification and updating of research and development needs for the SSTAR/LFR will be carried out as required. They will also initiate development of a plant dynamics analysis computer code for SSTAR that calculates transient thermal hydraulic conditions inside the lead-cooled primary coolant system, reactivity and power feedback of the autonomous power core in response to changes in the core fuel and coolant temperatures, and thermal hydraulic conditions inside of the turbomachinery, heat exchangers, and piping of the supercritical CO_2 Brayton Cycle. The code will incorporate detailed one-dimensional modeling of the off-design performance of the turbine and two compressors, heat exchange in the recuperators, cooler, and in-reactor Pb-to-CO_2 heat exchangers, as well as S-CO_2 Brayton Cycle control strategies. The plant dynamics analysis code will be applied to SSTAR to calculate a set of representative operational transients and postulated accidents.

JRC-IE researchers will continue their analyses and experiments. More tests are planned to investigate iodine, cesium iodide, and cesium behavior in LBE and Pb coolants under severe accident conditions for an oxide-fueled reactor at 900°C. Of particular interest is the behavior of iodine under these conditions, since the melting point of PbI is 854°C. JRC-IE will provide additional results from various experiments to ANL researchers. This includes earlier experiments on the injection of 5 liters of high-pressure sub-cooled water (6 MPa) at coolant temperatures of 200-260°C into Lead/Lithium (83/17 percent) with temperatures between 350-500°C that were performed for fusion blanket safety. In the EU integrated project, a specialist group (IP EUROTRANS) has formed to address the problem of heat exchanger tube failures leading to the injection of high-pressure secondary coolant into lead- or LBE-cooled systems. JRC-IE is involved and is considering funding an experiment with prototypical materials, temperatures, and pressures. Earlier and more comprehensive creep failure data at high temperatures have also been retrieved and will be transmitted to ANL.

Proliferation Resistance and Physical Protection Assessment Methodology

PI (U.S): Jordi Roglans, Argonne National Laboratory (ANL)

PI (Europe): Giacomo Cojazzi, Joint Research Center of the European Commission (JRC)

Collaborators: None

Project Number: 2004-004-E

Project Start Date: January 2004

Project End Date: September 2006

Research Objectives

The Technology Goals for Generation IV nuclear energy systems, developed during the roadmap project, highlight proliferation resistance and physical protection (PR&PP) as one of the four goal areas for Generation IV nuclear technology, along with sustainability, safety and reliability, and economics. On the basis of these four goal areas, an evaluation methodology was developed which contributed to identification of the nuclear energy systems options currently under consideration by the Generation IV International Forum (GIF). The Generation IV Roadmap recommended the development of a comprehensive evaluation methodology to assess PR&PP of Generation IV nuclear energy systems.

An Expert Group for the development of an Evaluation Methodology for proliferation resistance and physical protection of Generation IV Nuclear Energy Systems, reporting to GIF Expert Group, was created in December 2002. This Expert Group currently includes U.S. participants from national laboratories (ANL, BNL, INL, LANL, LLNL, PNNL, and SNL), academia, international experts from six additional GIF member countries (Canada, European Union, France, Japan, Republic of Korea, and the United Kingdom), the International Atomic Energy Agency, and observers from the U.S. State Department and the U.S. Nuclear Regulatory Commission.

The PR&PP Expert Group has been tasked to develop a systematic method for evaluating and comparing proliferation resistance and physical protection of Generation IV nuclear energy systems, including their fuel cycle facilities and operations. The methodology must be applicable to the evaluation of nuclear systems from the early development stages throughout the full lifecycle. A main aim is to establish an iterative process in which the PR&PP performance of the system is included in the evolution of the design.

Research Progress

To focus the development of the methodology, the expert group first developed and adopted definitions of proliferation resistance and physical protection, as follows:

- **Proliferation resistance** is that characteristic of a nuclear energy system that impedes the diversion or undeclared production of nuclear material, or misuse of technology, by the host State in order to acquire nuclear weapons or other nuclear explosive devices.
- **Physical protection** is that characteristic of a nuclear energy system that impedes the theft of materials suitable for nuclear explosives or radiation dispersal devices, and the sabotage of facilities and transportation, by sub-national entities and other non-host State adversaries.

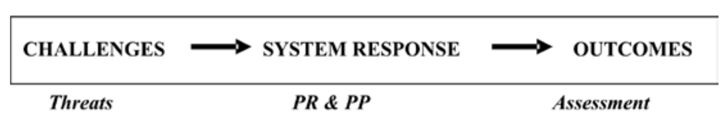

Figure 1. Framework for PR&PP evaluation.

Figure 1 illustrates the methodological approach. For a given system a set of **challenges** is defined, the **response** of the system to these challenges is assessed and expressed in terms of **outcomes**.

The methodology is organized as a progressive evaluation approach that will allow evaluations to become more detailed and more representative as the system's design progresses. This approach will maximize early, useful feedback to designers from basic process selection through detailed layout of equipment and structures and to facility demonstration testing.

The initial step in the evaluation (see Figure 2) is to identify the threat space. The next step, system response, has three main elements:

1) **System Element Identification**. The nuclear energy system is decomposed into smaller elements (subsystems) at a level amenable to further analysis.
2) **Target Identification**. A systematic process is used to identify targets, within each system element, that actors (proliferators or adversaries) might choose to attack or use.
3) **Pathway Identification and Refinement**. Individual pathway segments are developed through a systematic process, analyzed at a high level, and screened where possible. Segments are connected into full pathways and analyzed in detail.

A system pathway analysis for a set of threats consists of identifying potential sequences of events and actions that lead to the undesirable outcome (proliferation, sabotage, or theft) and evaluating the system response. Given that there are uncertainties associated with predicting the response of the system with respect to a given set of threats, a probabilistic pathway analysis is a natural structure for assessing system response to different types of threats.

The system response is expressed in terms of proliferation resistance and physical protection measures. The term measures identifies the few, high-level parameters (measurable factors) that can be used to express proliferation resistance (PR) or physical protection (PP). (This usage differs from another meaning that indicates the set of external actions or procedures applied to material and facility control and protection.) First these measures are evaluated for segments and then they are aggregated for complete pathways, as appropriate, to permit pathway comparisons and system assessment.

For proliferation resistance, the measures are:

- Proliferation Technical Difficulty
- Proliferation Resources
- Proliferation Time
- Fissile Material Quality
- Detection Probability
- Detection Resources

For physical protection, the measures are:

- Probability of Adversary Success
- Consequences
- Physical Protection Resources

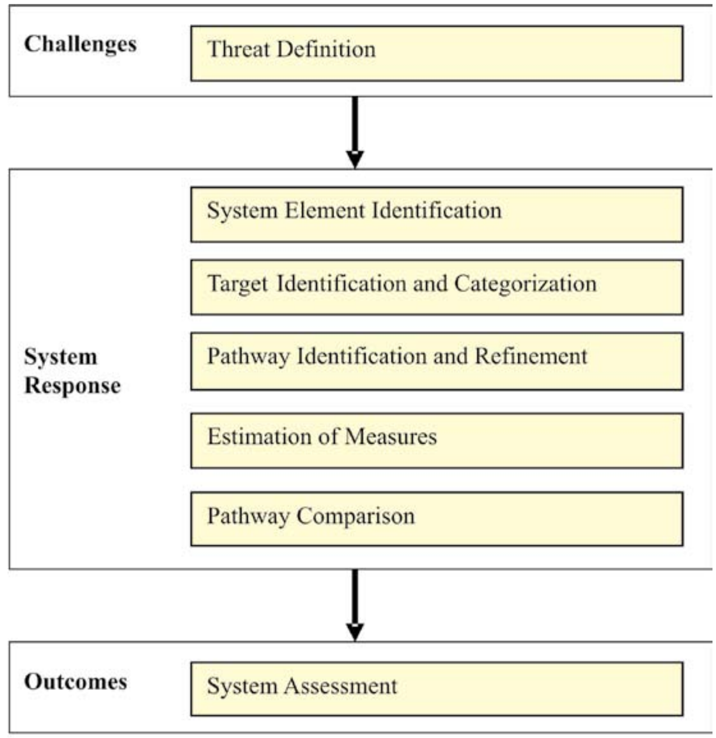

Figure 2. Framework for PR&PP evaluation.

Researchers are developing specific quantitative indices to facilitate the evaluation of proliferation resistance measures (metrics). In particular, they have improved the integration with safeguards approaches through the definition of a "safeguardability concept," defined as the ease of putting an effective safeguards system into operation.

Further development of the methodology is taking place through the example application to a demonstration study. The demonstration study consists of applying the methodology to a hypothetical nuclear energy system and performing additional specialized studies.

This year the PR&PP Expert Group also began to develop the framework for an implementation guide for PR&PP evaluations. A candidate approach and an initial description have been developed. The guide is intended to be a repository for detailed instructions and supplemental information for performing PR&PP evaluations.

Planned Activities

The expert group will continue developing the PR&PP evaluation methodology.

Major milestones are:

- Preparing a methodology update in early 2006 to incorporate improvements to the current status of the framework and methodology
- After completing the demonstration study, completing an updated methodology and initial implementation guide by the end of September 2006

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Characterization of Nuclear Waste Forms and Their Corrosion Products

PI (U.S.): B. Finch, Argonne National Laboratory

PI (Europe): V. Rondinella, Joint Research Center Institute for Transuranium Elements (JRC-ITU)

Collaborators: Pacific Northwest National Laboratory

Project Number: 2004-005-E

Project Start Date: January 2005

Project End Date: December 2007

Project Abstract

The objective of this project is to understand and describe the conditions for the formation and overall effects of altered or secondary phases on the behavior of waste form (spent fuel and/or conditioning matrix) during storage and/or in contact with groundwater. The main processes being investigated are the development of waste alteration caused by large accumulation of alpha decay damage (structural, property changes) and the formation of secondary phases on the waste form surface and its effect on the waste corrosion behavior (e.g., corrosion rate, formation of layers blocking further corrosion on the waste form surface, etc.).

1) Monitor the effects of radiation damage accumulation through measurement of relevant quantities/properties (e.g., lattice parameter, macroscopic swelling, hardness, thermophysical properties, etc.) and through microstructure characterization (e.g., transmission electron microscopy [TEM]). Investigate recovery mechanisms and study the accumulation/release behavior of He in different materials (comparison among irradiated fuels and alpha-doped fuels/matrices).
2) Evaluate possible relationships between observed property changes and corrosion behavior through experiments of aqueous corrosion of "aged" materials (e.g., preferential etching sites, isotopic fractions of released actinides, etc.).
3) Examine corrosion mechanisms and characterize solid corrosion products formed during the aqueous alteration of spent nuclear fuel (e.g., using x-ray photoelectron spectroscopy, transmission electron microscope/energy-loss spectroscopy [TEMEELS], scanning electron microscopy and energy dispersive spectrometer [SEM-EDS], and x-ray diffraction [XRD]). Determine the fates of various radionuclides following their release from altered spent fuel, especially in terms of secondary phase formation and co-precipitation phenomena. Characterize re-precipitated phases on leached surfaces in terms of composition and potential effects on corrosion.

The relevant experimental capabilities for microstructural and macrostructural analysis of the E.U. and U.S. partners will be applied to the abovementioned fuel investigations. Experimental setups and data obtained will be jointly discussed. This will include the possible exchange of suitable samples (e.g., "alpha-doped" materials) for full characterization by the U.S. and E.U. facilities or the acquisition of suitable samples.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Nitride Fuel Fabrication Research

PI (U.S): S. Voit, Los Alamos National Laboratory

PI (Europe): S. Fernandez, Joint Research Center Institute for Transuranium Elements (JRC-ITU)

Collaborators: None

Project Number: 2004-006-E

Project Start Date: October 2004

Project End Date: September 2007

Project Abstract

Implementation of accelerator-driven systems (ADSs) for the purpose of burning americium and degraded plutonium may possibly enable a reduction of radio-toxic inventories directed to geological repositories by a factor of 100. ADSs are designed to operate on uranium-free fuels in order to maximize transuranic (TRU) destruction rates and thus minimize added costs to the nuclear fuel cycle induced by ADS operation and recycling of the higher actinides. The particular choice of fuel type, however, remains an open question, since very little experience on the performance of uranium-free fuels is available.

While conventional oxide fuels have an indisputable advantage in terms of the vast experience accumulated, the low solubility rate of plutonium oxide in nitric acid appears to require a large-scale development of non-aqueous reprocessing methods with much smaller secondary waste streams than has been achieved to date.

Uranium-free nitride fuels, on the other hand, appear to be compatible with the industrialized PUREX process. They further have the advantage of allowing higher linear ratings, typically a factor of two higher than corresponding oxide or metallic fuels. Thus, the number of fuel pins needed to be fabricated and irradiated in ADS facilities can be halved, with a corresponding beneficial decrease in the number of advanced cores and pump systems subject to potential failure.

The lack of data on uranium-free nitrides necessitates a significant R&D program before nitrides can be qualified and validated as a suitable ADS fuel. Completion of this program will result in generation of comparative data on the fabrication and properties of nitrides. This data will provide valuable information on the feasibility of nitrides for plutonium and minor actinide management in ADS reactors.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Molten Salt Technology for Reactor Applications

PI (U.S.): D. F. Williams, Oak Ridge National Laboratory (ORNL)

PI (Europe): R. Konings, European Union's Joint Research Center - Institute for Transuranium Elements (JRC-ITU)

Collaborators: None

Project Number: 2004-007-E

Project Start Date: October 2004

Project End Date: September 2008

Research Objectives

Molten fluoride salts have been studied for use as a fuel and as a coolant for nuclear reactor systems in the past, and a considerable development program has been performed at Oak Ridge National Laboratory (ORNL). In addition, clean molten salts are a candidate to transfer heat from a Very High-Temperature Reactor (VHTR) to a thermochemical hydrogen production plant. In the United States, the VHTR and hydrogen production are high-priority activities. The fusion community also considers molten fluorides an important option for use as coolants and tritium-breeding media for fusion power chambers.

Present research activities in this area include operating the molten-salt corrosion test loop to develop clean molten salts for heat transfer, such as between a VHTR and a hydrogen production plant, and developing a conceptual design of a modern Molten Salt Reactor (MSR) as part of the Generation IV program. There is a growing interest in these and other applications of molten salts. The renewed interest in the U.S., Europe, and Japan in molten salt coolants and the MSR concept in Generation IV plants and in partitioning and transmutation (P&T) studies has led to new research programs at several institutes, among them the Institute for Transuranium Elements (ITU) of the European Union's Joint Research Center (JRC). ITU's research activities on molten salts for reactor technology are emerging. They focus on the assessment of the physicochemical properties and the calculation and measurement of phase diagrams of fluoride salts. Fuel salts for thorium/uranium (Th/U) fuel cycles, transuranium transmutation cycles, and coolant salts are also being studied.

The objective of this I-NERI project is to enhance the collaboration between ORNL and ITU through a common work program. Both organizations are involved in the review of molten salt reactor technology (MOST) project, a shared cost action of the 5th Framework program of the European Union. The extent and scope of this effort will depend on an eventual follow-up project to MOST. A total of six tasks have been identified: four represent activities that will strengthen the scientific basis for molten salt technology and two address the important technological issues of salt purification and on-line impurity removal. A firm scientific basis is essential for molten salt technology, as recent developments indicate higher demands due to the higher operating temperatures and larger temperature gradients. These have an impact on the behavior of the salt itself and the structural materials of the reactor, primarily as a result of corrosion, which is one of the key issues.

Research Progress

Work has progressed to evaluate candidate coolant salts for the liquid-salt-cooled VHTR and next-generation nuclear plant (NGNP). Researchers have conducted a comprehensive evaluation of coolant salts on the basis of physical properties and issued a report. These properties included: melting point, vapor pressure, density, heat capacity, viscosity, and thermal conductivity. Neutron moderation, absorption, and activation metrics were also developed. A summary of the results is shown in Table 1. For most cases, researchers found that salts with lower atomic number had superior heat-transfer and neutronic performance.

				Heat transfer properties at 700 °C					
Salt [a]	Formula weight (g/mol)	Melting point (¼C)	900¼C vapor press (mm Hg)	Density (g/cm^3)	ρ*Cp Volumetric heat capacity (cal/cm^3-¼C)	Viscosity (cP)	Thermal conductivity (W/m-K)	Neutron capture relative to graphite [b]	Moderating ratio [c]
LiF-BeF_2	33.0	460	1.2	1.94	1.12	5.6	1.0	8	60
NaF-BeF_2	44.1	340	1.4	2.01	1.05	7	0.87	28	15
LiF-NaF-BeF_2	38.9	315	1.7	2.00	0.98	5	0.97	20	22
LiF-ZrF_4	95.2	509	77	3.09	0.90	> 5.1	0.48	9	29
NaF-ZrF_4	92.71	500	5	3.14	0.88	5.1	0.49	24	10
KF-ZrF_4	103.9	390	--	2.80	0.70	< 5.1	0.45	67	3
Rb-ZrF_4	132.9	410	1.3	3.22	0.64	5.1	0.39	14	13
LiF-NaF-ZrF_4	84.2	436	~ 5	2.79	0.84	6.9	0.53	20	13
LiF-NaF-KF	41.3	454	~ 0.7	2.02	0.91	2.9	0.92	90	2
LiF-NaF-RbF	67.7	435	~ 0.8	2.69	0.63	2.6	0.62	20	8

Nuclear calculations used 99.995% ^{7}Li

Table 1. Summary of properties of candidate coolant salts for the LS-VHTR/NGNP.

Researchers conducted a comprehensive review of ORNL's experience in the area of high-purity salt preparation. They found that fluorine-containing reagents other than HF, such as ammonium hydrogen fluoride, were never used to produce high-purity salts and offer no advantages over HF. Ammonium hydrogen fluoride is a room temperature solid and was only used for synthesis of certain complex corrosion products (e.g., Na_3CrF_6). At molten salt temperatures, ammonium hydrogen fluoride decomposes to yield HF. HF has technical advantages over ammonium hydrogen fluoride in the areas of dosing, measurement, control, and potential recycle. Previous ORNL reports cover the basic hydrofluorination technology (ORNL-4616, GLOBAL 2003 paper).

The relevance of experience with the molten salt breeder reactor (MSBR) and molten salt reactor experiment (MSRE) to the clean-up of coolant salts was presented in an ORNL report (ORNL/TM-2004/104). Areas that will need to be addressed in future studies were identified.

The report includes a discussion of methods used to make thermal conductivity measurements and estimation methods. The researchers identified flaws in the earlier literature and explained the reasons for their inconsistency. The hypothesis of a heat-transfer film resistance in a molten fluoride system is completely refuted by the experience during the MSRE and by follow-up studies.

Planned Activities

Researchers plan to conduct a review of the levels of purity of the reagents used to prepare high-purity salts so that recommendations can be made. They will assess the potential for recycling reagents for industrial-scale preparation of salts and will also review the analytical methods needed to assess salt purity.

The team plans to make specific recommendations for research on the behavior of noble metal fission products in salts to identify methods that will effectively remove them or control their behavior. They will update property data-sources and estimation methods used to establish a set of basic physical-chemical property data.

They will also propose a plan for improving the accuracy of the thermal conductivity database by identifying methods that should be used to improve the poor agreement among various investigators. A more detailed assessment of models to predict thermal conductivity should be conducted.

Finally, although the phase diagrams of nearly all of the fluoride systems of interest as coolants have been investigated, there are some ternary-fluoroborate and

Safety Calculations for Gas-Cooled Fast Reactors (GFRs)

PI (U.S.): T.Y.C. Wei, Argonne National Laboratory

PI (Europe): H. U. Wider, Joint Research Center of the European Commission, Institute for Energy-Petten (JRC-IE), The Netherlands

Collaborators: None

Project Number: 2004-008-E

Project Start Date: November 2004

Project End Date: September 2007

Research Objectives

The objective of this project is to optimize the design of the gas fast reactor (GFR) by performing core design and transient analyses and evaluating the design's safety approach. The two participants will optimize the reactor core design for the 2400 MW_{th} GFR plant and evaluate the safety response, considering integrated system behavior.

Research Progress

For a preliminary 600 MW_{th} design, previous HEXNODYN calculations had shown good agreement with published results in the case of the Doppler reactivity. However, researchers strongly underestimated the positive voiding reactivity. Since the problems appeared to be due to a too small group cross section set in the HEXNODYN code, they acquired a new, larger and validated cross section set. After considerable efforts, these new cross sections are working but the space-time kinetics is not yet completely operable.

Researchers are benchmarking calculations for comparison of systems codes for a protected loss-of-flow accident including emergency decay heat removal in the 50 MW_{th} Experimental Technology Demonstration Reactor (ETDR) design. They have also established a GFR 2,400 MW_{th} unit core design and have obtained both a primary system design and a guard containment layout for this 2,400 MW_{th} plant. The accident of focus is a station blackout with a leak. Researchers are performing STAR-CD computational fluid dynamics (CFD) calculations for the guard containment to scope decay heat removal performance for this accident. For the larger plant unit sizes currently under consideration, the project goal calls for optimizing the design to enhance core performance, increasing fuel margins, and improving safety response. Additional mechanical design work was performed on the 100 W/cm^3 core design with vertical pins and a 0.5 bar pressure drop. The power density was defined to be compatible with the core pressure drop for the selected semi-passive safety approach to decay heat accidents. Researchers studied arrangements of the fuel element in a "practical" sub-assembly design. The "reference" design accounts for such factors as the SiC cladding, control rod implementation in the core layout, and practical fuel handling. To some extent, researchers selected the design based on engineering judgment. The work includes a characterization of the core configurations based on simplified computational models (2D-HexZ neutronics using REBUS-3/DIF3D and 1D-Z thermal-hydraulics).

The case for a low-pressure drop core can be improved by minimizing pressure drop sources such as the number of required fuel spacers in the subassembly design and by the details of the fuel pin design. The fuel pin design is determined by a number of neutronic, thermal-fluid, and fuel performance considerations. Structural mechanics factors are now included in the design assessment. In particular, thermal bowing establishes a bound on the minimum of fuel pin spacers required in each fuel subassembly to prevent the local flow channel restrictions and pin-to-pin mechanical interaction. There are also fabrication limitations on the maximum length of SiC fuel pin cladding which can be manufactured. This geometric limitation affects the minimum ceramic clad thickness which can be produced. This ties into the fuel pin heat transfer and temperature thresholds. All these additional design factors were included in the current iteration of the subassembly design to produce a lower core pressure drop.

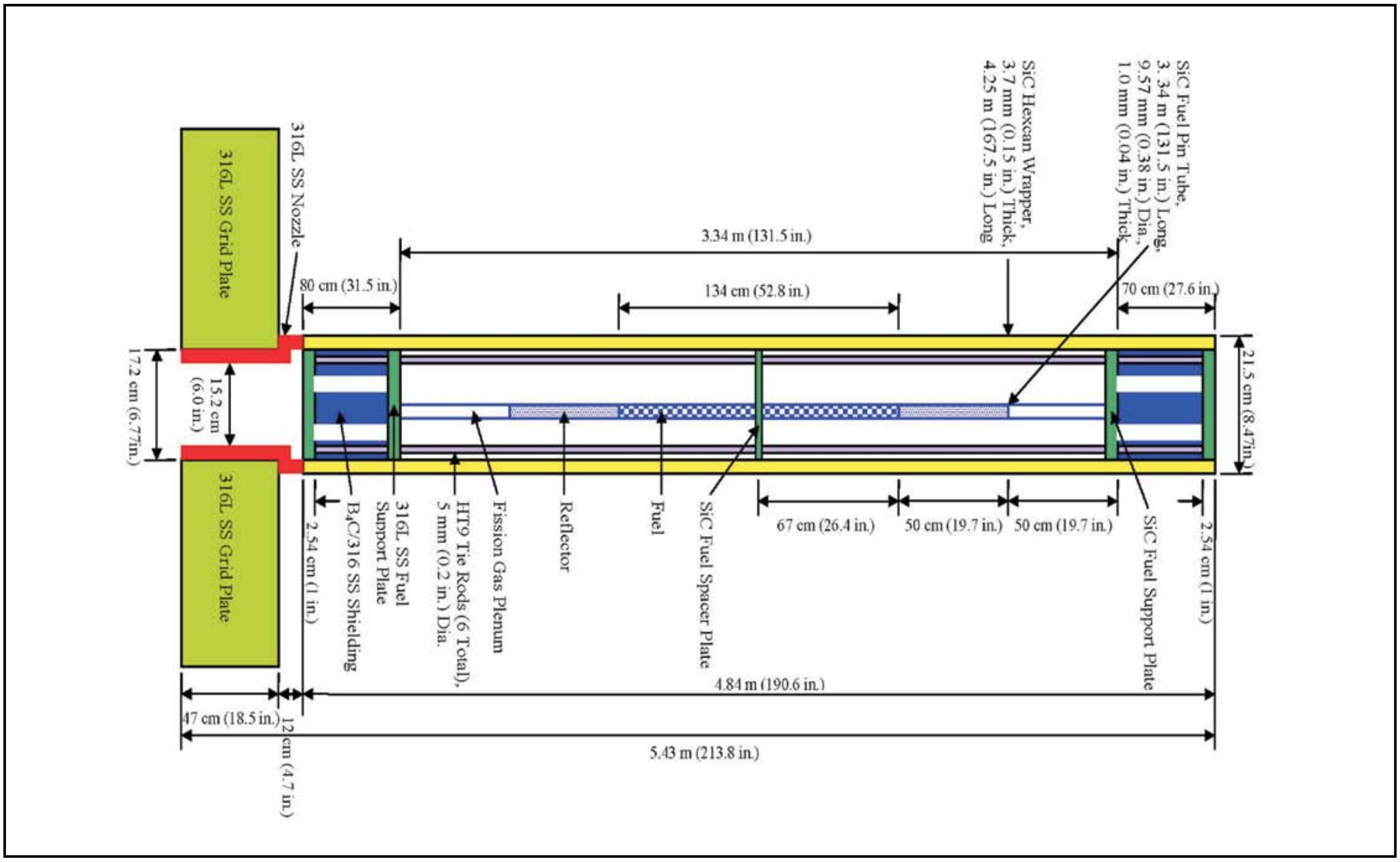

Figure 1. Subassembly layout.

A more detailed definition of the fuel pin/subassembly design is shown in Figure 1.

Planned Activities

Researchers will evaluate the subassembly design under low pressure, natural convection conditions to assess its acceptability for the decay heat removal accidents. They will perform a number of CFD calculations to scope the thermal-hydraulic response of the guard containment design to the accidents of interest. Safety calculations for control rod ejection accidents are also to be performed. Possible design modifications to mitigate sensitivities will be explored under the auspices of the International Generation IV GFR collaborative R&D plan.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Use of an Ionization Chamber in Fission Cross-Section Measurements

PI (U.S.): T. Hill, Los Alamos National Laboratory

PI (Europe): P. Rullhusen, Joint Research Center of the European Commission-Institute for Reference Materials and Measurements (JRC-IRMM), Belgium

Collaborators: None

Project Number: 2004-009-E

Project Start Date: October 2004

Project End Date: October 2007

Research Objectives

The objective of this project is to improve fission cross section data files for major and minor actinides which will be needed for the design, optimization, and safety assessment of accelerator-driven systems, fast reactors, and waste transmuters, as well as relevant actinides for the thorium-uranium fuel cycle. The aim of this project is to produce accurate data files for several key isotopes, which will contribute to the new ENDF B/VII and JEFF 3.1 libraries.

Research Progress

The initial phase of the project included receiving and installing a double-gridded ionization chamber to make it operational for benchmark testing. Many of the delicate components of the chamber were damaged or destroyed in shipping (Figure 1). All of the damaged and destroyed parts have been repaired or replaced. The commissioning of the chamber has started and so this task is not too far off schedule.

Researchers measured the protactinium (^{231}Pa) fission cross-section at incident neutron energies E_n=0.8 up to 3.5 MeV relative to a neptunium (^{237}Np) reference sample in back-to-back geometry. The detector was a double Frisch-grid ionization chamber. Due to a very high alpha-activity of the sample available at IRMM, a collimator had to be used. Researchers verified the results by using two different collimators at E_n=2 and 3 MeV. In addition, they set up a special alpha-spectrometer to determine the effective mass used in the measurements. The results of the cross-section measurements were presented at the NEMEA-2 workshop in Bucharest and are presently in press at *Annals of Nuclear Energy*. The shape of the cross-section in this energy range confirms results obtained from a recent particle transfer reaction.

The individual cross-section data obtained had an uncertainty of less than 5 percent which meets the accuracy required by the International Atomic Energy Agency (IAEA) described in the 1999 summary report, ”Assessment of Nuclear Data Needs for Thorium and other Advanced Cycles.” With the new data, the currently large spread between evaluated data files may be removed.

Researchers continued the cross section measurements in the energy range E_n = 15 to 21 MeV. The cross-section values obtained below 16 MeV are considerably lower than

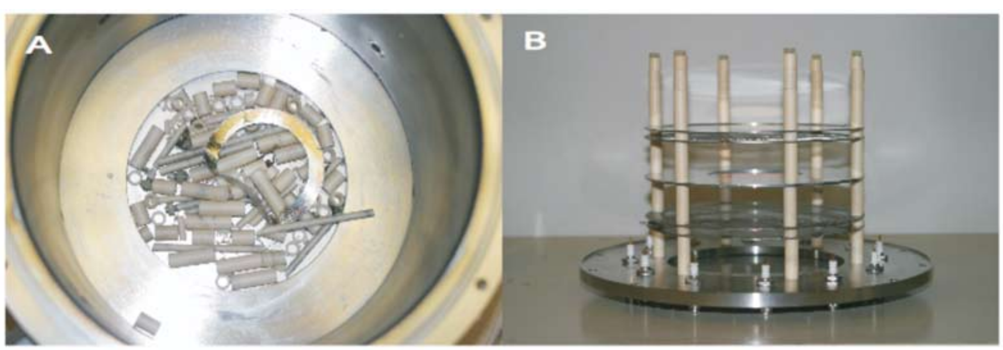

Figure 1. (A) Inside of the fission chamber with end flange removed after delivery, showing broken and damaged parts at the bottom of the vessel. (B) The end flange, used to seal the chamber and support the fission foils and read-out plates, shown with the fully reconstituted foil stack.

most of the other values found in literature, although they agree with recent calculations made in collaboration with scientists from Bucharest University. For energies above 16 MeV, a correction is necessary to account for the contribution of low-energy neutrons from secondary reactions. Determination of this correction is in progress.

Researchers measured the ^{237}Np fission cross-section at the Los Alamos Nuclear Science Center (LANSCE). The measurement, shown in Figure 2, spans 10 decades in incident neutron energy by using two high-neutron flux facilities at LANL—the Lujan Center and the Weapons Nuclear Research (WNR) facility. Both facilities provided high-flux neutron beams from spallation when 800 MeV protons impinge on tungsten targets. The experiments at WNR are exposed directly to the spallation neutrons, which range in energy from 50 keV to nearly 800 MeV, and the Lujan experiments see a beam moderated by light elements, providing neutrons from thermal energies to several hundred keV. Combining the data from the two facilities provides complete coverage from thermal energies to several hundred MeV. Researchers used a parallel plate ionization chamber running in trigger mode for this measurement due to the low activity of the sample. They measured the cross-section to better than 1 percent statistically at all energies above 100 keV incident neutron energy, with systematic errors below 2 percent everywhere else in that region, meeting the AFCI requirements for high-precision data. This data, which spans over 10 decades in incident neutron energy, is a first-of-a-kind measurement, and will be included in the new ENDF/B-VII release. Researchers will submit a paper documenting the experiment to *Physics Review*.

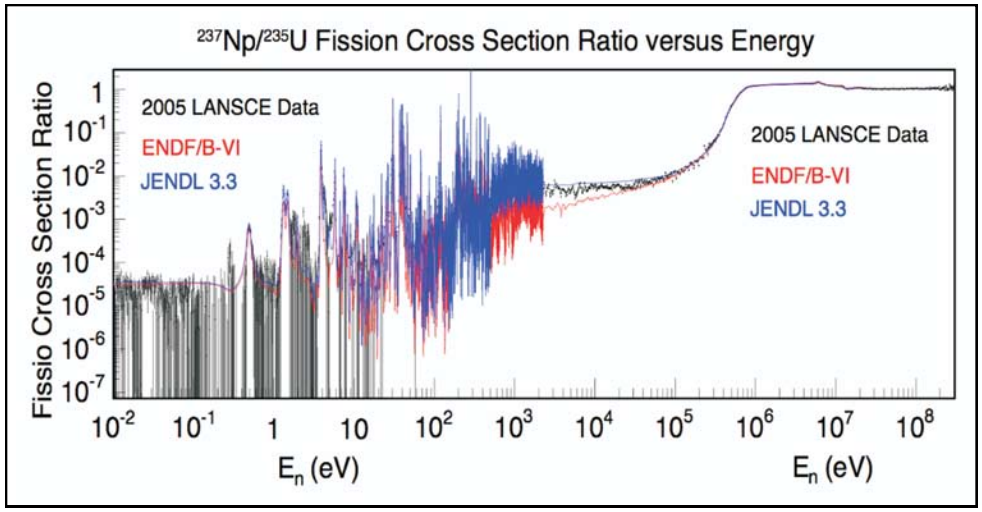

Figure 2. $^{237}Np(n,f)/^{235}U(n,f)$ cross section ratio as a function of incident neutron energy. The data (black crosses) were taken at the WNR and Lujan facilities at LANSCE. Two different evaluations are overlayed to show the level of discrepancy that this experiment was intended to address.

Planned Activities

The commissioning of the double-gridded chamber will continue so that design benchmarks can be developed. The goal is to use the chamber to carry out precision fission cross section measurements on highly active targets by combining signals from both fission fragments for triggering against radioactive alpha decays. Successful comparisons with well-measured cross sections will be required before a larger chamber is designed and built. The advanced detector will allow data to be taken on many samples simultaneously.

Researchers will complete the ^{231}Pa fission cross section measurement and submit the results for evaluation. A new measurement campaign will begin for the fission cross section of ^{233}U at EC-JRC-IRMM. Data for ^{233}U will also be taken at LANL so that inter-lab comparisons can begin. Also, fission cross section measurements on ^{242}Pu and ^{240}Pu will be carried out at LANSCE to provide the high-fidelity data required for the AFCI program.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Nuclear-Assisted Hydrogen Storage and Safety Issues

PI (U.S.): R. Vilim, Argonne National Laboratory

PI (Europe): H. Wilkening, Joint Research Commission–Institute for Energy (JRC-IE)

Collaborators: None

Project Number: 2004-010-E

Project Start Date: May 2005

Project End Date: September 2006

Research Objectives

The objectives of this project are to identify and assess the key issues associated with demonstrating the technical and economic viability of generating nuclear hydrogen, and with defining the analytical and experimental work needed to achieve maturity of the nuclear hydrogen process. These assessments usually involve engineering design studies and rule-of-thumb cost analyses. Researchers on this project will work with thermochemical cycles previously identified as having a reasonable basis for technical and economic viability. The three main tasks are to:

- Perform analytical research on the safety aspects of hydrogen production, storage, and transport
- Compare the efficiency, complexity, reliability/availability, and economy of different hydrogen production and distribution systems
- Conduct comparative analysis of Generation IV reactor types for hydrogen generation focusing on the engineering linkage between the hydrogen production plant and the nuclear heat source

Research Progress

Research work completed in FY 2005 suggested that low-temperature hydrogen production cycles may be more cost-effective than high-temperature thermochemical cycles because of challenges with structural materials that severely constrain performance with increasing temperature. Figure 1 illustrates how material capabilities decrease exponentially with temperature, while thermodynamic efficiency increases only linearly. Researchers explored the advantages of a low-temperature thermochemical process coupled to a direct-cycle gas reactor for hydrogen production. They reached a

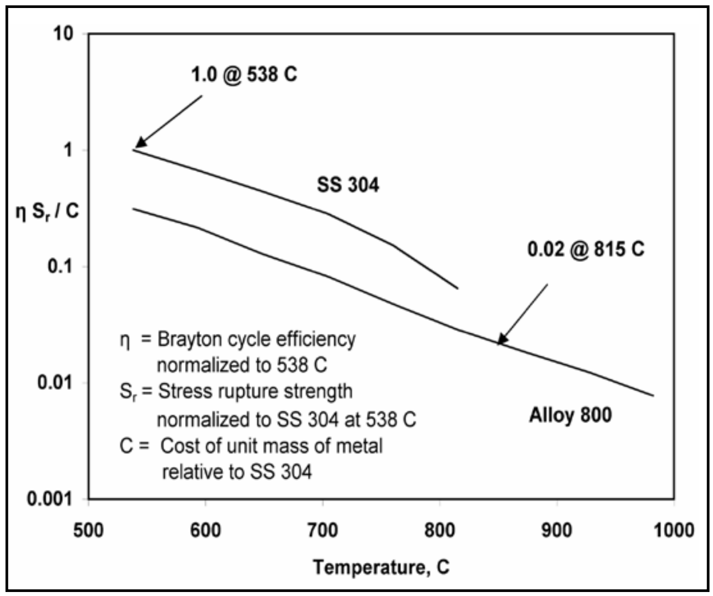

Figure 1. Index reflecting cycle efficiency, creep rupture stress, and cost per unit mass as a function of temperature.

preliminary conclusion that the hydrogen product cost in a cogenerating plant would be less using a low-temperature cycle.

The researchers identified several potential advantages for the low-temperature copper chlorine thermochemical cycle. These include potentially higher combined electricity/hydrogen production efficiency, reduced chemical plant complexity, less challenging materials requirements as a consequence of operation at reduced temperature, and less noxious intermediate products. They designed a combined plant layout that takes advantage of these observations (shown in Figure 2). They performed an analysis of efficiency and operability at full power and partial powers for the combined plant using the GAS-PASS/H computer code. The analysis confirmed the advantages seen initially. Figure 3 indicates that overall plant efficiency

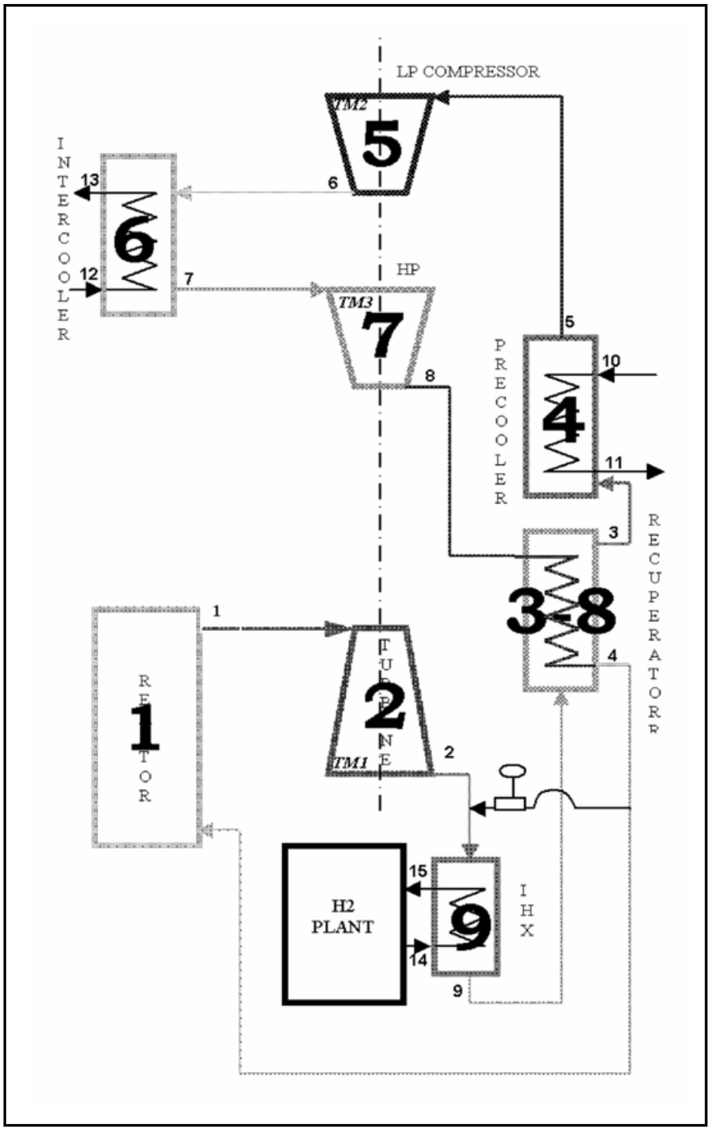

Figure 2. Schematic of 600 MW_t direct-cycle, series arrangement, low-temperature thermochemical cycle plant.

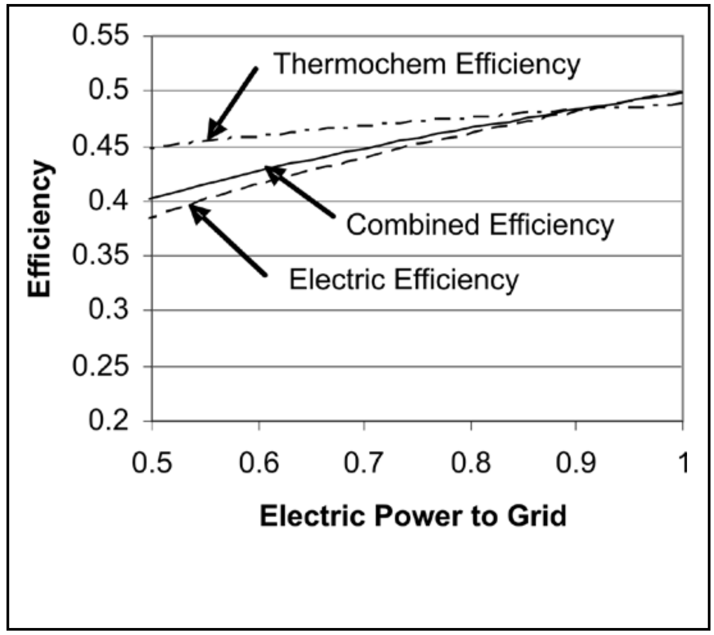

Figure 3. Hydrogen process and electrical efficiencies as a function of fractional power production sent to grid.

falls off with partial power. Current work is aimed at developing alternative control schemes that will reduce the efficiency loss at partial powers.

Planned Activities

The separation distance between the nuclear plant and hydrogen plant is dictated in part by hypothesized hydrogen plant accidents that could damage the reactor. The project team brings extensive expertise in hydrogen safety, including plume dispersion and consequences of hydrogen detonation, which they will apply to this separation issue. Researchers have already estimated the hydrogen inventory for the ANL design of the copper chlorine cycle, a key input parameter.

8.0 U.S./France Collaboration

U.S. Secretary of Energy, Spencer Abraham, and CEA Chairman, Pascal Colombani, signed a bilateral agreement on July 9, 2001, to jointly fund innovative U.S./French research in advanced reactors and fuel cycle development. The U.S./France collaboration was the first I-NERI agreement to be fully implemented; 16 U.S./France collaborative research projects have been awarded since FY 2001.

8.1 Work Scope Areas

R&D topical areas for the U.S./France collaboration include:

- Advanced gas-cooled reactors
- Advanced fuel and materials development
- Radiation damage simulation
- Hydrogen production using nuclear energy

8.2 Project Summaries

In FY 2001, the initial year of the collaboration, four research projects were awarded, with one additional project in FY 2002. Both remaining projects initiated in FY 2001 and the FY 2002 project were completed during the past year. Work on 11 collaborative projects initiated in FY 2004 is continuing.

A listing of the I-NERI U.S./France projects that are currently underway and those completed last year follows, along with summaries of the accomplishments achieved in FY 2005.

Directory of Project Summaries

Development of Generation IV Advanced Gas-Cooled Reactors with Hardened/Fast Neutron Spectrum

PI (U.S.): T.Y.C. Wei, Argonne National Laboratory

PI (France): J. Rouault, Commissariat à l'Energie Atomique (CEA) Cadarache

Collaborators: Brookhaven National Laboratory; General Atomics; Massachusetts Institute of Technology; Oak Ridge National Laboratory; Framatome – ANP (Fra-ANP), Lyon

Project Number: 2001-002-F

Project Start Date: March 2002

Project End Date: February 2005

Research Objectives

The Gas-Cooled Fast Reactor (GFR) is one of six systems selected for viability assessment in the Generation IV program. It features a closed nuclear fuel cycle, consisting of a high-temperature helium-cooled fast spectrum reactor, coupled to a direct-cycle helium turbine for electricity production. The GFR combines the advantages of fast spectrum systems with those of high-temperature systems. It was clear from the very beginning that the GFR design should be driven by the objective to offer a complementary approach to liquid metal cooling.

On this basis, CEA and the U.S. DOE decided to collaborate on the pre-conceptual design of a GFR. This reactor design will provide a high level of safety and full recycling of the actinides, and will also be highly proliferation resistant and economically attractive. The goals of the project were to perform exploratory studies on neutronics, safety, core, and fuel form (year 1); to conduct trade studies on design concepts with high potential (year 2); and to characterize point designs (year 3). Researchers from CEA and DOE continually exchanged information on fuel and structural materials throughout this work to ensure the coherency of the project.

Research Progress

This three-year project has been completed and two unit sizes, 600 MWt and 2,400 MWt, have been selected as the focus of the design and safety studies. Researchers studied fuel forms, fuel assembly/element designs, core configurations, primary and balance-of-plant layouts, and safety approaches for both of these unit sizes. Results regarding the feasibility of this GFR design are encouraging. For example, sustainability and non-proliferation goals can be met and the proposed concept has attractive safety features. These features take advantage of the helium in terms of its neutronic quasi-transparency as well as the enhanced Doppler Effect in connection with candidate fuel aocess has been developed for coating particle fuel.

To summarize, the research team assembled point designs from different options and combinations, as described below:

- **Fuel choice**: Dispersed fuel in plate sub-assemblies as the reference, SiC-cladded pellets in pin sub-assemblies as a back-up. The selected actinide compound was carbide in the design studies, but nitride remains a possible candidate.
- **Unit size**: 2,400 MWt
- **Power density**: 100 MW/m^3
- **Decay heat removal**: Natural convection passive approach, which should be combined with active means (low power circulators) in a well balanced mix to be refined. This does not exclude alternative options (search for conduction paths, heavy gas injection, etc.) on which some future effort should still be devoted.
- **Balance-of-plant**: Direct Brayton cycle balance-of-plant option remains the reference, but consideration of the indirect super-critical CO_2 cycle with an equivalent cycle efficiency has also been included.

Even though the trade studies have confirmed the neutronic flexibility of the GFR for burning and the potential for minor actinide management, no further work has been planned on this alternative. More effort has been concentrated on details of the core design tying together core neutronics, assembly thermal-hydraulics and fuel element structural design, and fuel performance. Concurrently, a list of accidents/transients has been developed, consistent with this licensing basis, which will be used by all of the project participants to perform the design basis accident evaluations and simulations necessary to set the various design parameters, performance limits/specifications, and threshold.

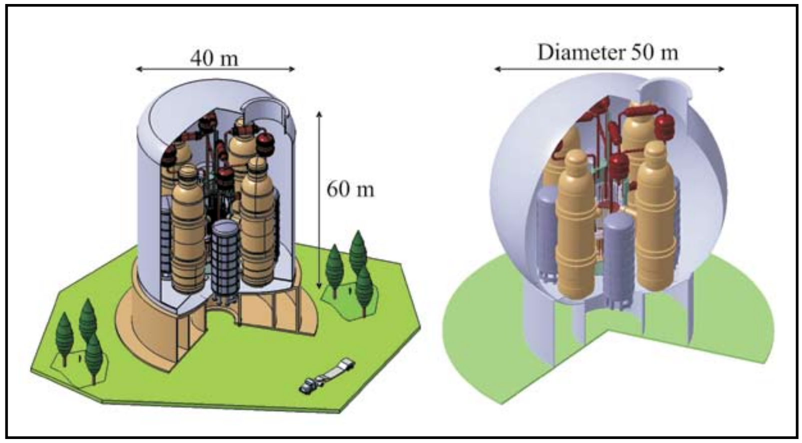

Figure 1. Possible layouts for the 2,400 MWt reactor plant.

Researchers reached consensus on the safety approach to mitigating depressurized decay heat accidents. The approach of using only natural convection has been fully characterized and all the essential transient calculations performed for the 600 MWt plant. However, total reliance on natural convection has economic drawbacks because of the need for a costly containment vessel that is able to ensure a 2.0 Mpa back-up pressure. Researchers also evaluated an alternative based on a well-balanced combination of both active and passive means. This is a semi-passive approach. The containment will still be utilized, but it will be sized for 0.5 to 0.7 Mpa backup pressures. The 5 bar back-up pressure plus whatever natural convection is available at this pressure will significantly reduce the blower power of the active DHR system sized to remove 2-3 percent decay power. The objective is to have such low power requirements that batteries can supply the total load. This 5 bar back-up pressure should be sufficient to support natural convection removal of 0.5 percent decay heat, which occurs at approximately 24 hours into the accident.

Therefore, there should be no more need for active systems or power supplies after the initial period of one day. Furthermore, since there will be a decay of the after-heat from 2-3 percent to 0.5 percent in this time period, credit should be taken in probability space for loss of active systems during the 24 hours. This safety approach is probabilistic—work can begin on the active systems and the PRA. The proximate vessel confinement should be significantly cheaper and could be either of metal or concrete. Refueling will be carried out at 5 bar and actions should be taken to rule out double containment bypass. The issue of water flooding will be investigated for shutdown worth requirements. (See follow-on I-NERI project 2004-008-F.)

In conclusion, researchers believe that evaluation of the GFR design, based on the 2,400 MWt plant size, has yielded promising results. This design uses less challenging fuels that meet both the high temperature and fast flux requirements, due simply to the larger size of the core. The larger size of the core leads to lower neutron leakage and less-than-maximal specifications on the fissile loading density. As an improvement on the 600 MWt design, a larger unit size with a larger core would prove less challenging to the fuel development due to decreased density loading requirements. At the same time, a larger unit size would also benefit from economies-of-scale. Modularity of the PCU could still be maintained by simply adding additional loops to the one loop/PCU 600 MWt design and utilizing a multiple number of 600 MWt PCUs. Unlike the VHTR, which would have difficulties scaling up in current size and still maintain the same safety case for conduction cooldown, the GFR can scale up with the same safety approach of natural convection from the 600 MWt unit to the larger 2,400 MWt unit. Unlike the HLM coolant reactors, vessel scale-up should not pose special difficulties. For these reasons, the 2,400 MWt GFR has been recommended as the reference design case. It will provide an option to the smaller modular reactor plant designs with the other primary coolants being considered by the Generation IV initiative and allow an economics-of-scale comparison. Figure 1 shows possible layouts of this plant design.

Planned Activities

This project has been completed. Follow-on work will be performed under I-NERI project 2004-008-F.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Nano-Composited Steels for Nuclear Applications

PI (U.S.): Roger E. Stoller, Oak Ridge National Laboratory

PI (France): Ana Alamo, Commissariat à l'Energie Atomique (CEA)

Collaborators: University of California, Santa Barbara

Project Number: 2001-007-F

Project Start Date: October 2001

Project End Date: September 2005

Research Objectives

The objective of this I-NERI project was to develop the required knowledge base of material processing, deformation mechanisms, fracture behavior, and radiation response of existing oxide dispersion strengthened (ODS) steels in order to guide future development of advanced alloys capable of meeting the Generation IV reactor needs for higher operating temperatures. In particular, the goal was to discover the thermomechanical processing required to prepare new alloys with properties comparable to a reference 12Cr ODS steel (12YWT) that had been fabricated in Japan in the late 1990's.

Research Progress

The primary goal of this project has been achieved. Researchers have developed a recipe for reproducibly fabricating an advanced oxide dispersion strengthened (ODS) alloy with the desired microstructure that includes high-density nanometer-sized oxide clusters. The new alloy, and the variants that were also produced, have high-temperature strength, making them good candidates for further development and ultimate application to Generation IV reactors or other advanced energy systems.

Researchers examined alloy processing and fabrication variables in an extensive investigation that employed a range of mechanical alloying and alloy consolidation methods available at the three participating institutions. They applied advanced microstructural analysis techniques to develop an improved understanding of how and when the nanometer-sized oxide clusters form in the mechanically alloyed materials. New insight into the differences and similarities of the ODS alloys MA957 and 12YWT was obtained and an improved mechanical property database on these materials was developed.

Further refinement of the processing recipe for the developmental alloy was carried out and the mechanical properties of the as-processed alloys were investigated. Specimens were fabricated and included in long-term irradiation experiments to examine the stability of the oxide nanoclusters. Because of the extended irradiation time and reactor operating schedules, it was not possible for these irradiations to be completed within the time frame of the original project. In addition, specimens of the developmental alloy were prepared for corrosion testing in Pb, PbLi, and under supercritical water conditions. These corrosion tests are ongoing under separate funding.

Four variants of the prime developmental 14Cr ODS alloy were prepared and the temperature dependence of the unirradiated tensile properties was measured. The four ODS alloys were first annealed in vacuum at 1,000°C for 1 hour and then warm rolled to approximately 40 percent reduction in thickness in several passes. After fabrication, the tensile specimens were annealed at 1,000°C for 1 hour before testing. The tensile tests were conducted at room temperature (~22°C) and from 360°C to 800°C in air using a strain rate of 10^{-3}/s.

Figure 1 shows the stress-strain curves that were recorded for the alloy variant designated OE14YWT-SM4. The 12YWT yield strength is indicated by the red bar. The results indicated that the new alloys containing the nanoclusters showed high yield and ultimate tensile strengths from room temperature up to 800°C. More importantly, the yield strength of the developmental alloy at room temperature was substantially greater than the reference 12YWT alloy.

While irradiation experiments involving the developmental alloys are ongoing, the effects of neutron irradiation on tensile properties and microstructure of the reference ODS alloy MA957 have been assessed in irradiations performed at 325°C in the Osiris reactor (CEA-Saclay) at 2 and 5.5 dpa, as well as in the BOR60 fast reactor up to 42 dpa. Data obtained for MA957 were compared with that from a conventional 9Cr1Mo steel and reduced activation ferritic/martensitic (RAFM) steels of 9CrWTaV-type irradiated under the same conditions. Figure 2(a) presents the radiation-induced increase in yield stress of these materials as a function of the dose. The initial yield strength at 325°C of ODS-MA957 is 895 MPa and 445-460 MPa for RAFM and 9Cr1Mo steels. As expected, irradiation induced an increase of the tensile strength, but despite the high chromium content, the lowest hardening was obtained for the ODS alloy. Moreover, the MA957 exhibited greater post-irradiation ductility with the highest values of total elongation, as shown in Figure 2(b), and also the highest uniform elongation and reduction in area level after irradiation to 42 dpa. Such results are promising indicators for application of the advanced ODS alloys in nuclear energy systems.

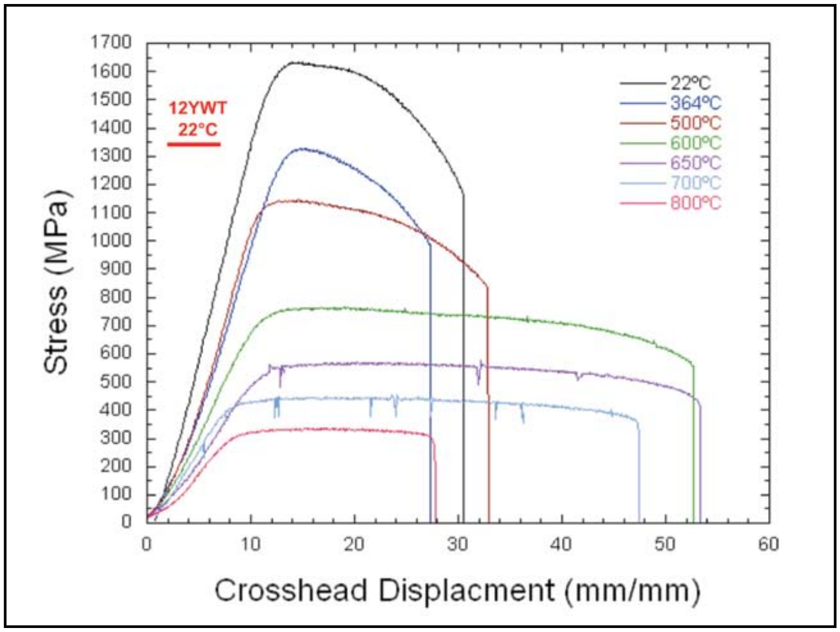

Figure 1. Stress-strain curves as a function of temperature for OE14YWT-SM4.

Planned Activities

No further work is planned directly under this project. Formal funding ended September 30, 2004, with some additional work being completed under a no-cost extension through FY 2005. Long-term irradiation of specimens fabricated from the developmental alloy is continuing, and post-irradiation examination of the specimens will be carried out under other funding. Similarly, results from the extended corrosion experiments will become available as these exposures are completed.

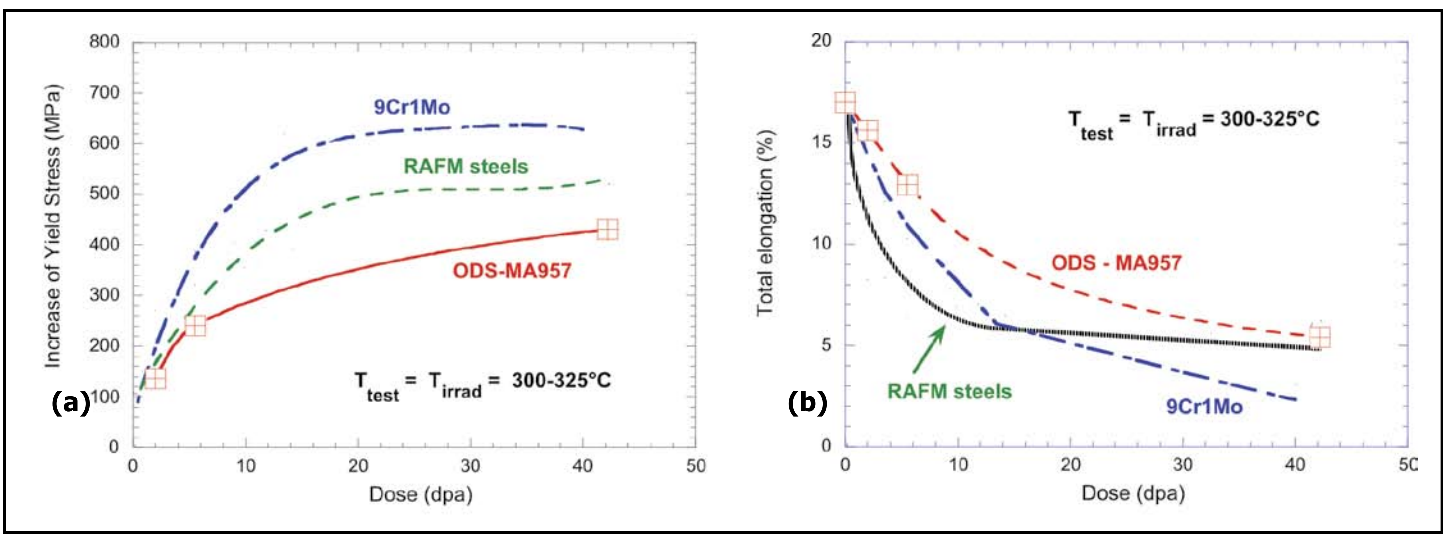

Figure 2. Radiation-induced strengthening (a) and total elongation (b) of the ODS MA957 alloy at 325°C compared to 9CR1Mo conventional and reduced activation martensitic (RAFM) steels as a function of dose.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

High Efficiency Hydrogen Production from Nuclear Energy: Laboratory Demonstration of S-I Water Splitting

PI (U.S.): P. Pickard, Sandia National Laboratories (SNL)

PI (France): P. Carles, Commissariat à l'Energie Atomique (CEA)

Collaborators: General Atomics (GA)

Project Number: 2002-001-F

Project Start Date: October 2002

Project End Date: September 2005

Research Objective

The objective of this project was to investigate the sulfur iodine (S-I) thermochemical water splitting cycle and assess the potential application of this cycle to nuclear hydrogen production. The project approach was to design, construct, and test the three major component reaction sections that make up the S-I cycle: 1) the primary (Bunsen) reaction section, 2) the HI decomposition section, and 3) the H_2SO_4 decomposition section. The researchers also evaluated process chemistry and materials of construction. Although this I-NERI project addressed only the development of stand-alone sections, the sections are being designed to facilitate later integration into a closed-loop demonstration. During this three-year project, researchers completed flowsheet analyses of the S-I cycle to examine process configuration options and designed and performed experiments on the three primary reaction sections.

Research Progress

The following sections describe the experiments performed on each of the primary reactions sections of the S-I cycle: the Bunsen section, the HI decomposition section, and sulfuric acid decomposition section.

Bunsen Section. Researchers at CEA completed experiments to support the design of the Bunsen section. In order to optimize the stoichiometry of the Bunsen reaction and the efficiency of the overall S-I process, they performed the following tasks:

- Defined appropriate analytical methods to fully characterize the different liquid phases sampled from the reactors
- Studied the distribution of iodine and sulfur between each of the two liquid phases obtained by mixing the final products of the Bunsen reaction
- Investigated Bunsen reaction chemistry with varying I_2 and H_2O amounts and SO_2 pressure

They constructed benchscale experimental devices, generally corresponding to these three steps, with post-test diagnostics to determine the chemical composition of the resulting liquid phases. Results from these experiments were consistent with published data.

A key issue in evaluating the S-I process has been the lack of basic thermophysical data to support flowsheet analyses of alternative configurations. Researchers are developing experimental capabilities to provide vapor-liquid equilibrium data for the HI-I_2-H_2O system and have completed experiments on the HI-H_2O system (Figure 1).

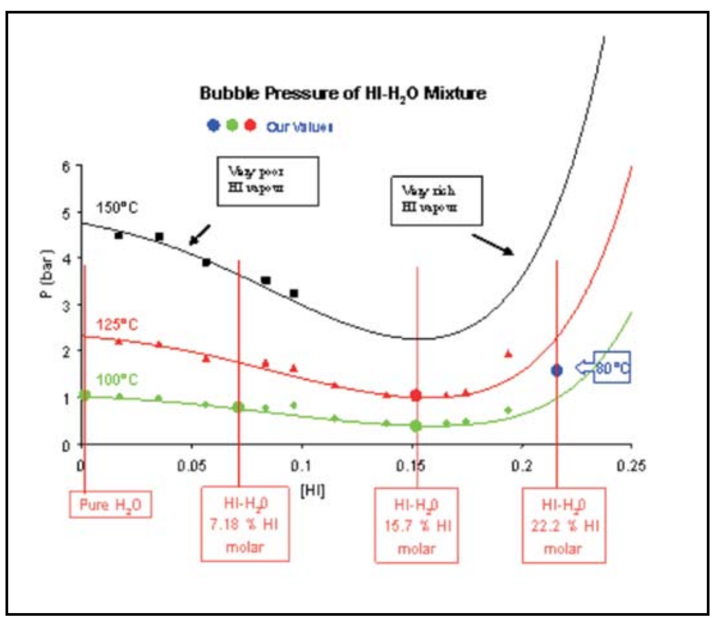

Figure 1. Total pressure measurements: comparison between experimental and calculated (ASPEN code) values.

Researchers also developed techniques to measure the total and partial pressure and temperature of the ternary system using three novel experimental devices, including a tantalum micro-autoclave and a vapor optical chamber. For real-time measurements of vapor phase concentrations in the Bunsen section of the S-I process, they developed UV-Visible spectrometry for measuring the iodine concentration and Fourier transform infrared spectroscopy (FT-IR) for measuring the hydrogen iodide and water concentrations. Raman spectroscopy is also under evaluation for high pressure measurements and speciation in the gas phase. Initial results indicated that a better knowledge of the vapor phase for HI concentration above the pseudo-azeotrope is needed. The HI content of the vapor phase appears to be higher than predicted by current models, which is advantageous if reactive distillation is utilized in the S-I process.

HI Decomposition Section. Researchers at General Atomics have completed analyses and experiments to evaluate two approaches for constructing and operating the HI decomposition section, that is, reactive distillation and extractive distillation. They constructed a reactive distillation apparatus and performed HI distillation experiments for both HI/H_2O and $HI/H_2O/I_2$. Results show high levels of H_2 production with HI/H_2O, but production was significantly reduced with I_2 present in the mixture (Figure 2). Experiments with an extractive apparatus proved to be more efficient. Based on the results, extractive distillation was selected as the distillation method for further development. Corrosion testing for this section has identified several Ta-and Nb-based alloys that appear promising as materials of construction for this section.

Sulfuric Acid Decomposition. SNL researchers completed two series of experiments on high-temperature sulfuric acid catalytic decomposition. They performed tests at absolute pressures of 2, 6, and 11 bars, and at temperatures varying from 750–875°C. Real-time measurements of acid conversion were used to determine SO_2 conversion as a function of temperature in a single experiment. These experiments resulted in the expected increasing acid conversion fraction with increasing temperature, but the measurements were not precise enough to accurately confirm the variation of conversion efficiency as a function of pressure. For acid vapor temperatures varying from 750°C–875°C, measured conversion fraction ranged from 0.4 to 0.45, respectively, at 6 bars and from 0.3 to 0.5, respectively, at 11 bars. These values were bounded by the thermodynamic equilibrium limit for acid conversion. Real-time diagnostics were used for the first time in these types of experiments, which allowed the conversion fraction to be available within seconds for process control and chemical composition data to be available in minutes.

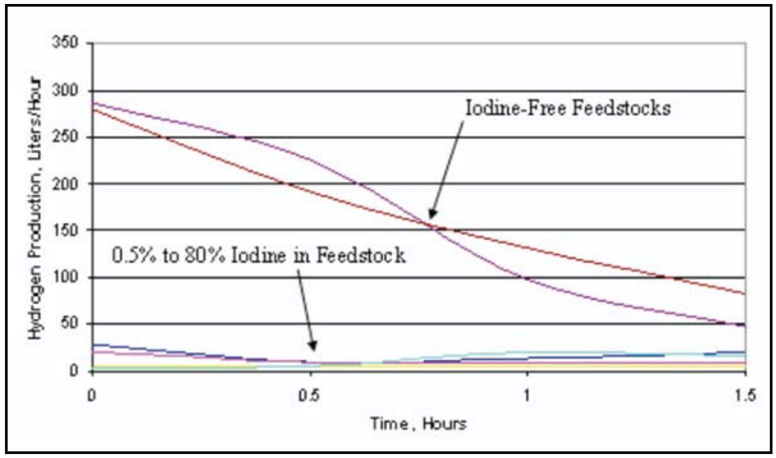

Figure 2. Hydrogen production rate from reactive distillation tests.

Based on these results, researchers have designed decomposers capable of supplying SO_2 at rates consistent with a 500 L/hr hydrogen level. The next series of tests will demonstrate a concentrator to receive dilute acid from the Bunsen section, and a direct contact heat exchanger (DCHX) to recover both heat and undecomposed acid from the decomposer. Additionally, FT-IR spectroscopy will be used for in-situ, real-time measurements of gas concentrations at the inlet and outlet of the catalyst decomposer.

Planned Activities

Although the scope of this I-NERI project was limited to constructing and testing the stand-alone reaction sections for the S-I cycle, the sections were designed to facilitate assembly into an integrated, laboratory-scale experiment. It is anticipated that a collaborative follow-on project will be defined which will complete testing of the three sections, and transport the three sections to a single site to perform an integrated laboratory demonstration. This integrated experiment will serve as a test bed for investigating process improvements, advanced materials, components, and operational and control issues.

In addition to addressing the key viability and performance issues for the S-I cycle, operation under closed-loop conditions presents new issues that must be evaluated before decisions on scaling to higher production levels can be made. The key issues of coordination and control between sections, potential for contamination or crossover between sections, process fluid quality, degradation and makeup, and other issues must be demonstrated in a closed-loop experiment.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Hydrogen Process to High Temperature Heat Source Coupling Technology

PI (U.S.): Charles Park, Idaho National Laboratory (INL)

PI (France): Dominique Barbier, Commissariat à l'Energie Atomique (CEA) Cadarache

Project Number: 2004-001-F

Project Start Date: August 2004

Project End Date: July 2007

Research Objectives

This project will develop the technology necessary to couple a high-temperature heat source to hydrogen production processes for the Nuclear Hydrogen Initiative. The primary focus of this I-NERI research is to develop the Sulfur-Iodine (S-I) cycle process technology. Specific research objectives include:

- Propose design solution schemes, including component connections for these interfaces: reactor → intermediate heat exchanger → high temperature step → medium temperature step → low temperature step. Compare their characteristics and select a component arrangement that will reduce heat losses.
- Evaluate heat transmission and exchangers including technical and industrial feasibility, flexibility of coupling schemes, and conversion energy losses for the design solutions. Develop potential scheme designs.
- Develop and utilize a model to evaluate the complete heat balances for the different schemes, analyzing the use of energy (electricity and/or heat) in relation to hydrogen production. This model will permit an understanding of the process behavior during normal operation, transient, and accidental condition. The information from the models and simulations will provide the data needed to perform availability and safety analysis, as well as information and interface data for the economic evaluation and cost estimation work teams.

Research Progress

The most promising current process (in terms of efficiency for very high temperatures) is the Iodine-Sulfur closed thermochemical cycle. For this purpose, the CEA supported specific studies on the coupling of a nuclear and hydrogen plant. Following is a summary of this research team's progress.

- Researchers evaluated pre-design options of a co-generation plant, mainly based on efficiency optimization. They considered several design schemes in order to meet the very flexible operational requirements for nuclear electricity generation and hydrogen production. They took into account criteria on industrial feasibility and economics.
- The team developed a design of the whole fluid transfer circuits between the primary heat exchanger and the preliminary hydrogen plant chemical flow sheet. This design is closely linked to a safety approach based on defense-in-depth principles, allowing researchers to analyze all the system configurations under normal, incidental, and accidental operating conditions.
- They developed a dedicated multi-code platform. This platform mainly concerns the use of the codes developed within the CEA framework:
  - Pre-design codes for stationary nuclear plant operation (links to H_2 plant with mainly heat sinks and source boundary conditions)
  - Conceptual design of the coupling fluid circuits
  - Hydrogen plant design
  - Nuclear safety codes extended to chemical plant operation for the final safety report
- Researchers focussed on an alternative hydrogen production process - High Temperature Electrolysis. CEA is developing a specific electrolyser model to improve thermodynamic efficiency and to develop a flow sheet compatible with industrial-scale massive H_2 production.
- Researchers evaluated the feasibility of some specific components, mainly the high-temperature heat exchanger with the SO_3 decomposer and the design of a test loop for mock-ups.

The U.S. research team advanced the science of coupling a future large-scale hydrogen production facility to a high-temperature heat source (such as a Generation IV nuclear reactor), including work focused on:

- Materials
- Heat Exchanger Designs
- System Designs
- Safety

Researchers tested materials to determine their suitability to withstand the very high temperatures and aggressive environments of the coupling process. Testing included the tensile properties of Hastelloy C-22, C-276, Incoloy 800H, Waspaloy, Zr-705, and Inconel 617 at temperatures up to 600°C. The best performers were Inconel 617, Waspaloy, followed by 800H. Future measurements will be extended to 1,000°C. Researchers also studied high-temperature deformation of these materials, concluding that ductile failure modes were indicated at elevated temperatures. Optical microscopy revealed conventional solution-annealed microstructures. Ceramic and C/SiC materials were also tested to identify and test candidate fabrication methods for forming flow channels in plates and for laminating and infiltrating multiple plates. Thermal stress was analyzed at full heat exchanger scale. The high temperature heat exchanger plates need to be redesigned based on the stress analysis results.

The leading choice of liquid salt being considered for use as a heat transfer fluid for the system interface is FLiNaK (46.5 percent LiF, 11.5 percent NaF, 42 wt percent KF, 454°C). Researchers performed an initial study of FLiNaK to examine corrosion control mechanisms and methods for controlling HF formation upon H_2SO_4 in-leakage. A Molten Salt Working Group was also commissioned to bring together experts in liquid salt technology.

Compact heat exchanger designs were investigated including: thermal/mechanical stress modeling performed using ANSYS 9.0; fluid flow using FLUENT and MATLAB; parametric studies of strip fin thickness, gap length, channel dimensions, fin length, pitch, sizing, grid independence; and development of parallel processing capability. Intermediate heat exchanger research includes ceramic and composite material heat exchanger designs for helium/molten salt interactions and optimization of an offset strip fin design for compact ceramic composite HX.

Thermal-hydraulic modeling of system interface included: examination of relative efficiency differences between basic configurations; comparison of 2 MPa He, 7 MPa He, and liquid salt (FLiNaK, $NaBF_4$-NaF); and the evaluation of metallic material constraints. Some conclusions of this work indicated that an interface pressure of 7 MPa would exceed metal creep constraints in the interface/process heat exchanger using a simple HX design. Researchers also found that liquid salt would result in a 6 percent boost in efficiency over 7 MPa He with a 30 percent smaller system volume. Researchers studied aspects of the systems interface in more detail, including parallel versus concentric pipe arrangement, pipe diameters and temperature losses versus distance, and stress & creep rupture limits of printed circuit heat exchangers.

They also performed an initial study of the minimum separation distance required between the nuclear plant and the hydrogen facility, using a Probabilistic Risk Assessment approach. The analysis resulted in a minimum spacing of 110 meters. This may be reduced to as low as 60 meters with protective barriers and other technologies.

Planned Activities

This I-NERI project will continue R&D of hydrogen production technologies coupled with advanced nuclear energy systems. Planned work will support materials corrosion studies, studies of liquid salts and liquid salt redox control to reduce materials corrosion problems, and the design of laboratory-scale heat transfer loops for testing heat exchangers and other components. Future scope includes:

- Performing materials corrosion studies under static conditions to support system interface development and design of the sulfuric acid systems in the S-I hydrogen production process.
- Designing a sulfuric acid flow loop that would be capable of exposing test samples to liquid and vapor sulfuric acid with contaminants and under pressure for hundreds of hours and preparing the necessary safety analyses, parts lists, etc., to a sufficient level of detail to authorize construction and use.
- Studying liquid salt redox control methods for reducing materials corrosion problems. Investigators will synthesize or purchase FLiNaK and $NaBF_4$-NaF; characterize impurities in the salt; employ the salt purification techniques of hydrofluorination, filtration,

and electroplating; assess their effectiveness and utility at a larger scale; and construct test equipment for assessing materials corrosion, metals dissolution, and redox control for future experiments.

- Exploring different cladding techniques and clad material/base metal options with the goal of defining suitable combinations that can be used to fabricate HIx decomposition section components, such as boilers and heat exchangers. In addition, samples and prototypes will be made using the chosen fabrication routes and they will be tested for corrosion resistance and mechanical stability.
- Continuing to develop and improve steady-state models of the system interface and related components to support future safety analyses and estimates of process efficiencies.

OSMOSE - An Experimental Program for Improving Neutronic Predictions of Advanced Nuclear Fuels

Principal Investigator (U.S.): R. Klann, Argonne National Laboratory (ANL)

Principal Investigator (France): J. Hudelot, Commisariat à l'Energie Atomique (CEA) Cadarache

Collaborators: CEA-Valrho

Project Number: 2004-002-F

Project Start Date: October 2004

Project End Date: September 2007

Research Objectives

The goal of the OSMOSE program (Oscillation in Minerve of Isotopes in "Eupraxic" Spectra) is to create a database of the measured reactivity effect of minor actinides in known neutron spectra of interest to the Generation IV reactor program and other programs for use as an international benchmark. This project will measure very accurate integral reaction rates in representative spectra for the actinides that are important to future nuclear system designs. The work will provide experimental data needed for improving the basic nuclear data files. The OSMOSE program is generic; that is, it will measure reaction rates over a broad range of isotopes and spectra corresponding to specific experimental lattices in the MINERVE reactor (thermal, epithermal, moderated/fast, and fast spectra). The MINERVE experimental reactor is located at the CEA-Cadarache research facility. OSMOSE will provide precise experimental data (integral absorption cross-sections) for a majority of the heavy nuclides important to reactor and nuclear fuel cycle physics: ^{232}Th, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{243}Am, ^{244}Cm, and ^{245}Cm.

By producing very accurate measurements for the minor actinides in various spectra — from over-moderated thermal spectra to fast spectra — researchers can use this experimental data, in coordination with international nuclear data, to establish deficiencies in the basic nuclear data libraries, identify their origins, and propose paths towards correcting them.

Research Progress

Technical progress on the OSMOSE project was made in reactor modeling, sample fabrication, and experimental measurements during FY 2005.

Reactor Modeling. Monte Carlo and deterministic models of the MINERVE facility in the R1-UO2 and R1-MOX configurations were developed to assess core and safety parameters. The deterministic model was also used to calculate the reactivity worth of oscillation samples in the central channel of the core. The models are based on the composition and geometry specifications listed in the Material Specification Report for the MINERVE reactor.

The Monte Carlo calculation schemes were used for the determination of the following safety parameters: reactivity worth of the control rods, importance in fissions of the experimental zone versus the driver zone, reactivity excess of the core, and effective fraction of delayed neutrons (β_{eff}).

In addition to the safety authorization basis, the calculational scheme has been used to predict the reactivity effect of the OSMOSE samples in the R1-UO2 configuration. An initial series of calculations of the reactivity-worth of the OSMOSE samples in the MINERVE reactor with the R1-UO2 core configuration were completed using a deterministic model. The deterministic model is based on the REBUS code system. REBUS has been used to solve the diffusion equation in XYZ geometry with the finite difference method. The self-shielded cross sections used in REBUS are provided by the one-dimensional-transport-code-system WIMS-ANL 5.07. The calculations indicate a range of reactivity effect from -22 pcm to +25 pcm compared to the natural U sample. Deterministic models were used to calculate the reactivity worth of the oscillation samples because the estimates could not have been determined with enough accuracy by using Monte Carlo calculations (up to about 30 pcm only).

The safety report for the OSMOSE program in the R1-UO2 and R1-MOX core configurations was presented to the French safety authorities on April 28, 2005. Safety authorization for the start of the OSMOSE program was granted on June 21, 2005.

Sample Fabrication. The preparation of the OSMOSE samples is a multi-stage process which includes purification of the isotope feedstock materials, creation of an oxide material, mixing and fabrication of sintered oxide fuel pellets, assembly of the fuel pellets into the sample, and welding of the clad for double-encapsulation.

All of the isotopes have been purified except the ^{233}U sample. Because of the high activity due to the presence of ^{232}U decay products, the operation must be performed in a shielded hot cell and is scheduled at the end of 2006.

Sample	Target composition (g)	Mean Density (% of T.D.)	Mean Diameter (mm)	Variance in Diameter (mm)
UO_2		96.1	8.16	0.08
UO_2-^{232}Th	2.0	93.0	8.15	0.09
UO_2-^{234}U	0.3	95.6	8.13	0.08
UO_2-^{237}Np	0.1	95.6	8.15	0.08
UO_2-^{237}Np	0.6	95.1	8.12	0.08
UO_2-^{239}Pu	0.6	93.1	8.15	0.06
UO_2-^{242}Pu	0.5	93.7	8.01	0.20
URE	Pure	96.7	8.10	0.10
Specification		**>95%**	**8.0< Ø <8.2**	**D Ø < 0.1**

Table 1. Metrology of the first set of OSMOSE samples.

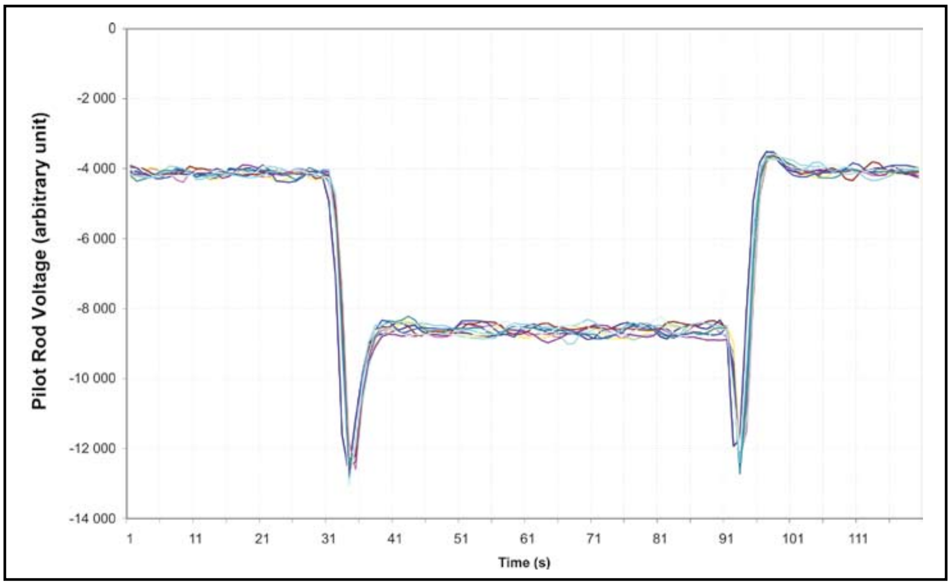

Figure 1. Signal of the Pu-239 OSMOSE sample during its oscillation in MINERVE R1-UO2 Configuration. (The change in the pilot rod voltage is measured as the difference between the two plateaus for a given sample. The voltage change is then related to a calibration curve to determine the reactivity effect due to the sample.)

The oven developed for OSMOSE sample fabrication has achieved 80 thermal cycles without major problems (i.e., 2,000 hours in working condition with 300 hours at high temperature). To prepare for fabrication of the samples in the shielded hot cell, researchers have produced a more efficient tool for the pressing step. The uniaxial press has been replaced by a new gear based on a tri-part (shell) design. With this new system, it is expected that very few out-of-specification pellets will be produced.

During FY 2005, the researchers manufactured eight complete samples including UO_2, UO_2 + $^{232}ThO_2$, UO_2 + $^{234}UO_2$, UO_2 + $^{237}NpO_2$ (1), UO_2 + $^{237}NpO_2$ (2), UO_2 + $^{239}PuO_2$, UO_2 + $^{242}PuO_2$, and $UreO_2$. URE is a sample containing ^{236}U that has been processed from spent nuclear fuel. Table 1 summarizes the characteristics of the first eight samples. With a few minor exceptions, the specifications were obtained for the density and the dimension of the pellet. Six of the samples were delivered to CEA-Cadarache in July 2005 and accepted. The two remaining samples (Np) were delivered in September 2005.

The isotopic and chemical analysis of the actinide stocks has been carried out for the remaining actinides. At the present time, only ^{243}Am, ^{233}U, and curium are still waiting to be analyzed by mass spectrometry techniques (IDMS). The ^{241}Am level (<500 ppm) has also been checked by alpha spectroscopy in all of the samples. The analysis of pellets from the first eight samples began in FY05.

Experimental Measurements. Oscillation measurements of the U-235 and borated calibration samples were conducted in July and August 2005.

Additional borated calibration samples are being fabricated and will be oscillated in October 2005.

The oscillation of the first series of the OSMOSE samples began on September 1, 2005. Each of the eight samples was oscillated 5 or 6 times inside the R1-UO2 configuration during September 2005. A measurement consists of 10 cycles with a cycle length of 120 seconds. Figure 1 shows an example of the signal obtained by oscillating the Pu-239 sample.

Planned Activities

The oscillation of the first eight OSMOSE samples in the R1-UO2 configuration will be completed in November 2005.

The next six samples–^{240}Pu, ^{238}Pu, ^{241}Am (x2), ^{241}Pu and ^{232}Th–will be fabricated in CEA-Valrho and shipped to CEA-Cadarache in February 2006. Pellet samples will also be shipped from CEA-Valrho to ANL for chemical analysis in February 2006. Chemical analysis should be completed by September 2006. The oscillation of these OSMOSE samples in the R1-UO2 configuration will begin in February 2006 and be completed by April 2006.

The core will be reloaded with the R1-MOX configuration and measurements using the first two sets of OSMOSE samples. The remaining samples will be performed from July 2006 through March 2007. Oscillation of the last five OSMOSE samples (^{243}Am (x2), ^{244}Cm, $^{244+245}$Cm, and ^{233}U) in the R1-UO2 configuration is scheduled from March 2007 through June 2007.

The OSMOSE samples will be oscillated in the R2-UO2 configuration from July 2007 to October 2007 and in the MORGANE-R configuration from February 2008 to July 2008.

Several activities related to reactor modeling are planned for FY06. Pre-analysis estimates of the reactivity effect of the OSMOSE samples in the R1-MOX core configuration will be performed. Additionally, the results of the OSMOSE samples in the R1-UO2 configuration will be studied and re-analyzed if the results of the chemical analysis become available in FY06.

Studies will be performed of the OSMOSE samples in the planned core configurations to determine the relevance of these configurations for the Generation IV program. Specifically, the configurations will be compared to block-type very high temperature and gas-cooled reactor systems.

Researchers will also evaluate the OSMOSE samples for use in Doppler-broadening measurements in MINERVE. Results of these efforts will lead to discussions between ANL and CEA on the future direction of the OSMOSE program and other potential related collaborative efforts.

International Nuclear Energy Research Initiative

Thermal-Hydraulic Analyses and Experiments for GCR Safety

PI (U.S.): Richard R. Schultz, Idaho National Laboratory (INL)

PI (France): Denis Tenchine, Commissariat à l'Energie Atomique (CEA)

Collaborators : Argonne National Lab (ANL), Utah State University (USU)

Project Number: 2004-003-F

Project Start Date: January 2005

Project End Date: January 2008

Research Objectives

The objective of this experimental and computational research project is to provide benchmark data for validating and improving thermal-fluid dynamics codes proposed for evaluating decay heat removal in gas-cooled reactor (GCR) designs. Researchers will consider several reactor designs under the international Generation IV Initiative, including the very high temperature reactor (VHTR) and the gas-cooled fast-reactor (GFR). These reactors feature complex geometries and wide ranges of temperatures, leading to significant variations of the gas thermodynamics and transport properties plus effects of buoyancy during loss-of-flow and loss-of-coolant scenarios and during reduced power operations.

Research Progress

This research effort is divided broadly into two areas: 1) benchmark analyses and validations and 2) benchmark experiments for complex GCR geometries. Following is a summary of the work performed under each to date.

Benchmark Analyses and Validations. Computational fluid dynamics (CFD) validation. Based on the identification of components, transients, limiting criteria, and phenomena for thermal-spectrum GCRs, the researchers have developed phenomena identification and ranking tables (PIRT) for the thermal fluid dynamics of prismatic and pebble-bed reactors. Because multi-dimensional CFD analyses may be needed in addition to conventional one-dimensional systems codes, the researchers reviewed the PIRTs to rank the importance of multi-dimensionality in the GCR applications.

CFD predictions for NSTF RCCS. Researchers conducted CFD analyses of a reactor cavity cooling system (RCCS) design for a GCR application and of its possible simulation with ANL's Natural Convection Shutdown Heat Removal Test Facility (NSTF). The purpose was to examine whether key fluid flow and heat transfer phenomena can be adequately simulated. Results indicate that NSTF simulations can cover all important phenomena and their expected ranges of variation.

GCR core modeling. Researchers have started developing a multi-scale, multi-resolution model for computing GCR core flows. It consists of a porous modeling of subassemblies coupled to an open modeling of the by-pass region between the subassemblies. Using this model, researchers will be able to model prismatic blocks, pin, or plate subassemblies and to couple the core model with the inlet and outlet plena.

Extension of TBLE to dilatable fluids. The researchers launched the development of specific wall functions called TBLE (turbulent boundary layer equations) to deal with dilatable fluids involved in GCRs. This special modeling technique was developed with the TRIO_U code to find the best compromise between physical modeling and CPU time.

CFD modeling of the HTR-10 benchmark. They have also performed CAST3M/ARCTURUS calculations of the Chinese HTR-10 reactor, under the framework of an IAEA benchmark. The reactor vessel is modeled as axisymmetric, using about 20,000 nodes and taking into account convection, conduction, and radiation. Some discrepancies remain between the calculated and the measured values, probably due to uncertainties in the reactor boundary conditions and measurements.

CFD predictions of complex geometries. Researchers are evaluating both the Reynolds-averaged Navier-Stokes (RANS) and the large eddy simulation (LES) techniques for a series of fundamental geometries.

Benchmark Experiments for Complex GCR Geometries.

Matched-Index-of-Refraction experiments. The research team is conducting particle image velocimetry (PIV) and laser Doppler velocimetry (LDV) measurements of flow phenomena expected in the lower plenum of a prismatic VHTR using INL's unique matched-index-of-refraction (MIR) flow system. Researchers will obtain measurements that are representative of the region away from a plenum outlet (where there is no significant cross flow) and the region near the outlet (where crossflow velocities are expected to be greater than the jet velocities). The experimental model has been fabricated, installed, tested, and operated with jet flow from two of the inlets in the configuration representative of the region away from a plenum outlet. They have completed initiation of measurements, both with flow visualization and the INL 3D-PIV system. The team will continue to obtain further measurements and will develop model modifications to better represent the region near the plenum outlet.

Supporting PIV measurements. Two-dimensional PIV measurements have been completed to determine the minimum Reynolds number required for crossflows to be in the mixed flow regime for the INL lower plenum model and to provide benchmark data for assessing CFD codes. Measurements are available for mean velocities, turbulent fluctuations, and Reynolds shear stresses in the plane of observation and for details of the boundary layer profiles around the circumference of support posts.

Planned Activities

Researchers will perform scaling analyses to demonstrate that the NSTF facility can be used for simulating a passive water-cooled RCCS system. More specifically, they will demonstrate that NSTF is capable of simulating all significant phenomena in a water-cooled RCCS and that these simulations can cover the whole range of variation in the parameters describing these phenomena.

Researchers will also initiate the following additional activities:

- A number of experiments will be performed in the MIR to examine the flow behavior in a typical lower plenum of a prismatic gas-cooled reactor system.
- The first TRIO_U computation will be performed. It will address the thermal fluid behavior in the pin-type core of a GFR demonstration reactor.
- The TBLE will be tested on analytical configurations and assessed with existing data.
- New HTR-10 calculations will be performed with new benchmark specifications.
- Studies for strongly heated circular tubes, annuli, and rod bundles are underway and will be extended to jets in crossflows through cylinder arrays (e.g., VHTR lower plenum).

SiC/SiC for Control Rod Structures for NGNP

PI (U.S.): William Windes, Idaho National Laboratory

PI (France): Jacques Lamon, University of Bordeaux, France

Collaborators: Pacific Northwest National Laboratory, Oak Ridge National Laboratory

Project Number: 2004-004-F

Project Start Date: January 2005

Project End Date: October 2007

Research Objectives

This research project will investigate issues surrounding the development of tubular geometry SiC/SiC composite material for control rod and guide tube applications in a Very High Temperature Reactor (VHTR) design. Fiber-reinforced ceramic composites are being considered for possible use as control rod cladding and guide tubes in the VHTR. Ceramic composites are considered the only viable choice for these primary safety components which need to be capable of withstanding the extremely high temperatures and dose levels inside the core. Researchers will study the mechanical, thermal, and radiation-damage response of both the U.S. and French fabricated composites.

This project will take full advantage of the innovative SiC/SiC technologies developed by the French collaborators whose research group has pioneered the use of 2D woven SiC/SiC composites and also nanoscale-multilayered pyrolytic carbon/silicon carbide interphases. The French emphasis on basic science and improved composite design will complement the U.S. program which focuses more on application-oriented testing and verification of these composites for use in the VHTR. This project will facilitate thermo-mechanical testing of improved composite designs in a full-scale test sample. Researchers have established a common working goal of validating these ceramic composites for use in a reactor environment. They will validate "preliminary" composite structures for use and develop more advanced designs that could yield dramatic improvements over the current structure.

Research Progress

Researchers have fabricated tubular test samples for ASTM-approved mechanical testing (Figure 1). These so-called "ASTM round-robin" tests will be used to develop testing standards required to validate the composites for use within a nuclear environment. Initial mechanical testing will involve only low-temperature tensile tests where the strength of the composite is determined. Later tests will be conducted at high (900ºC) and very high (1,100ºC) temperatures to determine the effects of temperature on composite strength.

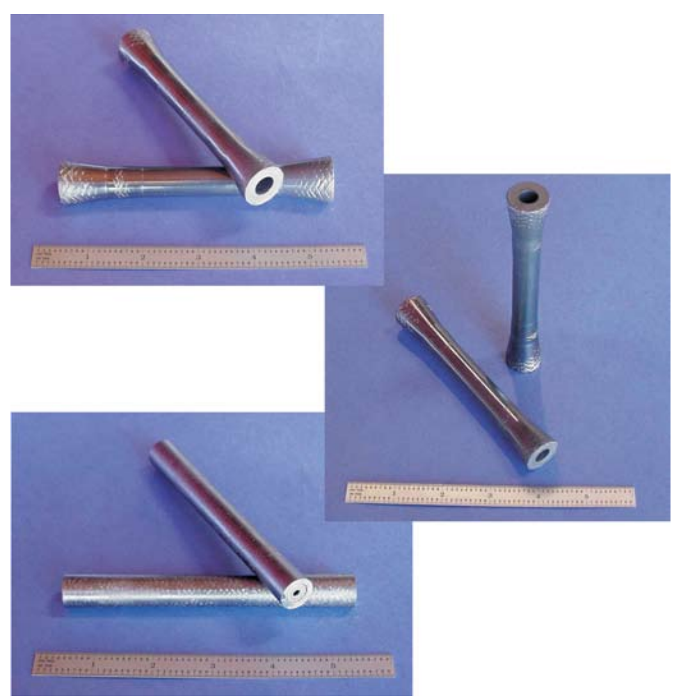

Figure 1. Tubular test samples fabricated for ASTM test standard.

In addition, the French collaborators will fabricate additional tubular test samples using similar fibers and fiber architecture to maximize compatibility with the current testing program. Since these composite structures are expensive, this will provide a valuable addition to the current matrix of composite tests.

Planned Activities

U.S. researchers will conduct an irradiation program for the French advanced composite designs. Since the control rods will receive the largest radiation dose of any component within the VHTR reactor core, it is necessary to determine the irradiation performance of these newer designs before thermo-mechanical testing can be conducted. Small "mini-composite" samples (single fibers embedded within a solid SiC matrix) will be subjected to high irradiation levels. Researchers will then examine the mini-composites to determine the structural stability of each sample type.

French composite designs that demonstrate superior irradiation stability will be added to the U.S. irradiation creep program where the composites will be tested under realistic conditions (i.e., under load, temperature, and irradiation). Small tensile bar composite samples will be tested and examined for structural stability after irradiation. Samples from the current composite design along with samples from at least one "advanced" composite design from the French are anticipated for these studies.

In addition, data exchanges, sharing modeling experience/results, and additional test sample exchanges between the two programs are anticipated. Further meetings in the coming months will provide detailed schedules and individual research plans for specific testing and sample fabrication.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Assessment of Existing Physics Experiments Relevant to VHTR Designs

PI (U.S.): Temitope A. Taiwo, Argonne National Laboratory

PI (France): Robert Jacqmin, Commissariat à l'Energie Atomique (CEA)

Collaborators: Idaho National Laboratory

Project Number: 2004-005-F

Project Start Date: October 2003

Project End Date: September 2006

Research Objectives

This project will identify and assess experimental data and benchmark tests applicable to the qualification of Generation IV system design and analysis physics tools. The research team will interface with U.S. and international groups to identify and assess existing data that could be used for the qualification and quality assurance of computer codes and databases for reactor physics analysis of the Very High Temperature Reactor (VHTR). This activity is expected to support subsequent efforts to document the benchmark specifications and measured results in a standard format for use in VHTR software quality assurance efforts. In this work, researchers will:

- Evaluate the adequacy of existing critical experiments and nuclear data
- Define target accuracies for pertinent core parameters
- Conduct sensitivity studies for assessing relevance of experiments to VHTR
- Identify additional integral experiments and/or nuclear data evaluation and measurements that are required
- Perform joint detailed analysis of selected physics experiments

Research Progress

Researchers have completed an assessment of experimental tests and measurements, performed since the early 1960's, that could be used to validate and verify reactor physics codes and data to be used for VHTR/NGNP analysis. This is documented in a report entitled "Preliminary Assessment of Existing Experimental Data for Validation of Reactor Physics Codes and Data for NGNP Design and Analysis." Based on this assessment, researchers determined that several specific sets of measurements should receive the highest priority for compilation as peer-reviewed benchmark specifications. For pebble-bed type cores, this includes measurements conducted at the following four facilities: HTR-PROTEUS, HTR-10, ASTRA, and AVR. For design and analysis of block-type next generation nuclear plant (NGNP) cores, the HTTR and VHTRC measurements were rated highly as benchmarks, based on the relevance and availability of measured data. An additional assessment resulted in the inclusion of the compact nuclear power source (CNPS)

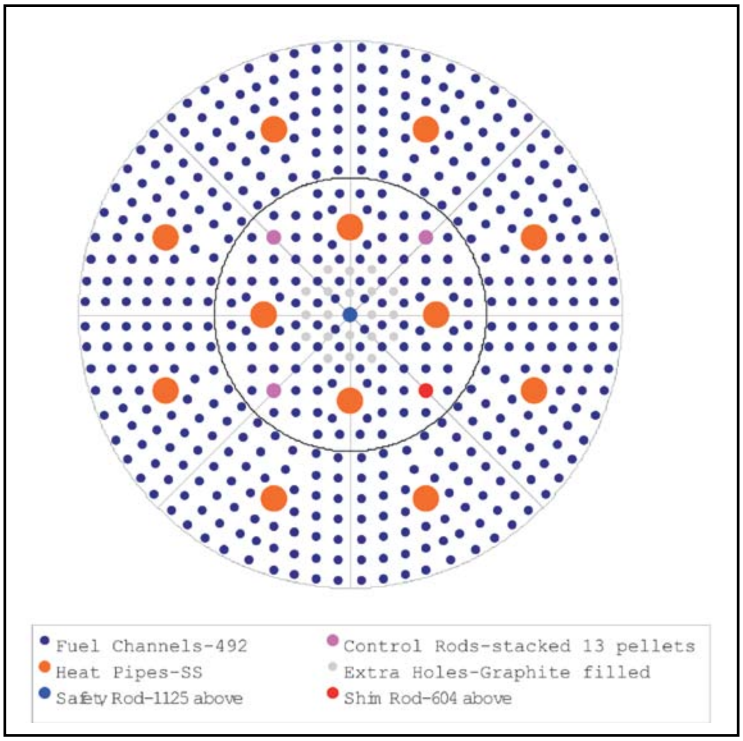

Figure 1. CNPS full critical core loading configuration.

experiment tests, performed in the late 1980's, in the high priority list. Figure 1 shows the CNPS core loading configuration.

CEA researchers independently assessed existing data to which they have access. Their search for experiments was limited to thorium-free, low-enrichment systems, in general. Based on the review, they identified seven experiments as potentially worthy of re-evaluation with modern codes and nuclear data. These are PROTEUS, ASTRA, MARIUS, VHTRC, UHTREX, HITREX-2, and CNPS. CEA analysts plan to further assess these experiments to determine if sufficient information is available (configurations, measurements, and uncertainties, etc.) to warrant a detailed analysis. Their initial efforts are focused on the PROTEUS, MARIUS, and ASTRA experiments, with the evaluations of PROTEUS and MARIUS to be pursued more vigorously in early 2006. From these first reviews, the researchers have concluded that there are a very limited number of relevant physics experiments worth analyzing in detail. In addition, they determined that important descriptive data are lacking on these few relevant experiments, with limited prospects of obtaining the missing information.

Researchers have also completed an evaluation of the potential impact of nuclear data uncertainties on a number of performance parameters (core and fuel cycle) for the prismatic block-type Very High Temperature Reactor (VHTR). Results of this evaluation are documented in a report entitled "Uncertainty and Target Accuracy Studies for the Very High Temperature Reactor (VHTR) Physics Parameters." They performed an uncertainty analysis based on sensitivity theory to identify the nuclides, cross-section types, and energy ranges responsible for the most significant uncertainties. In order to provide guidelines on priorities for new evaluations or validation experiments, researchers first derived required accuracies on specific nuclear data, accounting for target accuracies of major design parameters. Results from this extensive analysis indicate that only a limited number of relevant parameters do not meet the assumed target accuracies, implying that the existing nuclear cross-section data can be used for the feasibility and pre-conceptual assessments of the VHTR. However, as the results obtained depend on the quality of uncertainty data used, the researchers suggest focusing some future evaluation work on producing consistent, complete, and user-oriented covariance data.

In order to propose a credible program for new cross-section measurements, a study must show the impact of the existing cross section uncertainties on the relevant parameters, taking into account the target accuracies on the design parameters. For this purpose, the researchers have considered design target accuracies which could be relevant in successive design phases and have evaluated nuclear data improvement requirements. The resulting requirements indicated that a careful analysis is needed in order to define the most appropriate and effective strategy for reducing data uncertainty.

The research team has also performed a preliminary assessment of the relevance of the HTTR and CNPS experimental tests to a prismatic block-type VHTR, by comparing the values of core parameters for the systems to that of a representative reactor. This study found similarities between the HTTR or CPNS core and the VHTR core (e.g., the shape of the neutron spectrum). Some differences were observed, however, for the energy locations of the thermal neutron spectrum peak (due to different operating temperatures) and the resulting magnitude of the double heterogeneity effect.

The researchers further evaluated and analyzed results of three experimental tests (HTTR, HTR-10, and CNPS) to create standard benchmark problems that can be used to validate computer codes and nuclear data. Their findings are compiled in a report entitled "Evaluation of High Temperature Gas-Cooled Reactor Physics Experiments as VHTR Benchmark Problems." They also conducted a technical evaluation of the CNPS and HTTR measurements, including sensitivity studies, to understand discrepancies in data and the impact of modeling assumptions on the results. Due to insufficient data, particularly regarding the uncertainties associated with the design data, these efforts did not progress to the stage of defining standard benchmarks that follow the structure recently defined by the International Reactor Physics Experiments Preservation (IRPhEP) sub-group of the Nuclear Energy Agency (NEA), a specialized agency within the Organization for Economic Cooperation and Development (OECD). However, these models could be used for specifying numerical benchmarks based on the experiments. Researchers evaluated the available HTR-10 data and concentrated on developing a standard benchmark for the initial critical core.

After their preliminary evaluation, the research team has concluded that new, reliable, high-quality experimental data will be needed for validation purposes, unless core designers are willing to accept very large uncertainties that might exceed the requirements of the licensing authorities. The team is evaluating the feasibility of new experiments. If such an experimental physics program is feasible in one of the CEA facilities, it would be open to international participation.

The project participants have been engaged in international activities (those of the OECD/NEA groups and working parties and the Generation IV International Forum) dedicated to improving the analytical tools (code and data) for analyzing advanced reactor systems, with a focus on the VHTR. The OECD/NEA activities have centered on those of the NEA/NSC Working Party on Scientific Issues of Reactor Systems (WPRS), which have included definitions of benchmark problems, evaluations of the benchmark specifications, and analysis of benchmark problems for high-temperature gas-cooled thermal reactors.

Planned Activities

Obtaining all the pertinent data from foreign organizations is a potential problem for this I-NERI project because of the proprietary nature of the data. Bilateral or multi-lateral agreements to share this information will likely be needed, and will be pursued.

Based on current findings, the need for new integral measurements cannot be ruled out. Researchers will pursue cost-effective approaches for creating high-quality measurements in collaboration with other local and international organizations.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

GFR Physics Experiments in the CEA-Cadarache MASURCA Facility

PI (U.S): Temitope A. Taiwo, Argonne National Laboratory

PI (France): Robert Jacqmin, Commissariat à l'Energie Atomique (CEA)

Collaborators : None

Project Number: 2004-006-F

Project Start Date: October 2003

Project End Date: September 2006

Research Objectives

Gas-Cooled Fast Reactor (GFR) designs are being developed to meet Generation IV goals of sustainability, economics, safety, reliability, proliferation resistance, and physical protection. As a supplement to these design studies, CEA-Cadarache is planning experiments that will investigate the core physics issues relevant to Generation IV GFR designs that were not addressed in previous gas-cooled reactor experiments. The objective of that experimental program, designated the **E**xperimental **N**eutron **I**nvestigation on **G**as-reactors at **MA**SURCA (ENIGMA), is to define MASURCA configurations that are similar in their neutronic characteristics to the candidate GFR designs and to extend the validation domain of the neutronics tools to the design and licensing calculations of future GFRs. This I-NERI project builds upon ENIGMA research, with the goals of:

1) improving analytical models for GFRs based on evaluation of experimental results; and
2) establishing broader international participation in the ENIGMA program (including justification, definition, and design of experiments).

Research Progress

Researchers have completed their evaluation of the results of calculations that were conducted in FY 2004. This evaluation will support the development of core configurations and measurements for the first phase of the ENIGMA project, which will be conducted in the MASURCA facility at the CEA-Cadarache center. A report entitled "Investigation of the Similarity of Reactor Physics Experimental Configurations Planned in the CEA MASURCA Facility to Gas-Cooled Fast Reactor Concepts" discusses the findings of the sensitivity and similarity of these planned experimental configurations to GFR concepts. This evaluation was necessitated by the constraints imposed on the first phase of the experiments: limitations of core size, geometry, and core materials (e.g., unavailability of GFR-specific carbide and nitride fuel types and reflector material and the relatively large sizes of GFRs). The evaluation results showed that the significant material differences and neutronic characteristics between the GFR cores and typical sodium-cooled fast reactor cores justify the planned experimental campaign. The results also provided indications of the similarity of the planned MASURCA experiments to the GFR concepts and the potential contribution of the experiments to reducing uncertainties in core physics integral parameters.

The project team also analyzed past experiments in the ANL ZPR-9 gas-cooled reactor configurations. The results support the need for additional experiments for the advanced GFRs. This is because the existing data, although valuable, consist of just a few experiments and are not sufficient. Additionally, existing experimental data are only partly representative of prospective advanced GFRs, and their dataset lacks descriptive information regarding some measurements.

The researchers have outlined the planned ENIGMA experiments to facilitate the collaborative definition of the GFR physics measurements to be done as part of this project.

Researchers completed a study of possible configurations for the pre-experimental phase of the ENIGMA project. The findings are documented in a joint report entitled "Impact of Spectral Transition Zone in Reference ENIGMA Configuration," which discusses the impact of introducing a transition zone in the central region of the ENIGMA reference configuration on the flux spectrum, core reactivity, and spectral indices. The transition zone could be utilized for studying physics effects that might not be otherwise obtained in the initial phases of the ENIGMA program due to the potential lack of appropriate GFR design materials. The results show that significant variations in the neutron flux could be obtained by the use of transition zones, with small perturbation in the core reactivity state. The use of a graphite transition zone results in a significantly softer spectrum, while the use of the void transition zone produces a significantly harder spectrum compared to the reference case.

Planned Activities

The project team met to discuss the findings of joint studies for the project, along with the project status and future plans. They discussed the development of new measurement techniques and the design and options for future configurations. A first reference core will be loaded in MASURCA in 2006 for pre-experiment tests. This is required to support the safety checks needed for the program approval by the CEA safety authority. Only a limited number of characterization measurements are planned before the facility is shutdown later that year for a major upgrade. The first phase of the ENIGMA program will start after the upgrading work is completed, in early 2009.

Current manpower available for the ENIGMA tasks in the U.S. and in France is largely insufficient. Consequently, additional participants for the experiments are being sought. CEA has received expressions of interest from various organizations interested in joining the ENIGMA program (ANL, INL, PSI, JNC, Chalmers University, and BNFL). A technical seminar is planned in early 2006 in order to identify potential contributions by these groups.

Much more work is needed to define the experimental program in full detail, with inputs from measurement experts on either side. It is particularly important to establish what new materials and equipment will be necessary for subsequent phases of the ENIGMA program. CEA and ANL agreed that the coming two years should be used to strengthen the motivations for the program and prepare the various experimental phases in detail. The assessment of target accuracies on the basis of the CEA preliminary GFR concepts will be an important part of this work.

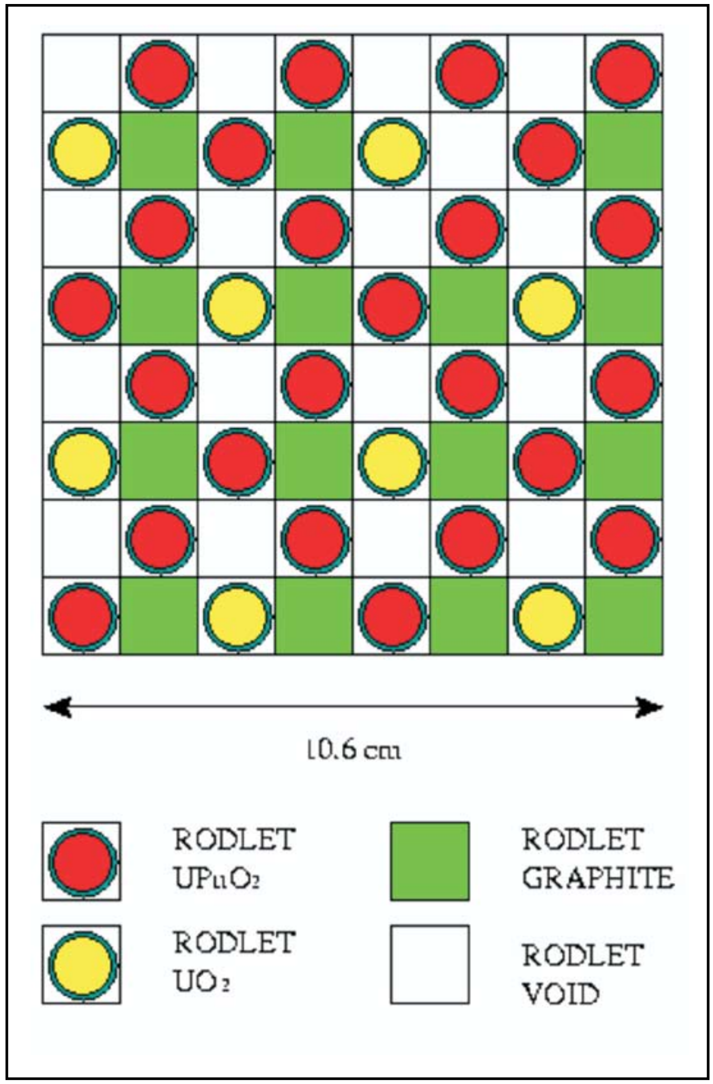

Figure 1. ENIGMA reference fuel assembly.

Preliminary studies at CEA show that, for the purpose of specific experiments, materials or equipment used in past U.S. fast critical reactor programs (e.g., ZPR-3, ZPR-6, ZPR-9, and ZPPR facilities) and stored at INL could be valuable to the ENIGMA program. This includes such materials as graphite moderators, refractory metals, zirconium platelets, and devices such as high-purity foils and back-to-back detector holders. ANL provided informal information on the inventory of some of these materials and the project team expressed interest in receiving additional information. It was noted that such information and material exchanges would necessarily include the U.S. DOE and INL, in addition to ANL. Additional discussion on this item is planned.

Innovative techniques are being considered to better characterize ENIGMA core parameters.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Evaluation of Materials for Gas-Cooled Fast Reactors

PI (U.S.): Thomas Y.C. Wei, Argonne National Laboratory (ANL)

PI (France): Jean-Louis Seran, Commissariat à l'Energie Atomique (CEA)

Collaborators: University of Wisconsin, University of Michigan, Pacific Northwest National Laboratory (PNNL)

Project Number: 2004-007-F

Project Start Date: August 2004

Project End Date: August 2007

Research Objectives

Both France and the United States have a shared interest in developing advanced reactor systems that employ inert gas as a coolant. Currently, there is an insufficient amount of physical property data to qualify candidate materials for gas-cooled fast reactor (GFR) designs. The goal of this project is to establish candidate metallic and ceramic materials for GFR designs and to evaluate their mechanical properties, dimensional stability, and corrosion resistance.

The first goal of this project is to improve high-temperature creep strength and resistance to environmental attack by optimizing grain boundary structural orientations, known as grain boundary engineering (GBE). Thermal-mechanical treatment is performed on GFR candidate alloys to maximize the fraction of low-energy boundaries. Following treatment, the changes to microstructure are characterized. Researchers will focus on Alloy 800H, which is an austenitic alloy designed for high-temperature boiler components, and on T-91, which is a low-carbon (9Cr-MoVNb) ferritic-martensitic alloy designed for lower temperature boiler components.

The second goal of this project is to characterize the radiation resistance of candidate GFR metallic materials. Metallic materials have not typically been used for high dose core components in GFR applications. Therefore, radiation response of these alloys will be characterized by examining the changes in the microstructure of samples that are irradiated with high-energy ions and when available, neutrons from a test reactor. The focus is on Alloy 800H.

Research Progress

Researchers performed grain boundary engineering, which involved developing a series of thermo-mechanical treatments designed to convert a fraction of the high-energy boundaries to low-energy boundaries (identified as Coincident Site Lattice [CSL] boundaries) to reduce cracking susceptibility and to improve creep strength. This project developed the first treatment to enhance the fraction of CSL boundaries in an advanced, ferritic-martensitic steel—T91. The challenge was to enhance the grain boundaries without disturbing the original microstructure.

Since the microstructure is critical to achieving high-temperature properties, the heat treatment process requires strict control. Researchers developed a treatment in which the CSL boundary fraction of T91 was enhanced over the as-received case without changing other critical features of the microstructure, such as grain size, carbide size and location, density, and hardness. As shown in Figure 1, improved creep strength results from preserving all the microstructural features decisive for creep strength in T91 and from increasing the fraction of low-angle boundaries. In addition to T91, the researchers also developed CSL-enhancement techniques for Alloy 800H, a higher temperature alloy seen as a candidate for high-temperature, gas-cooled reactors. Figure 2 shows the grain boundary distribution for the optimized heat treatment, consisting of a 6 percent thickness reduction via mechanical rolling followed by an anneal at 1,050°C for 90 minutes. Creep testing of GBE-treated samples is ongoing, as are radiation tests of mini-tensile samples.

To understand the radiation stability of 800H, researchers conducted nickel-ion irradiations using 5 MeV Ni ions at 500°C to 50 dpa (displacements per atom). They carried out microstructural characterization for unirradiated and irradiated samples using a transmission electron microscope. The high dose irradiated microstructure is dominated by faulted loops and small precipitates uniformly distributed throughout the sample. No cavities were detected at high dose. The uniformly distributed small precipitates are expected to play an important role in material mechanical properties.

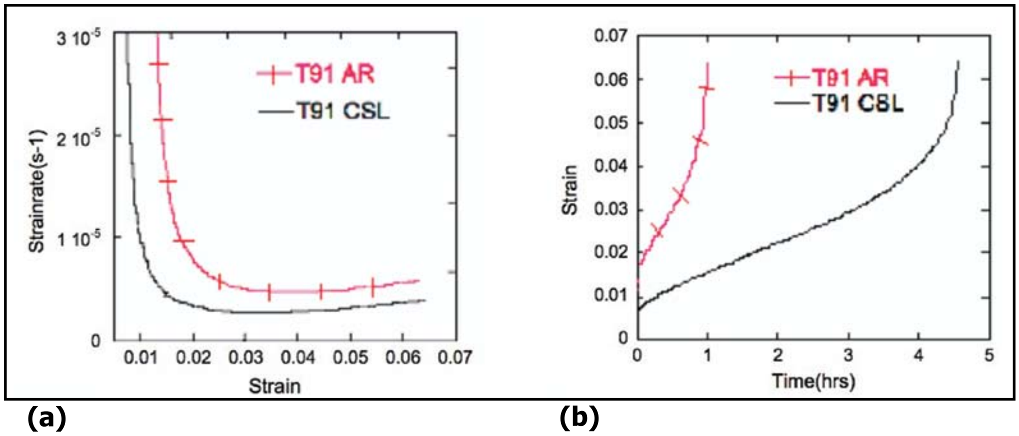

Figure 1. Plots of (a) strain rate vs. strain and (b) strain vs. time for creep tests of alloy T91 at 220 MPa (600°C, argon). AR = as-received, CSL = enhanced grain boundaries.

Planned Activities

Future work will examine the stability as a function of time at temperature of grain boundary treatments, the effect of GBE on creep in 800H, and the ability of applying GBE to other advanced steels.

Irradiation damage studies are complete under this I-NERI project, but samples of 800H being irradiated in the Advanced Test Reactor will be available for analysis at a future date.

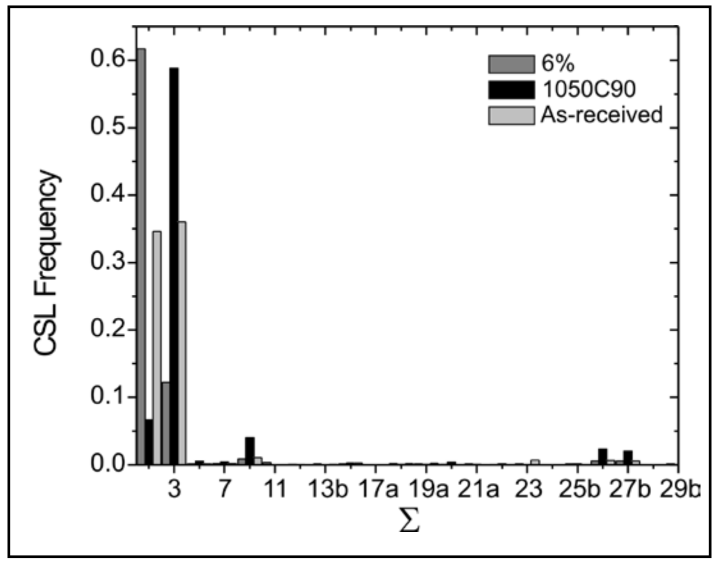

Figure 2. CSL frequency as a function of Σ1 and "special" boundaries (Σ3-Σ29b) of 6 percent, 1050C90, and as-received samples.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Development of Generation IV Advanced Gas-Cooled Reactors with Hardened/Fast Neutron Spectrum

PI (U.S.): T.Y.C. Wei, Argonne National Laboratory (ANL)

P.I. (France): J. Rouault, Commissariat à l'Energie Atomique (CEA) Cadarache

Collaborators: Brookhaven National Laboratory, General Atomics, Massachusetts Institute of Technology, Idaho National Laboratory

Project Number: 2004-008-F

Project Start Date: March 2005

Project End Date: February 2006

Research Objectives

The objective of this project is to design a Gas Fast Neutron Reactor (GFR) with a high level of safety and full recycling of the actinides, which will also be highly proliferation resistant and economically attractive. This project started as a continuation of I-NERI project 2001-002-F, which was completed February 2005. The original work began with a three-year CEA/ANL collaboration that evaluated possible GFR models for further consideration. It reached the stage when the effort focussed on the characterization of a 2,400 MWt GFR design. In this continuation phase of the project, the objective is to start with the following selected point design parameters and to proceed to a pre-conceptual design:

1) Fuel choice: Dispersed fuel in plate sub-assemblies as the reference, SiC cladded pellets in pin sub-assemblies as a back-up. The selected actinide compound is carbide in the design studies but nitride remains a possible candidate.
2) Unit size: 2,400 MWt
3) Power density: 100 MW/m^3
4) Decay heat removal: Natural convection passive approach, which should be combined with active means (low power circulators) in a well-balanced mix to be refined. This does not exclude alternative options (search for conduction paths, heavy gas injection, etc.).
5) Balance-of-plant: Direct Brayton cycle balance-of-plant option remains the reference design, but consideration of the indirect super-critical CO_2 cycle, and other combined cycle alternatives using gas mixtures with an equivalent cycle efficiency, have also been included.

The work on the design and safety of this plant option will proceed in coordination with the multilateral GIF (Generation IV International Forum) International Collaboration Plan. This is in anticipation of the successful completion of the Project Arrangement for the GFR design and safety effort. The goal is to perform work on the tasks of the International Collaboration Plan with respect to core and system design, safety rules and approach, safety systems, and transient analysis.

Research Progress

Researchers prepared documentation for the study of pin core alternatives for a 100 w/cc core design with vertical pins and a 0.5 bar pressure drop. The power density was defined to be compatible with the core pressure drop for the selected semi-passive safety approach to decay heat accidents. Researchers studied the arrangement of the fuel element in a "practical" sub-assembly design. They selected a "reference" design which accounts for such parameters as the SiC cladding, control rods implementation in the core layout, and fuel handling, and which incorporates a degree of engineering judgment. The work characterized core configurations based on simplified computational models (2D-HexZ neutronics using REBUS-3/DIF3D and 1D-Z thermal-hydraulics).

Structural mechanics factors are included in the design assessment. In particular, thermal bowing establishes a bound on the minimum number of fuel pin spacers required in each fuel subassembly to prevent local flow channel restrictions and pin-to-pin mechanical interaction. There are also fabrication limitations on the maximum length of SiC fuel pin cladding that can be manufactured. This geometric limitation affects the minimum ceramic clad thickness that can be produced and ties into fuel pin heat transfer and temperature thresholds. All these additional design factors were included in the current iteration on the subassembly design to produce a lower core pressure drop.

The plate core effort was concentrated on the 06/04 core characterization (case 3). Calculation of the equilibrium fuel composition, after multiple recycling, shows the minor actinide (MA) content increases up to about 1.2 percent of the heavy nuclides. Researchers determined the decay heat curve, considering various plutonium compositions and MA content ranging from 0 to 5 percent, and compared results against the ANS standard. The cases with 2 percent and 5 percent MA content lead to a higher decay heat value for cooling times of one hour or more. Finally, the case with 2 percent MA content was selected for additional transient analysis. Researchers performed a series of 3D Eranos calculations for the core characterization task, consolidating such core features as reactivity, power peaking factors, reactivity swing, and reactivity feedback. They determined that the core is less reactive by about 3,000 pcm, with the absorber located immediately above the upper axial fissile/reflector boundary. This is explained mainly by the neutron leakage and absorption due to the presence of the control rods.

Researchers also re-evaluated the balance-of-plant. They performed comparative and sensitivity studies of various power conversion cycles in terms of thermo-dynamical efficiency. For a core outlet temperature of 850°C, the direct cycle offers the highest efficiency. Nevertheless, the indirect/combined cycle with a tertiary steam/water loop could be almost equivalent in performance. It was concluded that the choice of the conversion process could be left open for the exploratory phase. A more general feasibility, safety, and economical assessment is to be performed to support a future decision.

The specific case of a lower core outlet temperature (680°C) was also studied, considering indirect supercritical CO_2 as the working fluid in the conversion cycle. For a 2,400 MWt direct cycle reactor, the researchers considered either four separate power conversion systems (PCS), each one similar in size and design to the GT-MHR secondary plant, or a single large PCS. The exploratory design study of such a machine was initiated.

In comparison, an indirect cycle offers the opportunity to simplify the nuclear part of the system. The design option of a compact primary system situated inside a guard vessel, itself limited in size, is potentially attractive for both economy and safety. Therefore, researchers concentrated their efforts on the indirect cycle system arrangement and conducted an exploratory design study of its components, pre-sizing and modeling the gas/gas intermediate heat-exchanger, the primary circulator, reactor vessel, and guard vessel. They have defined a workable design.

Figure 1. Guard containment flow distribution.

An effort was initiated to evaluate the impact of the passive approach to decay heat removal on safety and the design of the guard containment. Researchers identified thermal-hydraulic phenomena which would be assessed through the performance of multi-dimensional computational fluid dynamics (CFD) calculations. They completed the mesh layout for a CFD model utilizing the STAR CD computational fluid dynamics code. The General Atomics design for the 2,400 MWt plant option was selected as the reactor plant/guard containment design for the CFD calculations.

Researchers are focusing on the thermal-hydraulic response of the guard containment atmosphere during a particular class of beyond-design basis accident (BDBA), specifically a station blackout with leakage. In the current analysis, the containment atmosphere is a mixture of nitrogen and helium at a pressure of 6 bar. Results have been obtained for the long-term temperature distribution in the containment fluid (nitrogen-helium mixture). As expected, the hotter region is the area around the vertical side of the reactor vessel, which reaches a maximum temperature of 139°C. Most of the outer cavity has a temperature of about 75°C. The maximum containment wall temperature occurs on the inner surface above the reactor vessel, which reaches a temperature of 77°C. Figure 1 shows that gas flow in the section of the inner cavity above the reactor vessel is complex. Its main feature is two large vortices rotating in opposite directions.

Planned Activities

Researchers plan to complete the following exploratory studies (neutronics, safety, core, and fuel form) during the first year:

- Collaboration Integration
- Core Design
- Reactor Design Study
- Plant System Transient Analysis
- Safety Studies and Plant Transient Analysis
- Guard Containment Safety
- Guard Containment Structure Design
- PRA Aided Design of Advanced Reactors with an Application to GFR Safety-Related Systems
- System Transient Analyses Benchmarking

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Development of Fuels for the Gas-Cooled Fast Reactor

PI (U.S.): M. Meyer, Idaho National Laboratory (INL)

PI (France): N. Chauvin, Commissariat à l'Énergie Atomique (CEA)

Collaborators: Oak Ridge National Laboratory (ORNL), Los Alamos National Laboratory (LANL), Joint Research Center for Transuranium Elements (JRC)

Project Number: 2004-009-F

Project Start Date: October 2004

Project End Date: September 2007

Research Objectives

This project seeks to develop silicon carbide matrix, uranium carbide dispersion fuel in two forms: 1) a hexagonal block with coolant holes throughout and 2) a pin-type dispersion fuel utilizing silicon carbide and uranium carbide as the matrix and fuel phase respectively with an integral silicon carbide cladding suitable for gas-cooled fast reactor (GFR) service. Because fuel operating parameters and physical requirements for the GFR are outside of the current experimental nuclear fuel database, many basic viability issues will need to be addressed experimentally to demonstrate the feasibility of proposed GFR fuels. Two basic fuel types appear viable: refractory matrix dispersions and refractory metal or ceramic-clad pin-type fuels. Researchers will demonstrate the feasibility of these fuels by analyzing fuel requirements, simulating behavior using fuel performance models, fabricating fuel specimens, and characterizing microstructure and properties. They will conduct ion irradiation testing of materials to simulate material behavior at high irradiation doses in short times. The GFR-F1 test in the Advanced Test Reactor (ATR) and the FUTURIX-MI test in the Phénix reactor also address basic issues regarding the irradiation behavior of the "exotic" refractory materials required for GFR fuel service in a neutron-only environment. Ultimately, proof-of-concept for GFR fuel can only be demonstrated through irradiation testing of fissile-bearing specimens. The GFR-F2 fuel irradiation test in the ATR is planned as a fuel behavior test that will give the first true indication of fuel feasibility.

Research Progress

Current U.S. GFR fuel concepts are based on a dispersion of (U, Pu)C coated particles in a silicon carbide (SiC) matrix. The U.S. has two reference fuel forms, large hexagonal blocks with coolant holes drilled throughout or a refractory clad pin-type dispersion fuel. Both the block-type and the pin-type fuel will be fabricated through reaction bonding; however, the starting material preforms are fabricated in a slightly different fashion.

The method of reaction bonding used for the block-type fuel fabrication starts with a polymer-derived carbon preform. The polymer is produced with a specific amount of pore-forming agent that creates the appropriate porous microstructure. The polymer is cured and pyrolyzed to produce a porous carbon preform. The polymer can be cast its final shape or the preform can easily be machined. The preform is then infiltrated with molten silicon which reacts with the carbon to form SiC. The microstructure of the preform must be tailored to produce a fully infiltrated sample with minimal residual silicon (5-15 volume percent). The microstructure is dependent upon the amount of pore former used in the original polymer mixture. The disadvantage of this process for fuel fabrication is that the sample will shrink on the order of 50 volume percent during pyrolyzation. If fuel spheres are incorporated at this point, the preform will crack due to the shrinkage of the matrix around the stable fuel particles. Therefore, a filler is added to control shrinkage. A ratio of filler powder to polymer of 80:20 is required to maintain the shrinkage to less than 5 percent.

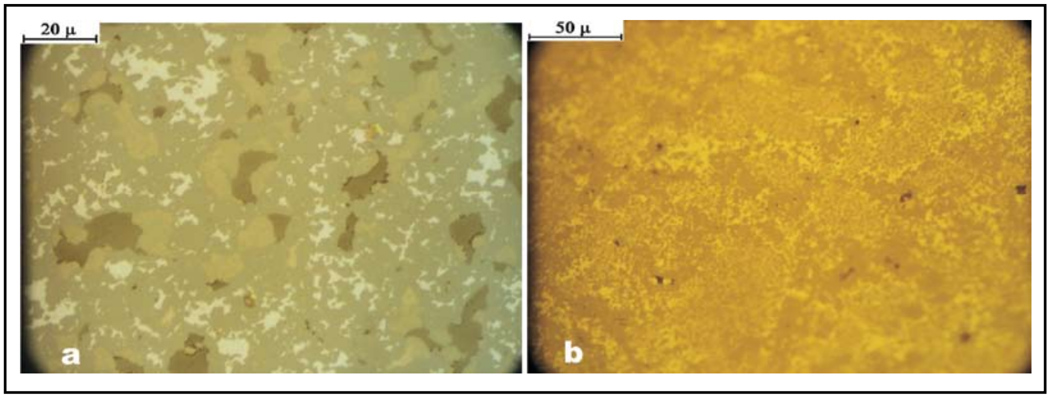

Figure 1a. Preform with no filler material; notice free carbon and large areas of residual silicon.

Figure 1b. Preform with filler material; notice no free carbon and a finer distribution of residual silicon.

The addition of filler materials affects the green, or pre-infiltrated, microstructure dramatically. If the microstructure is too coarse or too porous the final product may also be porous or may have a large amount of free silicon, which is detrimental to the high temperature properties. There may also be residual carbon which will affect the irradiation properties. Adding filler materials makes the microstructure much finer, but if the microstructure is too fine the porous networks are closed off by SiC formation during infiltration, stopping the infiltration process before the interior volume of the sample is infiltrated. This has been seen with the required high filler loading. Another possible outcome of too fine of a microstructure or insufficient porosity is that as the SiC is formed and expansion takes place, the sample falls apart or cracks. By using a combination of particles sizes in the filler material, the microstructure is refined sufficiently for full conversion of carbon, yet maintains complete infiltration of the pellet. Samples made with 80 weight percent filler made up of 68 percent SiC platelets (-100 mesh +200 mesh), 12 percent SiC powder (-325 mesh), 15 percent graphite (-325 mesh), and 5 percent carbon black have produced a dense, fully infiltrated sample. Samples have also been successfully fabricated using only SiC powders as filler. The resulting pellets, however, have more residual silicon when compared to samples with a mixture of SiC and carbon fillers. Samples have also been fabricated using SiC-coated spheres as a surrogate fuel phase. These samples used filler powders of SiC, graphite, and carbon black powders. Samples containing 35 weight percent filler and a low volume of spheres (~25 percent) have been fully infiltrated, producing a dense sample with little porosity. However, excessive shrinkage occurred because the filler amount was low, which opened large gaps between the sphere and the matrix and cracks were formed. These gaps and cracks were subsequently filled with silicon, which led to an excess of free silicon. Figure 1 contrasts the effect of adding 35 weight percent filler powder to the same polymer precursor. Even though it has been found that 35 percent inadequately controls shrinkage, the dramatic effect on the microstructure can be seen.

When sphere loading and amount of filler material are increased, porosity increases and the amount of material infiltrated and converted to SiC decreases. These effects are caused by the increased pressure needed to produce a pellet with the spherical particles fully surrounded by a consistent amount of matrix material. The increased pressure decreases the amount and size of open porosity. The porosity on the surface is closed off by SiC formation before the samples are fully infiltrated leaving a partially infiltrated sample. Samples have also been made using uranium carbide (UC) spheres. Further process development is required, however, to produce fully infiltrated dense samples. Because of the success seen in producing non- "fuel" loaded samples and the limited success seen in "fuel" loaded samples, this process is still a viable fuel fabrication route, but requires more process development.

Pin-type fuel fabrication by reaction bonding is also under development. In this fabrication process, the only carbon source is carbon powder added to SiC powder. Pin-type fuel fabrication starts by wet mixing fine powders of α-SiC and graphite along with surrogate fuel spheres. The mixture is dried and a binder (glycol) is added and pellets are made by uni-axial cold pressing. Debinding is done at 150°C in air, resulting in a material preform with interconnected porosity. Silicon infiltration is carried out by placing a preform in an argon atmosphere furnace along with silicon chips and heating to a temperature above 1,410°C. Parametric studies using various controlled precursor powder particle sizes, ratios of SiC and carbon powders, preform pressing pressure, and infiltration temperature have been performed to determine the optimum combination of material inputs and process variables. It was found that fine powders of α-SiC (70 percent of -100+200 mesh and 30 percent of -325 mesh) and graphite (-325 mesh) in a 75:25 ratio, mixed with 25 weight percent glycol, pressed at 9,000-18,000 psi, and infiltrated at 1,550°C yields well-infiltrated samples of matrix material, as shown in Figure 2. When spheres were added to the matrix, however, the infiltrated samples show severe cracking, indicating that further optimization is required in order to incorporate fuel particles into the matrix.

In conjunction with fuel fabrication activities, researchers have also performed several material irradiation experiments. Heavy ion irradiation studies of ceramics (ZrN, TiC, TiN, and SiC) in FY 2005 continue following the work on ZrC in FY 2004. The irradiation conditions were 800°C and doses of 10 and 70 displacements per atom (dpa). All the irradiations were conducted with 1-MeV Kr ions using the IVEM-TANDEM facility at Argonne National Laboratory. The results showed that the irradiation performance of ZrC and ZrN under these conditions was poor, with these materials showing severe lattice expansion. In the case of TiC, TiN, and SiC, the irradiation performance was much improved, with lattice expansion of TiC and TiN reduced by a factor of about four compared to ZrC and ZrN at 70 dpa. Virtually no lattice expansion was observed in the SiC samples.

The GFR-F1 is a low-dose materials experiment that was irradiated in INL's Advanced Test Reactor. The experiment is not instrumented and the specimen temperature is not actively controlled. Various fill gas compositions are used to vary the heat transfer from the experiment capsules, so that specimen temperature is calculated to be approximately 1,000°C. The first experiment capsules are currently in the Hot Fuel Examination Facility (HFEF) at INL and have been examined by neutron radiography, which showed the samples were intact with no gross material failures.

Planned Activities

The FUTURIX-MI materials irradiation experiment will be inserted in the Phénix reactor in France in 2007. Samples of various high-temperature materials including refractory ceramics and alloys and appropriate documentation were prepared by three DOE labs and were delivered to CEA for insertion.

Initial planning has started for the GFR-F2 fuel irradiation test, scheduled for fiscal year 2007. It is anticipated that the test configuration will mimic the existing AFCI hardware design and use a cadmium-filtered thermal neutron spectrum in the Advanced Test Reactor (ATR). The power, fuel loading, and target burnup will be prototypic of the reference GFR design. There will be two capsules destined for low (5 percent) and high (10 percent) burnup. The fuel samples will be representative of both block-type and pin-type fuel with two different fuel particle coatings. Fuel fabrication activities may carry into FY07.

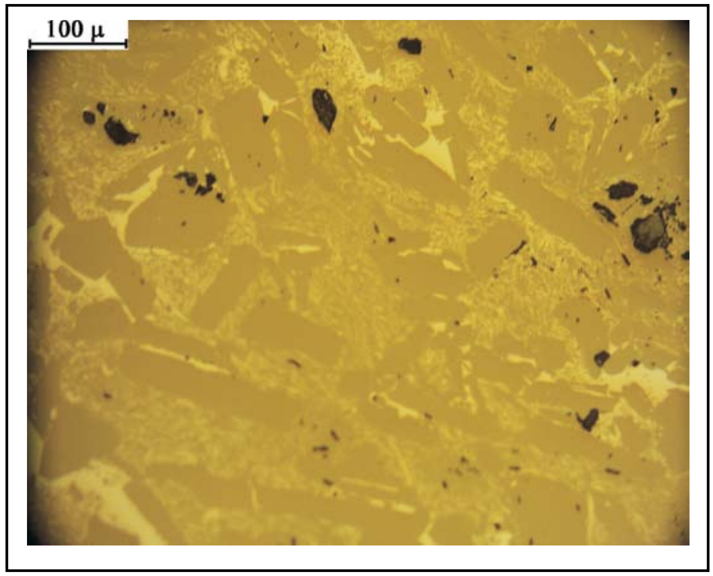

Figure 2. Microstructure of reaction bonded SiC using the proper ratio of particles sizes and compositions.

Work on both fabrication and materials irradiation will continue through next year, resulting in samples being prepared for inclusion in GFR-F2. Work is planned to further optimize the microstructure of the SiC matrix material through a series of parametric studies involving filler powder particle size distribution and composition. Thus far into the project, reproducibility has been an issue due to limitations in the processing equipment control system, which will be upgraded in FY06. Work will continue in this area to ensure samples are reproducible. Also, sphere particle distribution and packing will be examined in a series of parametric experiments to optimize the fuel particle distribution. Work will also continue on uranium carbide sphere production through a rotating electrode atomization process with the subsequent particle characterization.

Transmission electron microscopy characterization of the materials irradiated in the first GFR-F1 capsule will also take place.

PRA-Aided Design of Advanced Reactors with an Application to GFR Safety-Related Systems

PI (U.S.): T.Y.C. Wei, Argonne National Laboratory (ANL)

PI (France): N. Devictor and J. Rouault, Commissariat à l'Energie Atomique (CEA)

Collaborators: Massachusetts Institute of Technology (MIT)[1]

Project Number: 2004-010-F

Project Start Date: August 2004

Project End Date: August 2007

Research Objectives

This project focuses on formulating the conceptual design of decay heat removal systems for gas-cooled fast reactors (GFR) that will be effective during both normal modes of operation (including shutdown and refueling) and accident conditions (such as following a loss-of-coolant accident [LOCA]). Researchers will evaluate these systems under a range of scenarios, including station blackout and anticipated transients without scram (ATWS).

GFRs are contenders of international interest for advanced nuclear power service; however, particular attention must be paid to reliable decay heat removal if GFRs are to meet the high expectations for safety assurance established for new reactor designs. Probabilistic risk assessment (PRA) has matured over the last 30 years and is expected to play a key role in all aspects of system design and safety. The use of PRA will allow the designers to take advantage of lessons learned from the vast array of PRA applications already developed for light water reactors (LWRs) and other reactor types.

Two major issues must be addressed in order to take full advantage of PRA capabilities. First, since currently operating LWRs do not employ passive systems, PRA models for such systems will have to be developed for advanced reactors. Second, the use of PRA in design implies that there are probabilistic goals to determine which design is "good enough." Although there are activities by the U.S. Nuclear Regulatory Commission and the International Atomic Energy Agency to establish such probabilistic goals, the current licensing framework is largely "deterministic" and is not expected to change substantially in the near future. This raises the issue of whether the design should satisfy the deterministic criteria or the probabilistic goals, especially when a particular design option meets the probabilistic goals but fails the deterministic criteria. This project will also address these issues associated with PRA.

Research Progress

Passive safety systems are commonly considered more reliable than active ones. The lack of mechanical moving parts or other active components drastically reduces the probability of hardware failure. For passive systems, it is necessary to introduce the concept of "functional failure," i.e., the possibility that the loads will exceed the capacity in a reliability physics framework. In this work, researchers analyzed the passive cooling of a helium-cooled fast reactor in post-LOCA conditions. They used an importance sampling Monte Carlo technique to propagate the epistemic uncertainties and to calculate the probabilities of functional failures. The results showed that functional failures are an important contributor to the overall failure probability of the system and, therefore, should be included in PRA models.

Researchers also performed a comparison with an alternative active design. They quantified the risk of 2-, 3- and 4-loop designs considering functional failures. The passive system design has no hardware components that can fail; therefore, only functional failures due to epistemic uncertainty contribute to unreliability. For the actively cooled system (with blowers operating), blower failures were included, while functional failures are negligible. Table 1 shows the results for the passive and active systems.

[1] NOTE: The work at MIT is supported under NERI 05-044, "Optimized, Competitive Supercritical CO_2 Cycle GFR for GEN-IV Service."

While the passive system is always more reliable than the active one when functional failures are not considered, this is not the case if their impact is included in the analysis. A comparison of the mean values shows that the active system is actually more reliable than the passive one for the 2- and 3-loop designs. An increase in redundancy is more effective for functional reliability (affecting the passive system) than for hardware reliability (affecting the active system); therefore, for the highly redundant four-loop design, the passive system seems to be better than the active one. It should be pointed out that the calculated failure probability refers to the 72-hour, steady-state period after the initial transient. The results are conditional on the successful inception of natural (or forced) convection.

Researchers have proposed that the design process for the GFR reactor be accomplished in three phases:

1. From 2005–2007, researchers will conduct a more detailed analysis of potentially acceptable designs, with the objective of choosing a single reference design.
2. From 2008–2012, researchers will improve their analysis of the reference design, particularly improving and optimizing plant systems.
3. The last phase could be the licensing phase.

For each of these three phases, the research team has proposed a four-step risk-informed methodology that not only analyzes the optimization of systems, but analyzes the overall reactor as well.

The principles of the methodology are similar to the one proposed by MIT. The first issue studied was the practical usefulness of this methodology in the first phase. Work has been directed toward developing the proposed methodology with some preliminary studies. The methodology will be applied at the beginning of 2006 on the set of potential designs. The second issue is how to evaluate the reliability of thermal-hydraulic passive systems, such as the one that might be implemented in the GFR reactor, and how to integrate the results obtained into the subsequent PRA studies. Researchers completed initial work within the European RMPS project (Reliability Methods for Passive Safety) coordinated by CEA, which ended in 2004.

Special emphasis was placed on the problem of decay heat removal. Researchers showed that finding passive safety design solutions would be more challenging if helium were chosen as the coolant rather than carbon dioxide. Moreover, a fully passive system for decay heat removal may not necessarily be the safest and most economical solution. That is why PRA studies will be crucial in this decision-making process. In particular, researchers must find a way to account for the uncertainty in the reliability of passive systems.

		2 Loops	3 Loops	4 Loops
Passive design		4.76E-2	4.05E-4	7.19E-6
Active design	Mean	5.70E-3	1.58E-4	7.85E-5
	Median	3.00E-2	1.82E-3	1.14E-3
	5th percentile	3.00E-3	1.68E-4	1.06E-5
	95th percentile	5.70E-2	3.48E-3	2.18E-3

Table 1. Probability of failure results for the passive and active systems.

Researchers are evaluating the four-step risk-informed methodology developed at MIT to guide the design of future reactor systems. This methodology has many common features with the one proposed by French collaborators. The application of this methodology to the design of the GFR emergency core cooling system was analyzed. This analysis revealed the relevance of combining the rationalist and the structuralist approaches to defense-in-depth during the design process.

Planned Activities

Researchers are working on the time-dependent behavior of a passive decay heat removal system during LOCA transients in a helium-cooled GFR.

Considering the skills and abilities of the research partners, they have agreed to collaborate on the following tasks:

- Developing a risk-informed methodology for design
- Analyzing methodologies for including passive thermal-hydraulic systems in the PRA model, particularly the decay-heat removal system

Concerning the first issue, researchers are evaluating the similarities and differences of their different methodologies, with the objective of proposing (if possible) a common approach to risk-informed methodology for design.

Concerning the second issue, the CEA research team will work at a high level, developing and implementing the RMPS methodology for selection of potentially acceptable GFR designs. MIT's research team will work at a lower level, studying specific decay-heat removal systems, including the behavior of passive systems during LOCA transients and the performance of combinations of passive and active systems during these events.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Thermochemical Hydrogen Production Process Analysis

PI (U.S.): M. Lewis, Argonne National Laboratory

PI (France): P. Carles, P. Anzieu, and J.M. Borgard, Commissariat à l'Energie Atomique (CEA)

Project Number: 2004-011-F

Project Start Date: October 2004

Project End Date: September 2007

Research Objectives

There are two tasks in this I-NERI project. The objective of Task 1 is to develop a consistent methodology for evaluating the potential of a given thermochemical cycle to produce hydrogen with the use of nuclear heat. The objective of Task 2 is to use this methodology to identify which hydrogen cycles are the most promising among the 200+ that have been proposed in the literature. The metrics are chemical viability, energy efficiency, and engineering feasibility, as described within the methodology. In this way, all of the cycles will be compared on a consistent basis.

Research Progress

Argonne National Laboratory (ANL) and Commissariat à L'Energie Atomique (CEA) have collaborated in the identification of alternative thermochemical cycles and in the development of a consistent evaluation methodology. The method is based on the CEA concept of a cycle's efficiency changing as the level of knowledge increases.

The methodology was designed with two levels: Level 1 rapidly screens previously identified thermochemical cycles with reasonable realism; Level 2 identifies problems and unrealistic conditions. Level 1 only includes heat and work inputs and assumes stoichiometric reactions. The result is the maximum theoretical efficiency. Level 2 requires the same heat and work inputs but also includes equilibrium data that serve to identify unrealistic process conditions, problematic separations, unexpected by-products, etc. In Level 2, reaction conditions may be adjusted from values in the literature in order to maximize yields, minimize competing product formation, and reduce recycle. Available kinetic data may be used to adjust reaction conditions to provide reasonably fast reaction rates. Using the same methodology allows cycles to be compared on a consistent basis and focuses process development efforts. Components of the first two levels were defined in the scoping flowsheet methodology.

The researchers identified several alternative cycles as promising and evaluated them. These include the Cu-SO_4, Zn-SO_4, Mg-Cl, and Cu-Cl cycles. The efficiencies were calculated for both Level 1 and Level 2 analyses, as shown in Table 1. The data for the Cu-SO_4 cycle show a wide spread in calculated values, indicating that no optimization work has been done. More accurate efficiency calculations for the Cu-Cl cycle require new thermodynamic measurements, as well as further optimization work. The preliminary study of the Zn-SO_4 cycle indicates that the required reaction temperatures are too high for a nuclear heat source, while the efficiency for the Mg-Cl cycle is relatively low. Unless further compelling information

Cycle	Level	Efficiency % (LHV)	Maximum Temperature, °C	Other Conditions
Cu-SO_4	1	46.0	850	1 mol water
	2	38.1	1,100	1 mol water
	2	30.7	1,200	10 mols water
Zn-SO_4	1	40.5	850	1 mol water
	2	40.8	1,400	2.7 mols water
Cu-Cl	1	45.0	550	1 mol water
	2	43.9 From Aspen-Plus®	550	Excess water and HCl
Mg-Cl	1	35.2	600	1 mol water
	2	30.0 to 33.1	600	2 mols water

Table 1. Efficiency calculations for the alternative cycles evaluated with the scoping flowsheet methodology.

is obtained, these two cycles are no longer considered promising. Researchers are currently calculating the efficiency of the Ce-Cl cycle.

Proof-of-principle work for the Cu-Cl, Cu-SO_4, and the Ce-Cl cycles has either been completed or is nearly complete. The results of the laboratory work indicate that these cycles are chemically viable. Thus, several cycles have been identified as having promising efficiencies and are chemically viable. Further examination is therefore justified.

Researchers identified the key parameters that influence the costs of hydrogen production for high-temperature processes, such as thermochemical cycles and electrolysis. For thermochemical cycles, raw material investment and maintenance, heat exchanger costs, and energy recovery are the important parameters. For high-temperature electrolysis, the important parameters are the heat exchange and investment cost for the electrolyzer as well as the lifetime of the electrolyzer and its ability to handle shutdowns and recycle events. General screening criteria for potential thermochemical cycles are being quantified as part of this effort.

Planned Activities

In the original plans for Task 1, the research team specified that they would evaluate flowsheets for the baseline cycles, including one or more of the sulfur cycles and possibly high-temperature electrolysis. This work has been deferred until after the development of the methodology for a Level 3 analysis, which will consist of a detailed engineering feasibility study of the most promising alternative cycles. Components of the Level 3 methodology will include values for common engineering parameters, such as the efficiencies of pumps, compressors, and furnaces. In addition, boundary conditions, such as the hydrogen outlet pressure and hydrogen purity, will be fixed so that all cycles may be evaluated on a consistent basis. Some challenges associated with engineering feasibility include developing energy-efficient methods for separations and the removal of excess water, maintaining high-temperature operations under aggressive, oxidizing conditions, identifying corrosion-resistant materials for use at high temperatures and moderate pressures, and developing new technologies for difficult separations. The Level 3 evaluation will consider technical options to meet these challenges. This work will be done in conjunction with various American universities as well as with CEA.

9.0 U.S./Japan Collaboration

An exchange of notes was signed by U.S. Assistant Secretary John Wolf, for Secretary of State Colin Powell, and Mr. Keiichi Katakami, Minister of the Japanese Embassy, for Ambassador Kato, on April 22, 2004.

To implement this bilateral collaboration, the Japanese government decided to sign implementing arrangements using the following two organizations: the Agency of Natural Resources and Energy of Japan (ANRE) and the Ministry of Education, Culture, Sports, Science, and Technology of Japan (MEXT). ANRE is the office responsible for nuclear technology for the Ministry of Economy, Trade and Industry (METI).

On May 26, 2004, the implementing arrangement with ANRE was finalized and signed by Mr. William D. Magwood IV, Director of DOE-NE, and Mr. Kusaka, Director-General of ANRE. An annex regarding I-NERI collaboration was signed on June 10, 2004, by Mr. Shane Johnson, Deputy Director for Technology, DOE-NE, and Mr. Shigeru Maeda, Director for Nuclear Energy Policy, Nuclear Policy Division, ANRE/METI.

On February 8, 2005, the United States Department of Energy (DOE) and Japan's Ministry of Education, Culture and Sports, Science and Technology (MEXT) signed the Implementing Arrangement concerning cooperation in the field of research and development of innovative nuclear energy technologies (I-NERI).

9.1 Work Scope Areas

Areas of Collaboration with ANRE

- Supercritical Water-Cooled Reactor

Areas of Collaboration with MEXT

- Innovative nuclear reactor technologies
- Innovative processing technologies
- Innovative fuel technologies using solvent extraction

9.2 Project Summaries

The first project was awarded under this cooperative agreement in FY 2005, with the second awarded early 2006. An abstract of the project follows.

Directory of Project Summaries

Development of Materials for Supercritical-Water-Cooled Reactor

PI (U.S.): G. Was, University of Michigan

PI (Japan): H. Matsui, Institute for Materials Research, Tohoku University

Collaborators: Idaho National Laboratory; University of Wisconsin-Madison; University of Tokyo; Toshiba Corporation, Hitachi Works; Hitachi, Ltd.

Project Number: 2005-001-J

Project Start Date: October 2004

Project End Date: September 2007

Research Objectives

Advantages of the Supercritical-Water-Cooled Reactor (SCWR) design, including its high thermal efficiency, simplified systems, flexible core design, and minimized research and development (R&D) cost, prompted its selection as one of the promising candidates in the Generation IV program. Japanese R&D efforts aim to provide additional technical information in the areas of plant conceptual design, thermal-hydraulics, and materials that will be necessary for demonstrating SCWR technology.

Material development is a critical issue for further SCWR advancement. Previous studies in this area have been limited to screening commercial alloys and potential new materials via simulated irradiation tests and un-irradiated corrosion testing. To develop a detailed SCWR system design, a more thorough understanding of material behavior under specific SCWR conditions is necessary, along with development of a comprehensive materials database.

This project will evaluate the irradiation durability and corrosion performance of various materials, including resistance to stress corrosion cracking, by conducting neutron irradiation tests under simulated SCWR conditions. Selected commercial alloys and newly developed alloys will be subjected to micro-analysis and corrosion tests in supercritical water. Their long-term reliability will be evaluated via phase stability tests and long duration corrosion tests. Through these experimental studies, researchers expect to gain sufficient understanding of the material behavior under SCWR conditions. The accumulation of basic material data under SCWR conditions will enable the team to construct the materials database required for developing a more detailed design of fuel cladding and reactor core components.

Research Progress

Researchers completed the study of the temperature dependence of corrosion in ferritic-martensitic (F-M) alloys, and benchmarked the Irradiated Materials Testing Laboratory for conducting tests on neutron-irradiated material in supercritical water. They conducted an experiment consisting of a constant extension rate tensile (CERT) test on three F-M alloys and an exposure test at 600°C for 191 hrs. As shown in Figure 1, oxidation at 600°C was extremely rapid, resulting in weight gains that were 4-5 times that at 500°C and almost 20 times that at 400°C. Weight gain follows an Arrhenius behavior, as shown in Figure 2. The calculated activation energies were 189.29 kJ/mol for T91, 177.14 kJ/mol for HCM12A, and 172.60 kJ/mol for HT-9. These values are consistent with either cation outward diffusion or inward diffusion of oxygen by a short circuit (e.g., grain boundary diffusion) process.

Analysis of the oxide surfaces revealed a rough and porous morphology. The oxide subgrains on 400°C specimens were granular in shape. At 500°C, the subgrain size and porosity increased, reaching and average size of about 5 micrometers at 600°C. Microcracks appeared on surface oxides for the first time at 600°C. X-ray diffraction (XRD) characterization identified these surface oxides as magnetite (Fe_3O_4) in all alloys and at all temperatures.

Researchers determined oxide composition on cross-section samples using energy dispersive spectrometry. The outer oxide oxygen-to-metal ratio of approximately

1.3 is consistent with the Fe_3O_4 structure confirmed by XRD. The oxygen-to-metal of the inner layer is 1.1 to 1.3, which corresponds to a spinel oxide, $(Fe,Cr)_3O_4$. At 500°C, a transition region emerged beneath the inner oxide, where the metal content increased to bulk values and the oxygen content decreased to nearly zero, becoming more pronounced at 600°C. In addition, researchers observed a chromium-enriched layer between the transition layer and the alloy substrate in some parts of the coupon.

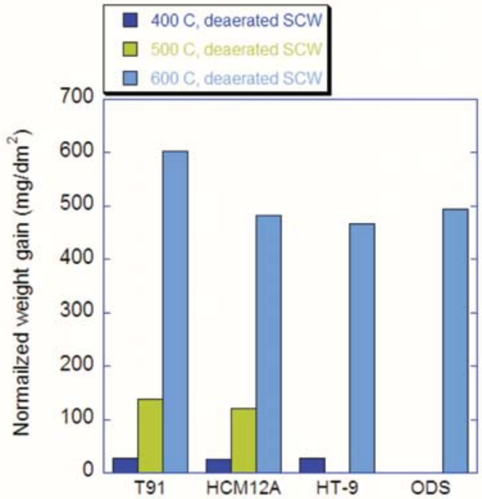

Figure 1. Oxide weight gain in F-M alloys and ODS at temperatures between 400 and 600°C.

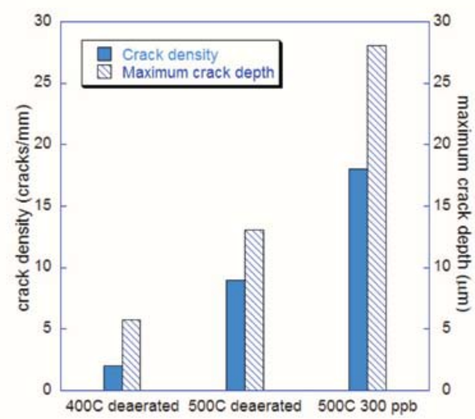

Figure 2. Crack depth and crack number density for HT-9 test in CERT mode at following exposure in deaerated SCW, 3 x 10^{-7} s^{-1} in SCW normalized to a 182 hr exposure time.

The CERT test was conducted at a strain rate of 3 x 10^{-7} s^{-1}. The stress-strain behavior of the F-M alloys in this study followed the trends previously documented in the literature very closely, with drops in yield strength and maximum strength between 400°C and 500°C, along with a decrease in uniform elongation but an increase in total elongation. At 600°C, the yield and maximum strengths dropped to less than half that at 400°C. In CERT tests in all environments, the yield strength and maximum stress for HT-9 was highest, followed by HCM12A and T91. All F-M alloys exhibited ductile failure at all temperatures in supercritical water (SCW). However, alloy HT-9 exhibited shallow inter-granular (IG) cracks that increased in depth and number density with increasing temperature and dissolved oxygen content (Figure 2).

In summary, the latest results through 600°C confirmed the Arrhenius behavior of oxidation of F-M alloys. The activation energy for oxidation is consistent with either cation outward diffusion or inward diffusion of oxygen by a short circuit process. The oxide is composed of between 2 and 4 layers depending on the temperature. CERT results showed that all three of the F-M alloys failed by ductile rupture. However, alloy HT-9 exhibited shallow IG cracking that was more severe at higher temperature and higher dissolved oxygen content. Grain boundary engineering will be explored to determine if the inter-granular stress corrosion cracking (IGSCC) susceptibility of this alloy can be addressed.

The benchmarking of the Irradiated Materials Testing Laboratory was completed in 2005, following a successful test on unirradiated samples in 500°C SCW and a dry-run loading and SCC test initiation and unloading of a set of samples that were treated as if they were radioactive. The SEM was also installed and operated in the hot cell. The facility is ready to accept irradiated samples for CERT tests in support of the SCWR program.

Collaborators at Wisconsin completed a single corrosion exposure at 500°C with a dissolved oxygen content of 25 ppb for 1,026 hours. They performed a detailed analysis of samples from this exposure, as well as samples exposed in FY 2004 at 500°C with a dissolved oxygen content of 2 ppm for 576 hours.

The weight gain due to oxidation in supercritical water is typically smaller but less predictable in austenitic alloys than in F-M alloys. The oxide layer in most austenitic steels exhibits a tendency to spall with increasing exposure time. Such spallation may be related to fine-scale porosity that develops in the spinel layer and may account for the lower predictability. To improve the oxide scale adherence, alloy 800H samples were thermo-mechanically processed to reduce the fraction of high-energy grain boundaries. Such a modification may reduce the anisotropy in the oxide layers and mitigate the effect of differential thermal expansion between hematite and magnetite by increasing the fraction of hematite, thereby improving the oxide adherence.

All the tested F-M steels after exposure to supercritical water at 500°C with 25 ppb dissolved oxygen show a typical dual layer, which is composed of an outer Fe-O magnetite layer and an inner Fe-Cr-O spinel layer. Among the test F-M alloys, the 9Cr ODS alloy showed the lowest weight gain due to oxidation, even though the 9Cr ODS alloy had less bulk Cr (9 wt% Cr) than HCM12A (12 wt% Cr), see Figure 3. Researchers also tested three Ni-base alloys: C22, INCONEL 625, and 718. All the samples showed a fairly good corrosion resistance in supercritical water environment. However, they observed pitting in all these Ni-base alloys.

The researcher also studied radiolysis in SCW. Several experiments have been performed to study the critical hydrogen concentration (CHC) under supercritical water pressures at 3,600 psi (25 MPa) and various temperatures. The results indicated that the CHC is approximately 2E-5 molar hydrogen and is dependent on the temperature. As the temperature increased toward the critical point, the presence of a CHC became less evident. At present, the reason for this is still unknown and further experiments are underway to help understand these observations.

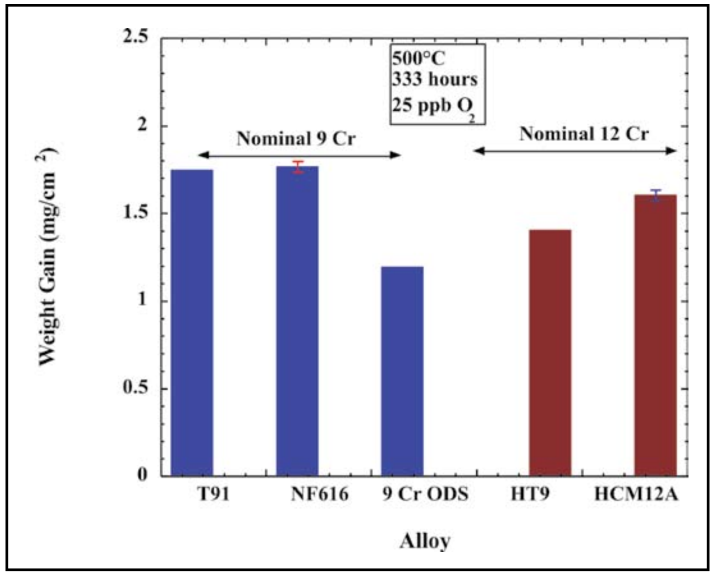

Figure 3. Superior corrosion resistance of the 9 Cr ODS alloy relative to other other ferritic-martensitic steels.

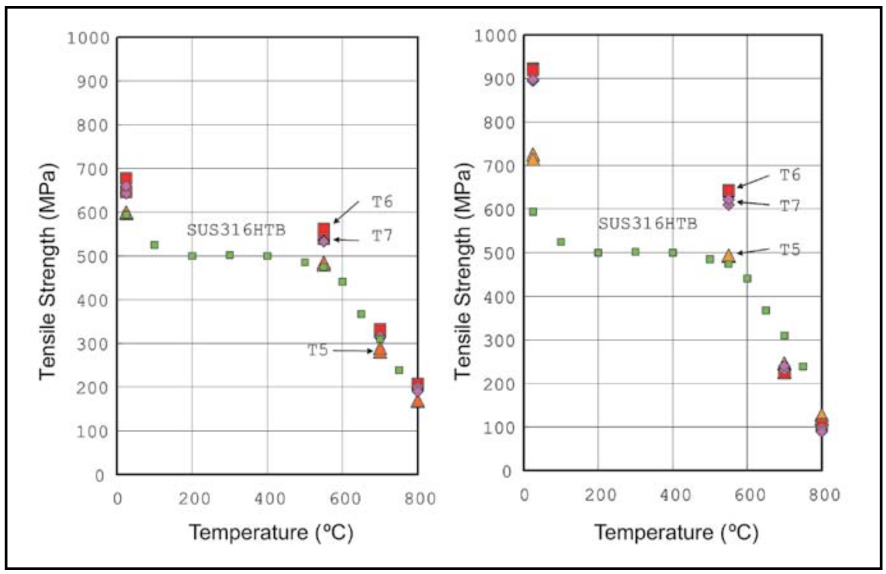

Figure 4. High-temperature mechanical properties of reference alloys and modified ones with two different grain sizes. Modified alloys show generally superior tensile strength in the standard grain size condition while, for refined grain size, tensile strength is slightly lower at temperatures above 600°C.

Activities conducted by the Japanese investigators are categorized into four subtasks: 1) Design compatibility, 2) Irradiation properties, 3) Corrosion properties after irradiation, and 4) Overall evaluation. Based on required specifications, researchers identified test items and conditions and carried out an evaluation of design compatibility with basic materials properties.

They prepared specimens for a variety of tests, including neutron irradiation. Alloy types chosen for irradiation tests were: SUS310, SUS316L, Alloy690 and five modified alloys derived from SUS 310 (i.e. T3, T5, T6, T7 and H2), and one derived from SUS316L (i.e. H1). Modifications were made to improve irradiation properties, corrosion properties, high-temperature strength, and creep properties. They demonstrated significant improvement in void swelling properties in T3, H1, and H2 modified alloys by electron irradiation tests, and neutron irradiations are planned to verify this result. Thermal creep tests on these alloys were started. High-temperature tensile properties have been obtained on these alloys both with the standard grain size (70 μm) and with refined one (<3 μm) as shown in the Figures 4a and b.

Irradiation tests in JOYO, the experimental fast reactor of the Japan Atomic Energy Agency (JAEA), are underway and specimens will be discharged from the reactor in FY 2006. Irradiation temperatures are 500°C and 600°C, with a neutron fluence up to 10^{22}n/cm^2. A second irradiation campaign is being prepared and the test matrix includes pressurized tube creep experiments up to 700°C. In order to evaluate materials response to thermal neutrons, another irradiation campaign is being prepared. Helium generation and its impact on high-temperature creep properties are to be examined in this experiment.

Researchers conducted corrosion tests up to 1,000 hours on austenitic stainless steels and nickel-based alloys. Among the three nickel-based alloys (Alloy 600, 625, and 690), weight loss was largest in Alloy 690. For the stainless steel samples, although SUS304 showed some weight loss after 1,000 hours, SUS316L and SUS310S showed weight gain and the normal behavior of weight loss has not yet been observed. The corrosion tests are still ongoing and further results will become available in FY 2006.

Design of a SCW-corrosion test loop to be installed in a hot cell facility in IMR Tohoku University has been completed and fabrication of significant fraction of the entire loop will be completed during FY 2006. In parallel with this activity, SCC tests as well as slow-strain-rate tensile tests in vacuum are being conducted with emphasis on the effect of impurities in the environment. Side cracking under SCW conditions is one of the important topics in this subtask area.

Planned Activities

Research activities planned for FY 2006 will focus on several areas. Researchers will conduct proton irradiation of austenitic alloys over a range of doses and temperatures to determine the role of irradiation in stress corrosion cracking in supercritical water. They will perform SCC tests on a sample of neutron-irradiated Japanese prime candidate alloy to begin determining the effect of neutron irradiation on SCC in supercritical water. In addition, they will initiate fatigue crack growth rate testing on compact tension samples of 316L to begin determining the effect of the supercritical water environment on the crack growth rate in unirradiated austenitic alloys.

Lastly, researchers also plan to conduct neutron irradiation and post-irradiation examination of some of the specimens, perform thermal creep tests and long-term general corrosion tests, construct and install an SCW corrosion test loop in the hot cell facility, and perform slow-strain-rate tensile tests in vacuum for the evaluation of micro-side crack formation.

10.0 U.S./Republic of Korea Collaboration

Director of DOE-NE, William D. Magwood IV, signed the first bilateral I-NERI Agreement on May 16, 2001, with Dr. Chung-Won Cho, Director General of Korea's Atomic Energy Bureau, signing for the Republic of Korea's Ministry of Science and Technology. The first U.S./Republic of Korea (ROK) collaborative research projects were awarded in FY 2002, with a total of 21 projects awarded to date.

10.1 Work Scope Areas

R&D topical areas for the U.S./Republic of Korea collaboration include:

2002 projects:

- Instrumentation, controls, and diagnostics
- Advanced light water reactors (LWR)
- Advanced LWR fuels and materials technology
- LWR safety technology
- Advanced LWR computational methods

2003 projects:

- Next generation reactor/fuel cycle technology
- Innovative nuclear plant design
- Advanced nuclear fuels and materials

2004 projects:

- Advanced gas-cooled fast reactor
- Hydrogen production by nuclear systems
- Advanced fuels and materials development
- Supercritical water-cooled reactor concepts

10.2 Project Summaries

In FY 2002, the initial year of the collaboration, six projects were awarded. Five additional projects were awarded in FY 2003 and six new collaborative projects were initiated in FY 2004. The final remaining FY 2002 project and three of the five FY 2003 projects were completed during the past fiscal year. Two FY 2003 projects received no-cost extensions for completion in FY 2006. Four new collaborative projects were awarded to Korean partners in FY 2005.

A listing of I-NERI U.S./ROK projects that are currently underway, completed last year, and newly awarded follows, along with summaries of FY 2005 accomplishments and abstracts of the new projects.

Directory of Project Summaries

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Advanced Computational Thermal Fluid Physics (CTFP) and its Assessment for Light Water Reactors and Supercritical Reactors

PI (U.S.): D. M. McEligot, Idaho National Laboratory

PI (Korea): J. Y. Yoo, Seoul National University (SNU)

Collaborators: Iowa State University, Korea Advanced Institute of Science and Technology (KAIST), Pennsylvania State University, University of Manchester, University of Maryland, Utah State University

Project Number: 2002-016-K

Project Start Date: December 2001

Project End Date: October 2005

Research Objectives

The goal of this project was to improve predictive methods for assessing Generation IV reactor systems (such as supercritical-pressure water reactors) in support of both the Advanced Fuel Cycle Initiative (AFCI) and the Nuclear Hydrogen Initiative (NHI). The objectives were to develop and to extend the supporting knowledge base of advanced computational techniques, such as direct numerical simulation (DNS), large eddy simulation (LES), and differential second moment closure (DSM) techniques, to treat supercritical property variation and complex geometries, thereby providing capabilities to:

- Assess predictive capabilities of current codes for supercritical-water reactors (SCWRs), very high temperature gas-cooled reactors (VHTRs), etc.
- Provide the basis for improving nuclear reactor thermal hydraulics, safety, and subchannel codes
- Provide computational capabilities where current codes and correlations are inadequate
- Predict Generation IV conceptual and preliminary design parameters for:
  - full power operation (LES, DSM, and Reynolds-averaged Navier-Stokes approaches)
  - reduced power operation
  - transient safety scenarios
- Handle detailed thermal-hydraulic flow problems for final Generation IV designs for improved performance, efficiency, reliability, enhanced safety, and reduced costs and waste

This project provided basic thermal fluid science knowledge to increase the understanding of the behavior of superheated and supercritical systems at high temperatures, to apply and improve modern computation and modeling methods, and to incorporate enhanced safety features.

Research Progress

Turbulence is one of the most important unresolved problems in engineering and science, particularly for the complex geometries and fluid property variation occurring in these advanced reactor systems and their passive safety systems. DNS, LES, and differential second moment closures (DSM or Reynolds-stress models) are advanced computational concepts in turbulence "modeling" whose development has been extended to treat complex geometries and severe property variation for designs and safety analyses of Generation IV reactor systems such as SCWRs. The basic thermal fluids research applied first principle approaches (DNS and LES) coupled with experimentally determined heat transfer and fluid mechanics measurements.

Variations of fluid properties along and across heated flows are important in all Generation IV reactor systems concepts, including SCWRs, VHTRs, and gas-cooled fast reactors (GFRs). Researchers found significant differences and uncertainties among thermal hydraulic correlations for these conditions. Developers of codes for reactor design and systems safety analyses need improved computational techniques and supporting measurements to treat the property variations and their effects reliably for operating conditions and hypothesized accident scenarios.

The geometries of the reactor cooling channels of some SCWR concepts are shown in Figure 1. Most of these geometries are more complex than those that have been used to generate the empirical correlations employed in the thermal hydraulic codes. Advanced computational techniques may be applied, but measurements with realistic geometries are needed to assess the reliability and accuracy of their predictions.

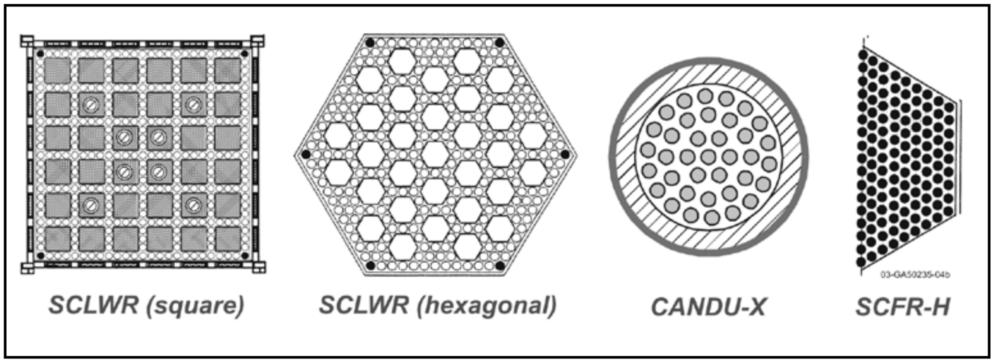

Figure. 1. Some proposed designs for fuel assemblies in supercritical water reactors.

The researchers extended LES and DNS to generic idealizations of such geometries with property variation. They developed DSM models and evaluated the suitability of other proposed RANS (Reynolds-averaged Navier-Stokes) models by applying the DNS, LES, and experimental results. They obtained fundamental turbulence and velocity data for an idealization of the complex geometries of these advanced reactor systems, and developed miniaturized multi-sensor probes to measure turbulence components in supercritical flows in tubes. Researchers also developed experiments on heat transfer with supercritical flows, provided industrial insight and thermal-hydraulic data needs, and reviewed the results of the studies for application to realistic designs and their predictive safety and design codes.

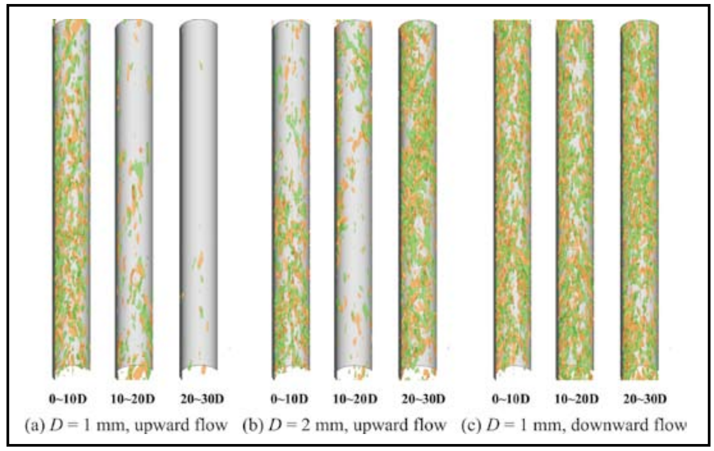

Figure 2. Direct numerical simulation of heat transfer to supercritical flow demonstrates sensitivity of turbulence (hence heat transfer) to fluid property variation and buoyancy influences.

DNS employs no turbulence modeling; it solves the unsteady governing equations directly. Consequently, along with measurements, it can serve as a benchmark for assessing the capabilities of LES, DSM, and general RANS techniques. It also can be applied for predictions of heat transfer at low flow rates in reduced power operations and transient safety scenarios, such as loss-of-coolant or loss-of-flow accidents, in SCWRs, GFRs, and VHTRs. Figure 2 indicates that, for SCWRs, it can handle sensitive situations that are difficult to treat properly with correlations or with many turbulence models. Once validated, LES and DSM techniques can be applied for predictions at higher flow rates, such as near normal full-power operating conditions, for these Generation IV reactor concepts. The flow facility developed at SNU provides a means of measuring heat transfer to supercritical fluids for assessing the effects of their property variations and the miniaturized multi-sensor probes from the University of Maryland permit measuring the turbulence which is modeled by the codes. The Matched-Index-of-Refraction flow system at INL, which uses optical techniques for measurements in small complex passages without disturbing the flow, provides the means to investigate the complex flow features of Generation IV reactor geometries. The INL experiment models the complex geometry of coolant passages in an SCWR concept to provide benchmark data.

During this collaborative research project researchers completed the following research activities.

- They extended the DNS code to obtain the first treatment of heat transfer to supercritical fluids and completed 17 cases with conditions spanning the pseudocritical temperature, demonstrated significant effects of buoyancy and property variation on the turbulence, compared predictions to measurements and extended the code to annular flow in the pseudocritical region with a heated central rod (Figure 3), and examined the effects of property variation on turbulent heat flux and other turbulent statistics.
- Researchers extended a quasi-developed code for circular tubes to include supercritical fluid properties (Figure 4) and validated its performance by comparing it to DNS and experiments. This was extended to developing flows and to complex geometries such as

annuli, ribbed annuli, and an idealization of flow phenomena in coolant channels of an SCWR concept.

- They applied a DSM code to examine the capabilities of a wide range of turbulence models for heat transfer to superheated gas flows and to supercritical flows — with and without buoyancy influences — and compared predictions to DNS and experiments (Figure 5). Results depended strongly on the individual models and researchers concluded that no single model could be chosen as the best because some predicted wall temperatures satisfactorily for some cases but not for others.
- INL installed a large-scale model for simulating flow in SCWR passages in their Matched-Index-of-Refraction flow system. They acquired two- and three-dimensional PIV data for the streamwise-periodic, three-dimensional region between successive grid spacers (Figure 6). Results of this benchmark database are archived electronically for assessment of DNS, LES, DSM, and RANS codes.
- Researchers developed two-sensor miniaturized hot-wire probes and a calibration facility (Figure 7) for use in supercritical CO_2 heat transfer experiments, calibrated the probes, derived response algorithms, and trained SNU students in the use of their probes for measuring instantaneous temperature and velocities in a supercritical fluid. They designed and constructed a mechanism to

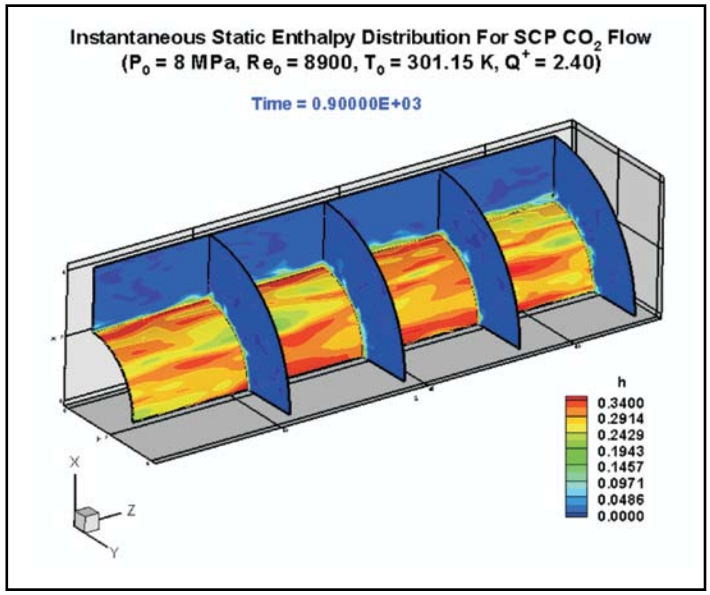

Figure 3. Direct numerical simulation of pseudocritical annular flow along a heated rod (h_{pc} = 0.0489). The gas-like region forms a very thin insulating layer near the heated surface, increasing the thermal resistance.

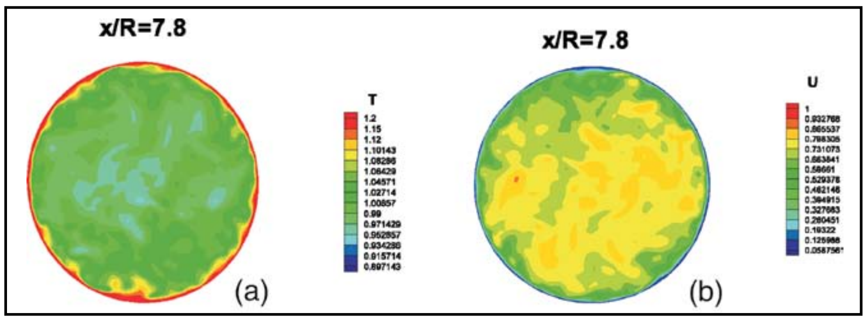

Figure 4. Large eddy simulations of SNU experiment on heat transfer to supercritical CO_2 at Re ≈ 28,700, instantaneous contours: (a) temperature and (b) streamwise velocity.

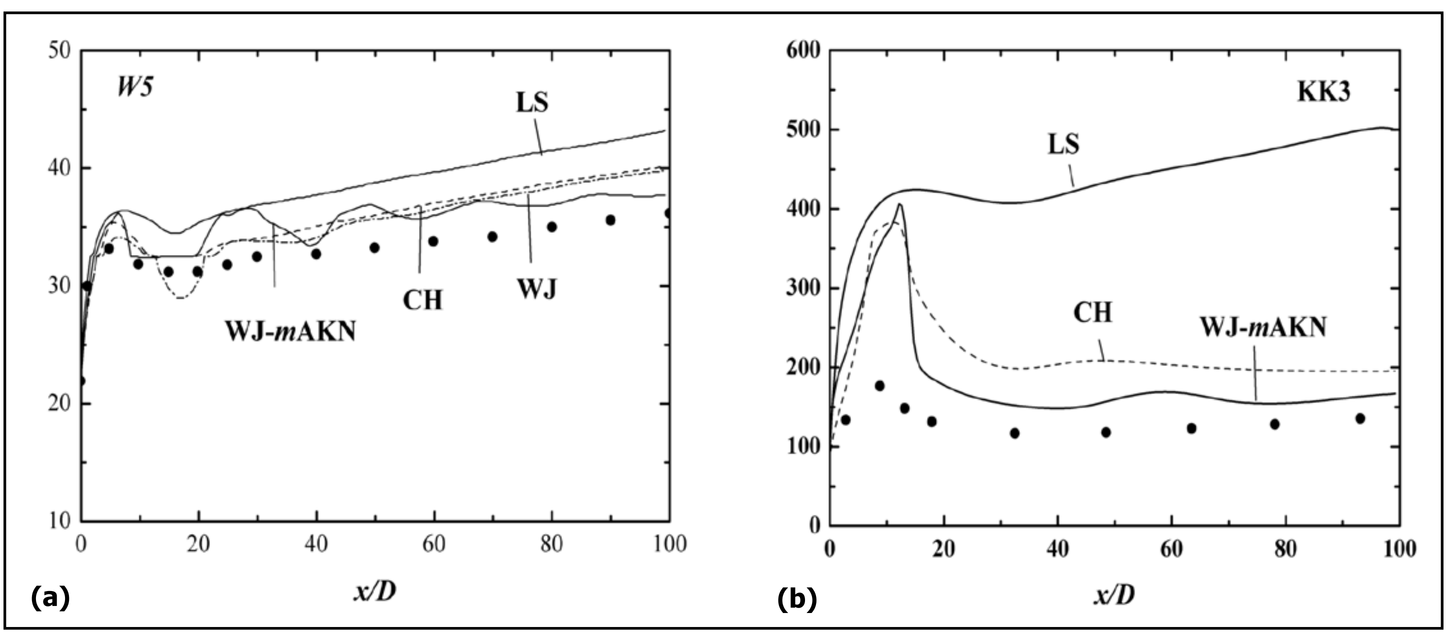

Figure 5. Comparisons of predicted wall temperature profiles for heat transfer to supercritical CO_2 flow and data of (a) Weinburg and (b) Kurganov and Kaptilnyi.

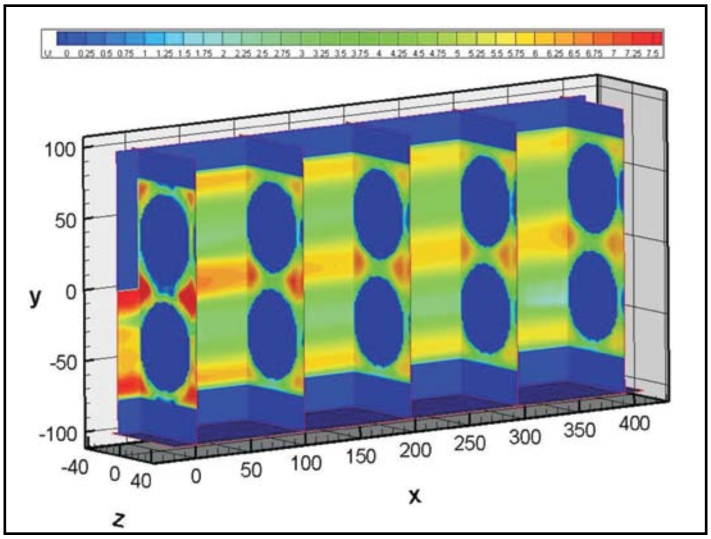

Figure 6. PIV (particle image velocimetry) measurements of flow features in a large-scale idealized model of coolant channels in an SCWR fuel assembly. Matching of the refractive indices of the fluid and rods allows undistorted access to the measurement region.

traverse the probe inside a high-pressure CO_2 flow and provided the designs to SNU.

- They built an experiment to measure heat transfer, pressure drop and velocity, and temperature distributions in supercritical CO_2 in tubes. They obtained the first measurements of heat transfer to supercritical flow in small square and triangular tubes (Figure 8) and measured heat transfer and pressure drop to supercritical CO_2 with small and large circular tubes for over 160 sets of conditions overall.

Since January 2002, the project partners had 33 archival papers published or in press, 58 conference presentations, and 23 invited presentations relating to this collaborative Korea/U.S. I-NERI project. They also had over 60 publications on other related topics.

Planned Activities

This project was completed on October 31, 2005, with submission of the final technical report, INL/EXT-05-00901.

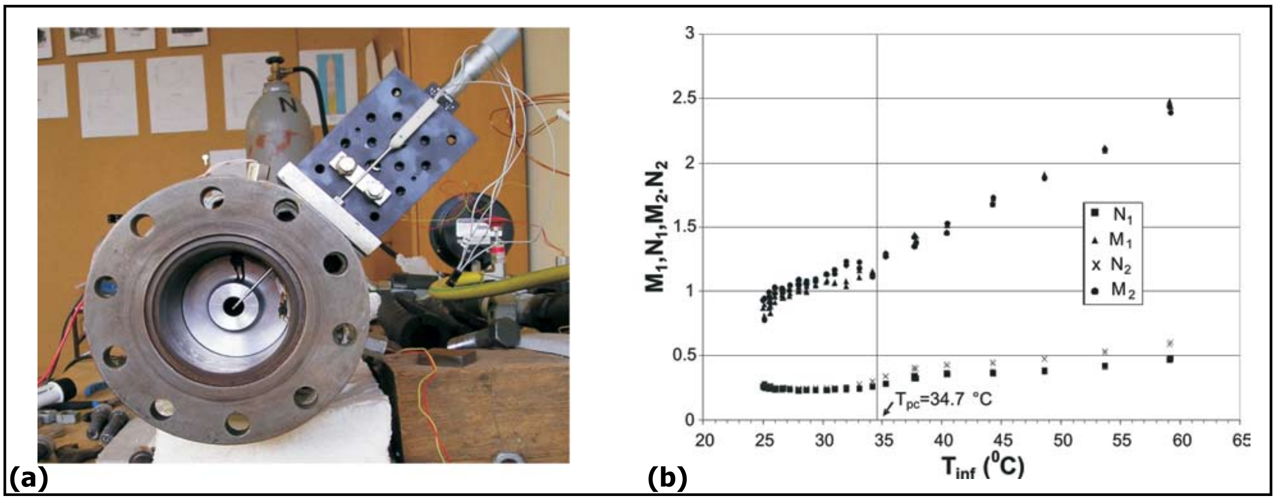

Figure 7. Calibration of two-sensor miniaturized hot-wire probe for determination of velocity, temperature, and their turbulent fluctuations in supercritical CO_2 flows, (a) photograph of probe mounted in front of nozzle for calibration in heated supercritical flow and (b) correlation of coefficients in convective heat transfer relation for sensor at P = 8 MPa.

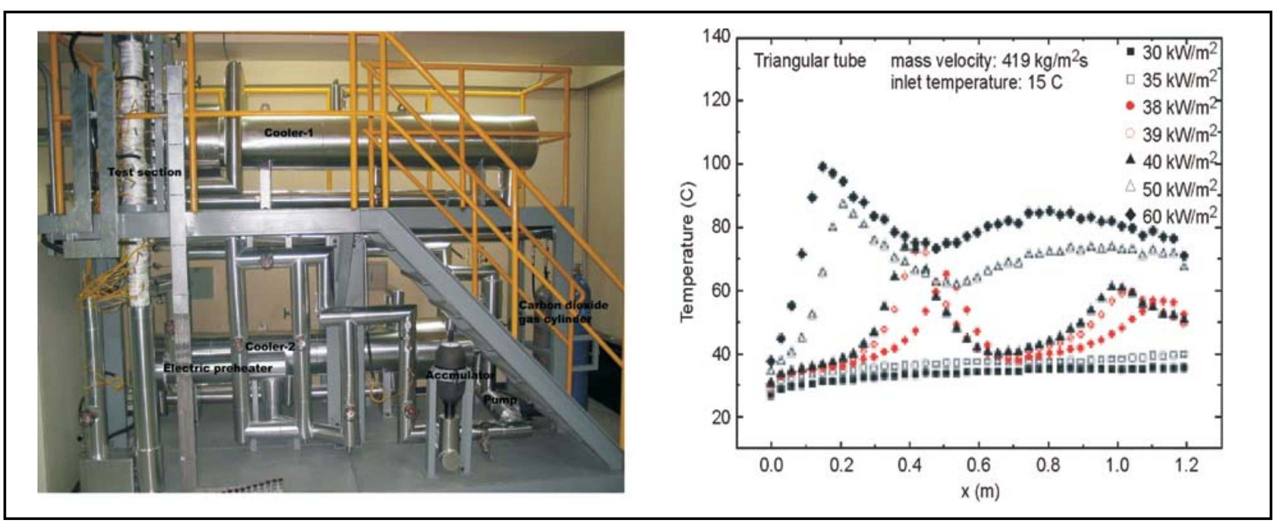

Figure 8. SNU facility for measurements of heat transfer to supercritical carbon dioxide and first measurements for small triangular tubes (hydraulic diameter = 9.7 mm). As with circular tubes, "deterioration" is sensitive to the surface heat flux.

Passive Safety Optimization in Liquid Sodium-Cooled Reactors

PI (U.S): J. E. Cahalan, Argonne National Laboratory

PI (Korea): D. Hahn, Korea Atomic Energy Research Institute (KAERI)

Collaborators: None

Project Number: 2003-002-K

Project Start Date: January 2003

Project End Date: December 2005

Research Objectives

This project was a three-year collaboration between Argonne National Laboratory (ANL) and the Korea Atomic Energy Research Institute (KAERI) to identify and quantify the performance of innovative design features in metallic-fueled, sodium-cooled fast reactor designs. The objective of the work was to establish the reliability and safety margin enhancements provided by design innovations offering significant potential for construction, maintenance, and operating cost reductions. The project goal was accomplished with a combination of advanced model development (Task 1), analysis of innovative design and safety features (Tasks 2 and 3), and planning of key safety experiments (Task 4). In 2005, the project concluded in its third and final year, with significant progress in all four tasks. The project was completed in December 2005.

Research Progress

In Task 1, the researchers collaborated on the development, implementation, and testing of a detailed, three-dimensional fuel subassembly thermal-hydraulic model. The objective of the model development effort was to provide a high-accuracy capability to predict temperatures in reactor fuel subassemblies, reducing the uncertainties associated with lower fidelity models previously used for safety and design analysis. The model that was developed computes steady-state and transient fuel, cladding, and coolant temperatures in each fuel pin and coolant sub-channel of the core. It also calculates coolant flow rates for each sub-channel, lateral flow between adjacent sub-channels, and duct wall temperatures for each flat of each subassembly. The model provides accurate and reliable data for calculations of reactivity feedbacks and safety margins. The project also included implementation and verification of the model by applying it to available reactor tests performed at EBR-II. Figure 1 demonstrates the model's accuracy as applied to EBR-II Shutdown Heat Removal Test 17.

In Task 2, researchers performed integrated safety assessments of innovative liquid metal reactor designs to quantify the performance of inherent safety features. The objective of the analysis effort was to identify the

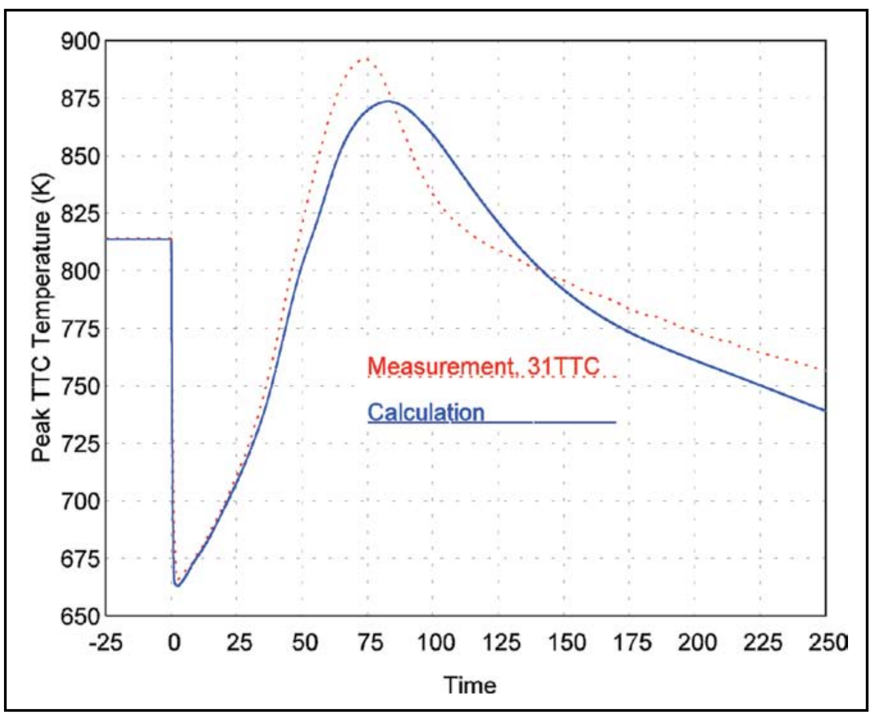

Figure 1. Transient peak coolant temperature near the top of the EBR-II fuel subassembly XX-09 in SHRT-17 (measured value compared to model calculations).

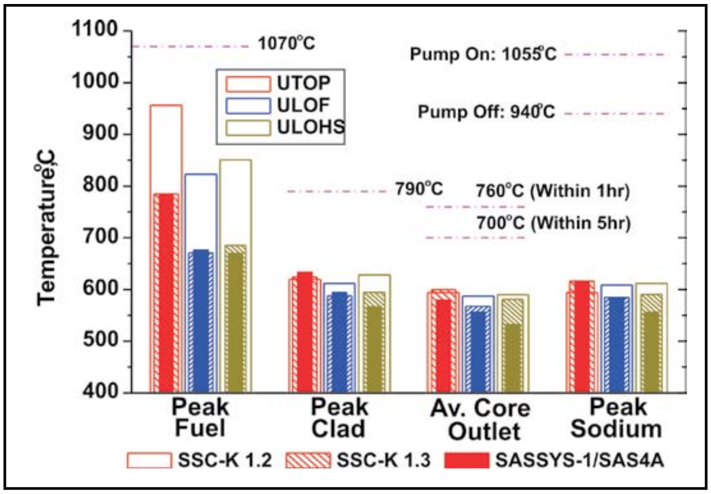

Figure 2. Summary of peak temperatures calculated by SASSYS-1 and SSC-K.

potential safety margin enhancements possible in a sodium-cooled, metal-fueled reactor design by using passive safety mechanisms to mitigate low-probability accident consequences. The project included baseline analyses using state-of-the-art computational models and advanced analyses using the new model developed in Task 1, as well as evaluation of passive safety design feature enhancements. Figure 2 shows the results of analyses of unprotected transient overpower (UTOP), loss of flow (ULOF), and loss of heat sink (ULOHS) accidents in an advanced reactor design using the KAERI SSC-K and ANL SASSYS-1 computer codes. The results indicate the high degree of self-protection available with sodium-cooled, metallic-fueled reactor designs during beyond-design basis accidents in which the plant safety systems fail.

In Task 3, the team investigated supercritical CO_2 gas turbine Brayton cycles coupled to the sodium-cooled reactors to discover new designs for high-efficiency electricity production. The objective of the analyses was to characterize the design and safety performance of equipment needed to implement the new power cycle. The project included considerations of heat transfer and power conversion system arrangements and evaluations of systems performance, as well as assessments of innovative concepts for sodium-to-CO_2 heat exchangers. Figure 3 provides a plant schematic for an optimized plant cycle arrangement.

In Task 4, the researchers developed test plans to measure phenomenological data needed for evaluation of

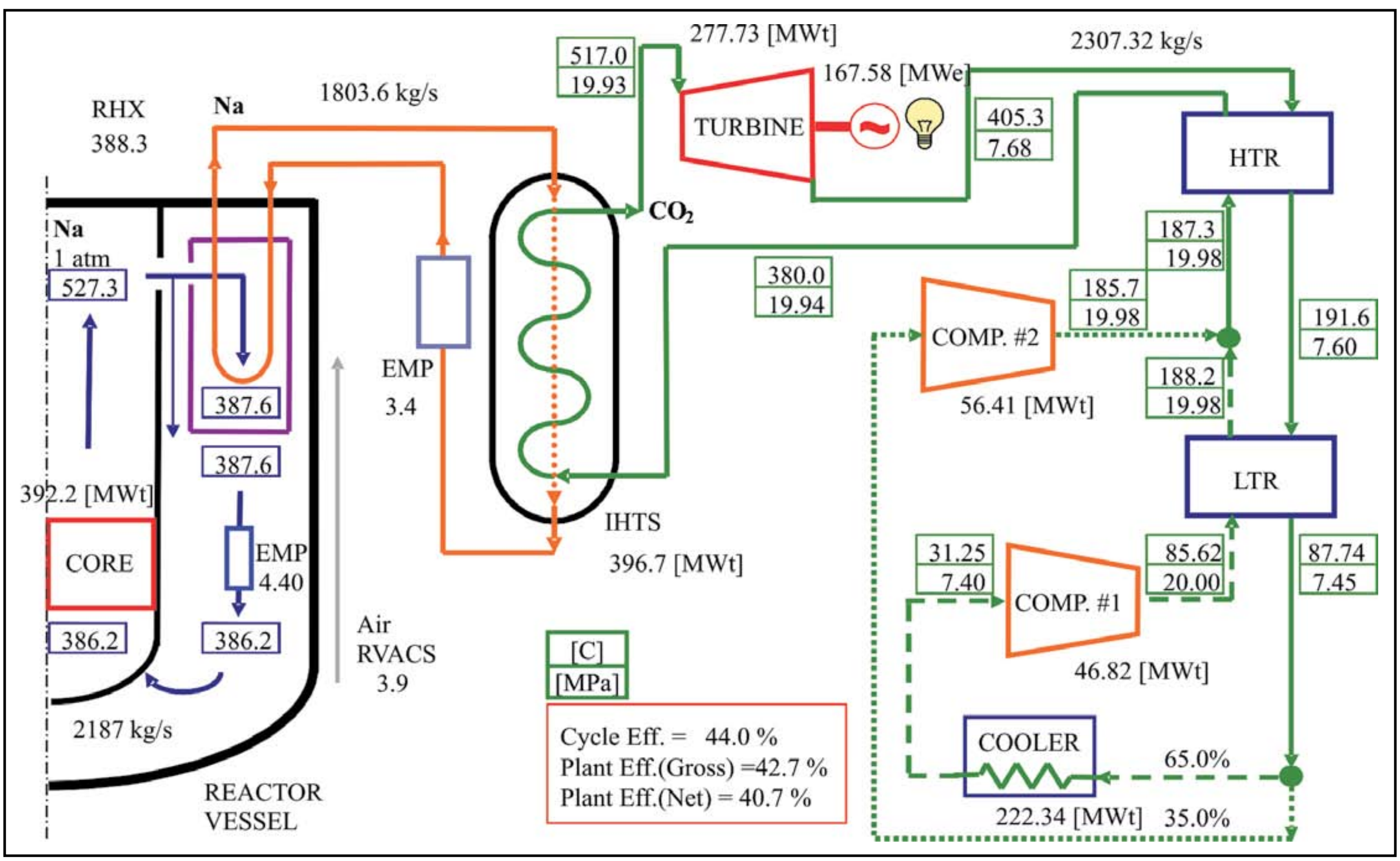

Figure 3. Schematic of supercritical CO_2 Brayton cycle coupled to a sodium-cooled reactor.

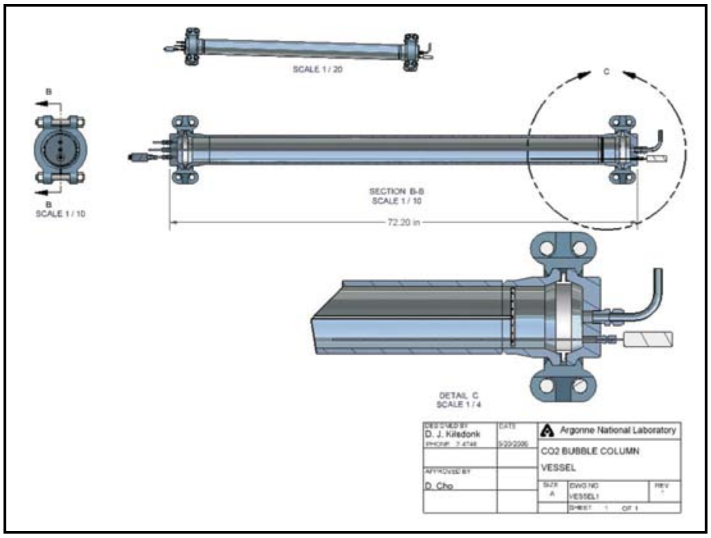

Figure 4. Test section for CO_2/sodium interaction measurements.

very low probability accident sequences unique to metallic fuel and CO_2 Brayton power cycles. The objective of the test plan was to provide all the planning necessary to conduct tests for measuring 1) freezing behavior of molten metallic fuel, 2) molten fuel relocation and interaction behavior with steel structures, and 3) mixing and interaction behavior of high-pressure CO_2 and liquid sodium. The project produced three test plans ready for execution. Figure 4 shows a drawing of the test section designed for investigating the injection of high-pressure CO_2 into liquid sodium.

Planned Activities

This project is complete. The collaboration concluded in December 2005.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Developing and Evaluating Candidate Materials for Generation IV Supercritical Water-Cooled Reactors

PI (U.S.): J. I. Cole, Idaho National Laboratory

PI (Korea): J. Jang, Korea Atomic Energy Research Institute (KAERI)

Collaborators: University of Michigan, University of Wisconsin, Korea Advanced Institute for Science and Technology

Project Number: 2003-008-K

Project Start Date: January 2003

Project End Date: December 2005

Research Objectives

The Generation IV Supercritical Water Reactor (SCWR) is being proposed as an advanced high-efficiency thermal reactor for baseload electricity production. One of the major unknowns with this reactor concept is the behavior of fuel cladding and structural components under the extremely aggressive supercritical water (SCW) environment. The objective of this project was to evaluate candidate materials for SCWR application. The work included efforts to evaluate alloys in terms of high-temperature mechanical properties, resistance to corrosion and stress corrosion cracking, radiation stability, and weldability. Two anticipated outcomes of the project were the production of information that can ultimately be used by SCWR system designers and guidance for future investigations involving in-reactor irradiation experiments. A chart of the sequence of project objectives is shown in Figure 1.

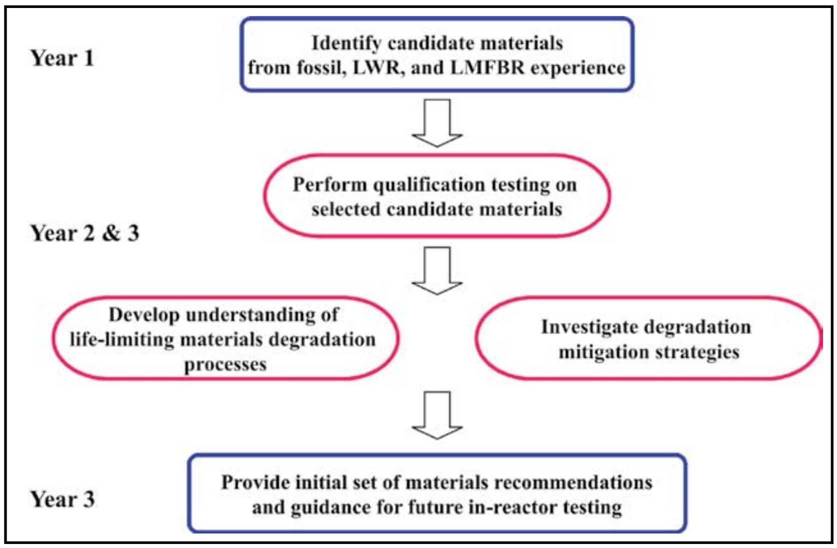

Figure 1. Chart of project objectives and research progress.

Research Progress

Over the last year of this effort, the research team conducted qualifications tests in several key areas where potential materials properties limitations may be encountered in the SCWR. The following sections, separated by task, highlight activities conducted and important results obtained.

High-Temperature Tensile and Creep Behavior. In order to evaluate the effects of the projected SCWR transient on the microstructure and properties of ferritic martensitic (F-M) steels, researchers subjected two representative alloys—modified 9Cr-1Mo-V (ASME Grade 91 steel) and HCM12A (ASME Grade 122 steel)—to a transient thermal cycle using a Gleeble thermal weld simulator to assess their microstructures, tensile properties, and creep properties. Different combinations of maximum transient temperature and number of transient cycles were first evaluated by microstructural analysis and hardness measurements, as reported in last year's annual report.

While the short-term transients up to 845°C did not appear to significantly affect properties, a marked increase in hardness and reduction in rupture life was found when the maximum cycle temperature increased from 860 to 870°C. Similarly, hardness increased and rupture life was reduced when hold times exceeded 10 seconds at 840°C.

Researchers also investigated high-temperature thermal properties for the modified 9Cr-1Mo-V and HCM12A alloys. They applied two methods available at Idaho National

Laboratory's (INL's) High Temperature Test Laboratory (HTTL) to estimate thermal diffusivity, thermal conductivity, and specific heat capacity.

Corrosion and Stress-Corrosion Cracking. The project has obtained substantial amount of corrosion and stress corrosion cracking (SCC) data. Three separate supercritical water corrosion and two separate SCC facilities were utilized for evaluating and qualifying the candidate alloys.

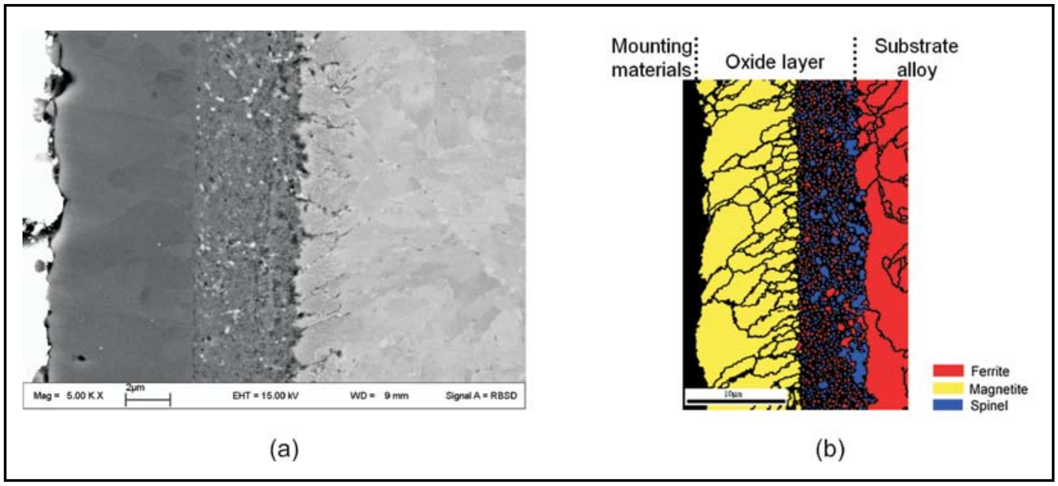

Figure 2. a) SEM image of oxide on surface of alloy HCM12A; b) EBSD generated image of corrosion oxide on surface of F-M alloy NF616. Grain boundaries are indicated by black curves.

Researchers conducted corrosion tests in supercritical water in the temperature range 350 to 550°C in both deaerated and non-deaerated water having various oxygen levels up to approximately 3,000 ppb. Samples were also SCC tested following exposure to high energy protons to emulate radiation damage that will be encountered in service. Overall, alloy HCM12A (12 percent Cr) oxidized less than T91 (9 percent Cr) in all environments. In addition, samples exposed to 100 ppb oxygen had a lower rate of oxidation than in the deaerated case. Researchers believe that the lower oxidation rate in the higher oxygen content supercritical water is due to the formation of a hematite (Fe_2O_3) layer in addition to magnetite (Fe_3O_4), which promotes a dense less permeable surface oxide thereby reducing corrosion. Tests conducted on the irradiated samples revealed the F-M alloys are highly resistant to SCC following irradiation. The results of these experiments indicated that, as with currently operating light water reactors and fossil plants, controlling water chemistry can be critical to minimizing internals degradation due to corrosion and stress corrosion cracking.

In another series of experiments, the corrosion and SCC susceptibility of alloys was tested following plasma source ion implantation. Results indicated that such surface modification can result in a lower rate of surface oxidation (as measured by weight gain) during long-term exposure tests. Detailed analysis to elucidate the mechanism of such changes in corrosion behavior revealed changes in formation morphology of the oxide on the surface of the implanted alloys versus the un-implanted alloys. Researchers measured these changes by examining the samples using electron backscatter diffraction (EBSD) in the scanning electron microscope to identify the spatial distribution of oxide phases forming on the surface of the alloys during exposure. An example of this analysis is shown in Figure 2.

Radiation Stability. F-M alloys T91 and HCM12 samples irradiated to 7 dpa using 2 MeV protons at 400°C were characterized using transmission electron microscopy. The microstructure of the irradiated alloy T91 contained dislocation loops, black dot damage, and precipitates. Alloy HCM12A contained these features as well as a population of voids. In addition to the microstructural analysis, researchers conducted grain boundary chemistry measurements on alloy T91. These measurements indicated a strong enrichment of chromium and depletion of iron at the grain boundary.

Planned Activities

This project continues through the end of calendar year 2005. Researchers will complete their efforts to retrieve additional candidate alloys which have been irradiated in the Advanced Test Reactor (ATR) in order to provide comparison to the proton and heavy-ion irradiation studies. Other remaining tasks include compiling the qualification

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Development of Safety Analysis Codes and Experimental Validation for a Very-High-Temperature Gas-Cooled Reactor

PI (U.S.): C. Oh, Idaho National Laboratory

PI (Korea): H. C. No, Republic of Korea Advanced Institute of Science and Technology (KAIST)

Collaborators: Seoul National University, University of Michigan

Project Number: 2003-013-K

Project Start Date: January 2003

Project End Date: December 2005

Research Objectives

The very high temperature gas-cooled reactor (VHTGR), operating with average coolant temperatures above 900°C or fuel temperatures above 1,250°C, provides the potential for increased energy conversion efficiency, high-temperature process heat application, power generation, and nuclear hydrogen generation. While all the HTGR concepts have sufficiently high temperatures to support process heat applications, such as desalination and cogeneration, the VHTGR's higher temperatures are also suitable for applications such as thermochemical hydrogen production. However, the very high-temperature operation can compromise safety following a loss-of-coolant accident (LOCA) initiated by pipe breaks caused by seismic or other events. Following the loss of coolant through the break and coolant depressurization, air from the containment will enter the core by molecular diffusion and ultimately by natural convection, leading to oxidation of the in-core graphite structures and fuel. This oxidation will release heat and accelerate the heatup of the reactor core.

Thus, without any effective countermeasures, a pipe break may lead to significant fuel damage and fission product release. The Idaho National Laboratory (INL) has investigated this event for the past three years for the HTGR. However, no available computer codes have been sufficiently developed and validated to reliably predict this event. New code development, improvement of the existing codes, and experimental validation are imperative to reducing the uncertainties in predicting this type of accident.

The objectives of this Korean/United States collaboration were to develop advanced computational methods for VHTGR safety analysis and to validate these computer codes.

Research Progress

This project consisted of six tasks for developing, improving, and validating computer codes for analyzing the VHGTR. These tasks were to: 1) develop a computational fluid dynamics code for benchmarking, 2) perform a reactor cavity cooling system (RCCS) experiment, 3) perform an air ingress experiment, 4) improve the system analysis codes RELAP5/ATHENA and MELCOR, and 5) develop an advanced neutronic model and 6) perform computer code verification and validation (V&V) was addressed within each task, as necessary. The primary activities and key accomplishments for each task are summarized below.

Task 1 – CFD thermal hydraulic benchmark code development. Researchers developed a multi-dimensional gas multi-component mixture analysis code (GAMMA) to predict the thermo-fluid and chemical reaction within a multi-component mixture system of an HTGR during an air/water ingress accident. The multi-dimensional governing equations consist of the basic equations for continuity, momentum conservation, energy conservation of the gas mixture, and the mass conservation of each species. GAMMA has the capability to handle the multi-dimensional convection and conduction behaviors as well as heat transfer within the solid components, free and forced convection between a solid and a fluid, and radiative heat transfer between the solid surfaces. Its basic equations are formulated with a porous media model to consider a pebble bed-type HTGR. Researchers performed the code V&V simulations for the various experiments and benchmark tests ranging from the basic simple problems to the integral test problems on the molecular diffusion, graphite oxidation, air ingress, heat transport in a pebble-bed, and the reactor cavity cooling system, etc. As a final step, they applied the GAMMA code to assess the system behaviors during the air ingress accident following the complete break of main pipes.

The researchers first performed the chemical reaction test for the VELUNA pebble oxidation experiment in order to select proper reaction models and then analyzed the air ingress accident for the 268 MW_{th} Pebble Bed Modular Reactor (PBMR). In the GAMMA analysis, significant rise in pebble temperature was observed at the bottom of the core due to graphite oxidation. Since the air ingress process depends on the vault conditions, further analysis coupled with more detailed vault or containment modeling would be necessary as a future study. As a further plant application of the GAMMA code, the researchers conducted two additional analyses - the International Atomic Energy Agency Gas-Turbine-Modular Helium Reactor (IAEA GT-MHR) benchmark calculation for the low pressure conduction cooldown (LPCC) accident, and an air ingress analysis for the 600 MW_{th} Prismatic Modular Reactor (PMR). Refer to Figure 1. The GAMMA code shows a comparable peak fuel temperature trend compared to results using computer codes of other countries. The analysis result for air ingress shows a much different trend from that of previous PBR analyses - later onset of natural circulation and a less significant rise in graphite temperature.

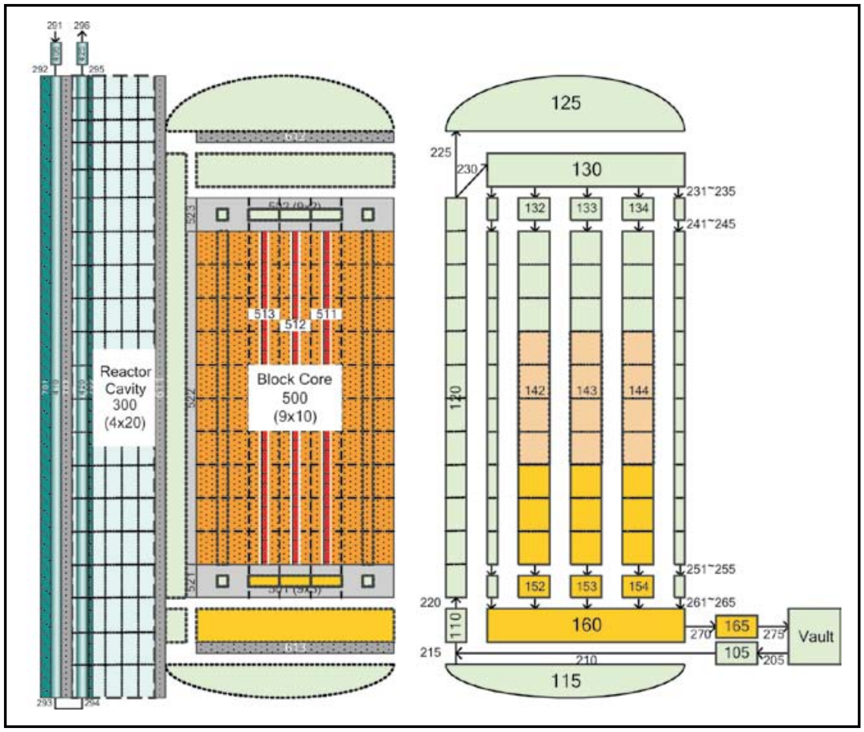

Figure 1. GAMMA nodalization for PMR 600 MW_{th}: solid and reactor cavity (left) and fluid component connection (right).

Task 2 – RCCS experiment. Researchers proposed a new kind of water pool reactor cavity cooling system (RCCS) to overcome the disadvantages of previous systems; specifically, the weak cooling ability of an air-cooled RCCS and the complex structure of a water-cooled RCCS. To estimate the feasibility of the system, they performed a series of experiments simulating the HTGR reactor vessel, cavity, and RCCS.

At first, separate effects tests for emissivity measurement were carried out to develop the testing method using an infrared thermometer in the RCCS environment. Then, the separate effects tests for water pool were performed with two different test devices (Figure 2). The objectives of this test were to investigate the heat transfer phenomena in both of the water pool and cooling pipe and the pressure drop between the cooling pipe inlet and outlet, especially the multiple U-bend type pipes. From the results, researchers concluded that if the total heat

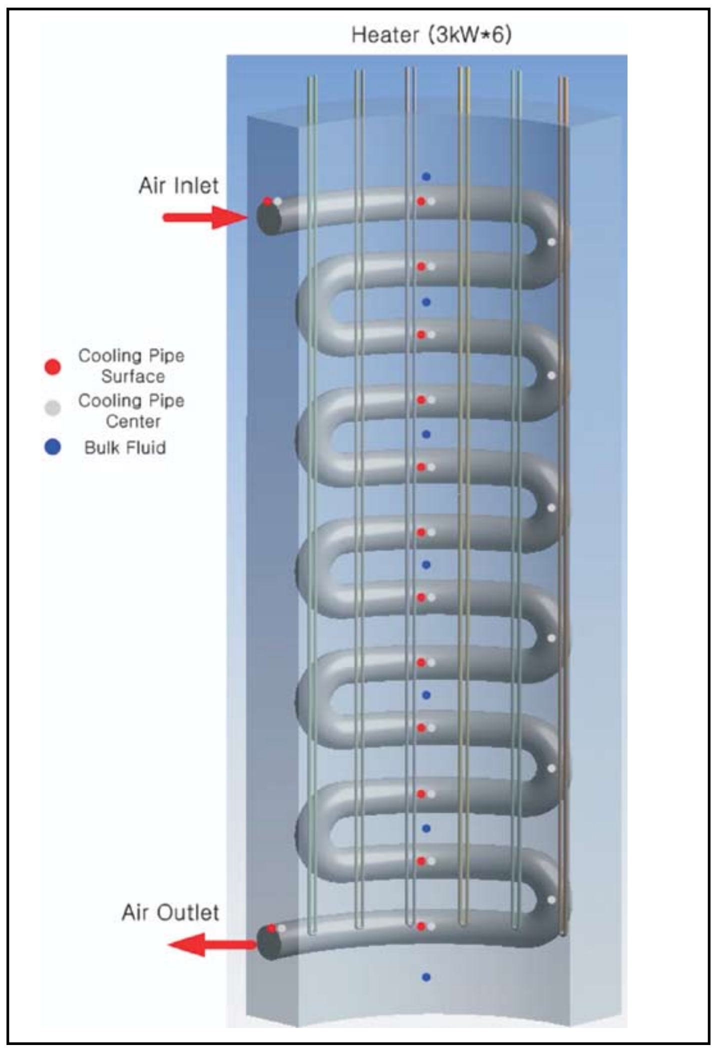

Figure 2. Schematic diagram of the new separate effects test device.

transfer area is preserved, reducing the total number of U-bends is advantageous for pressure drop, as well as heat transfer capability.

Finally, the researchers performed experiments in the SNU-RCCS integral test facility. Three categories of experiments were conducted in SNU-RCCS: normal operation tests, the RCCS active cooling failure test, and the Loss of Forced Convection (LOFC) test. In both the normal operation test and the active cooling failure tests, the maximum temperature of the reactor vessel wall was below the design limitation of the PBMR. From the LOFC experiment, researchers concluded that the passive heat removal capability of the water pool was not significantly retarded by the increase in the area of the uncovered cavity wall until this area attained approximately 12 percent of the total area of the cavity wall.

These experimental results were also used to validate the MARS-GCR code, as well as the thermal hydraulic code developed at KAIST. In addition, code-to-code benchmarks were carried out using CFX and MARS-GCR. Researchers found that MARS-GCR showed good agreement with experimental results at low power cases. However, in cases where the cavity wall temperature was high enough for sub-cooled nucleate boiling to occur, MARS-GCR over-predicted the vapor generation rate. Therefore, it is necessary to develop new correlations or modify existing correlations to precisely model sub-cooled boiling phenomena near the wall of water-pool type RCCS.

Task 3 – Air ingress experiment. In this task, researchers experimentally investigated the geometrical effect, burn-off effect, and minor chemical reactions due to air ingress. To investigate the geometrical effects on nuclear graphite oxidation in the regime where the chemical effect is the rate-controlling process, the concept of internal surface density was introduced into the Arrhenius-type reaction model. Using the 16 different samples of IG-110 graphite, which have different ratios of external surface to volume, the internal surface density was 17,260 m^{-1}. Researchers found that the external surface reaction was very small compared to the total reaction for the IG-110 graphite.

The burn-off effect on the rate of reaction was experimentally investigated and the modeling was performed. As a result, the time variation of the reaction rate was well predicted by the suggested numerical simulation.

Researcher investigated the chemical characteristics of the C/CO_2 reaction (Figure 3), finding that its activation energy was 295±8 kJ/mol and the order of reaction was 0.9. The C/CO_2 reaction rate was much smaller than the rate of the C/O_2 reaction, which was dominant in HTGR air-ingress below 1,400°C. Researchers developed a correlation of the C/CO_2 reaction rate.

Task 4 – Improvement of system codes. Researchers extended the RELAP5/ATHENA code to model the molecular diffusion of several species of gas through

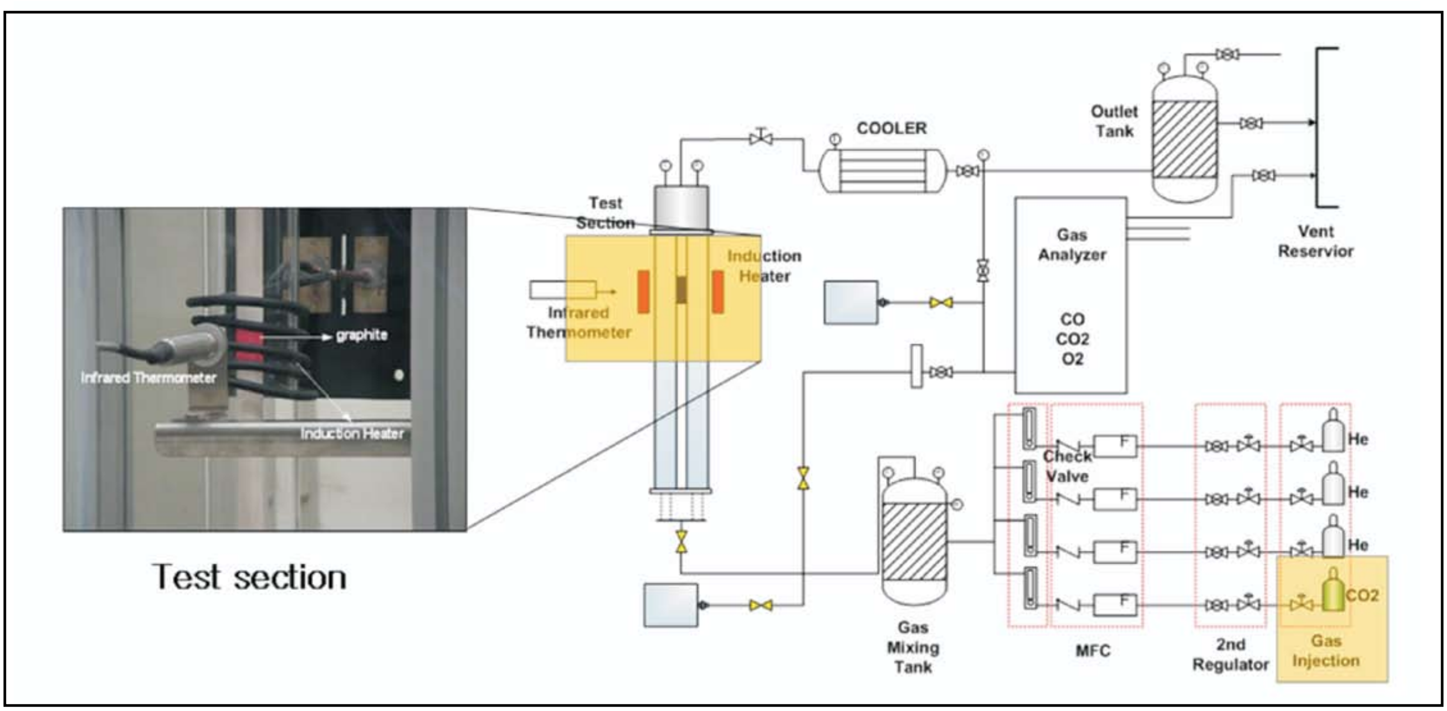

Figure 3. Schematic diagram of C/CO_2 reaction experiment.

a system represented by a general network of control volumes. These control volumes could be connected to several other control volumes on the inlet and outlet sides. Previously, the molecular diffusion modeling was applicable only to a gas mixture with two species of gas and to a pipe where each control volume was connected to only one control volume at each end. The extended code can model the molecular diffusion of up to five species of gas (He, N_2, O_2, CO_2, and CO) and any individual control volume may be connected up to 12 control volumes on either its inlet or outlet sides. Assessment of the updated RELAP5/ATHENA code was performed and the assessment of the diffusion modeling in the RELAP5/ATHENA code indicated correct modeling for a general system containing several species of gases. The Multiple Junction Test Problem showed correct modeling of diffusion in a network of control volumes with multiple inlet and outlet junctions. The Bulb Experiment Test Problem revealed that the calculated and measured results were in fair to good agreement for diffusion in a system with three species of gas and involving, for a period of time, the special case of diffusion against the concentration gradient.

Task 5 – Neutronic modeling. Researchers also made substantial progress in completing a full-core model of the VHTR. A neutronic model for particle fuel has been created and tested that accounts for the double heterogeneity posed by the particle fuel and is valid at all levels of analysis, from a microsphere cell to full core. They demonstrated that a two-region model of the six-region microsphere cell is an excellent model. They also examined the effect of "clipping" fuel particles on the surface of the compact cell and developed two approaches to eliminate clipped cells, which are artificial and have a substantial effect on the neutronic results. The researchers preferred model preserved the packing fraction of the particle fuel, resulted in no clipped particles, and maintained a simple cubic lattice within the compact fuel region. In addition, the research team completed the thermal/hydraulic feedback model and used this model to obtain a converged flux-power distribution for a full-core configuration at beginning of life. This will soon be extended to depletion with temperature feedback. Finally, researchers made substantial progress toward the goal of performing full-core depletion calculations with Monte Carlo, a necessary step to predicting the decay heat production source in the reactor. A preliminary full-core MONTEBURNS depletion with a constant temperature (900K) throughout the core has been completed using the team's parallel version of MONTEBURNS. This was used to predict the decay heat production source in the core as a function of burnup.

Planned Activities

This I-NERI project is complete.

International Nuclear Energy Research Initiative

Advanced Corrosion-Resistant Zirconium Alloys For High Burnup and Generation IV Applications

PI (U.S.): A. T. Motta, The Pennsylvania State University

PI (Korea): Y. H. Jeong, Korea Atomic Energy Research Institute (KAERI)

Collaborators: Westinghouse, University of Michigan, and Hanyang University

Project Number: 2003-020-K

Project Start Date: February 2003

Project End Date: July 2006

Research Objectives

The objective of this project is twofold:

- To demonstrate a technical basis for improving the corrosion resistance of zirconium-based alloys in the extreme operating environments present in severe duty fuel cycles (high burnup, boiling, and aggressive chemistry)
- To investigate the suitability of using advanced zirconium-based alloys in a supercritical water environment from a corrosion perspective

Researchers will compare corrosion kinetics and examine the fine structure of oxide layers formed in model alloys. These model alloys are designed to isolate specific features of the microstructure thought to affect formation of the protective oxide layer so that their effect on the corrosion rate can be studied individually.

A key aspect of the program is to rationalize the differences in corrosion kinetics between alloys through the differences in the structure and evolution of the protective oxide formed in each alloy. To find these structural differences in the oxides, the researchers will use advanced techniques to characterize both the metal and the oxide in order to relate differences in oxide structure to the original alloy microstructure. Characterization techniques include submicron-beam synchrotron radiation diffraction and fluorescence, cross sectional transmission electron microscopy (TEM), transmitted light optical microscopy, and nano-indentation.

This project consists of five tasks: 1) fabrication of model alloys, 2) autoclave testing, 3) testing in supercritical water, 4) characterization of alloys and oxide layers, and 5) data analysis and modeling.

Research Progress

Researchers have fabricated approximately 30 zirconium-based model alloys and conducted high-temperature corrosion testing. Three independent laboratories performed long-exposure testing in the following supercritical water (SCW), steam, or water environments:

- 150 days in a 500°C SCW flowing (dynamic) system and close to a year in a 500°C SCW static system, both at 24.13 MPa (3,500 psi)
- 240 days in a 500°C steam static system at 10.34 MPa (1,500 psi)
- 360°C in water for over one year

They are continuing to perform additional corrosion testing in pure water at 360°C and in supercritical water. Oxide characterization is currently underway on many corrosion samples that had been archived. The test results, as follows, show a range of corrosion behavior depending on the alloy composition:

- About half showed poor, non-protective corrosion behavior
- Approximately 10 alloys exhibited reasonable behavior (stable, protective oxide, but with higher rates)
- Six have shown excellent behavior (protective stable oxide, low rates, no breakaway)

Figure 1 shows the weight gain versus exposure time for the tests conducted on the lowest corrosion rate zirconium (Zr) alloys in this study, compared to those obtained for ferritic-martensitic and austenitic alloys that are also under consideration for the SCWR. It is clear from the plot that the three autoclave conditions (shown in different shades

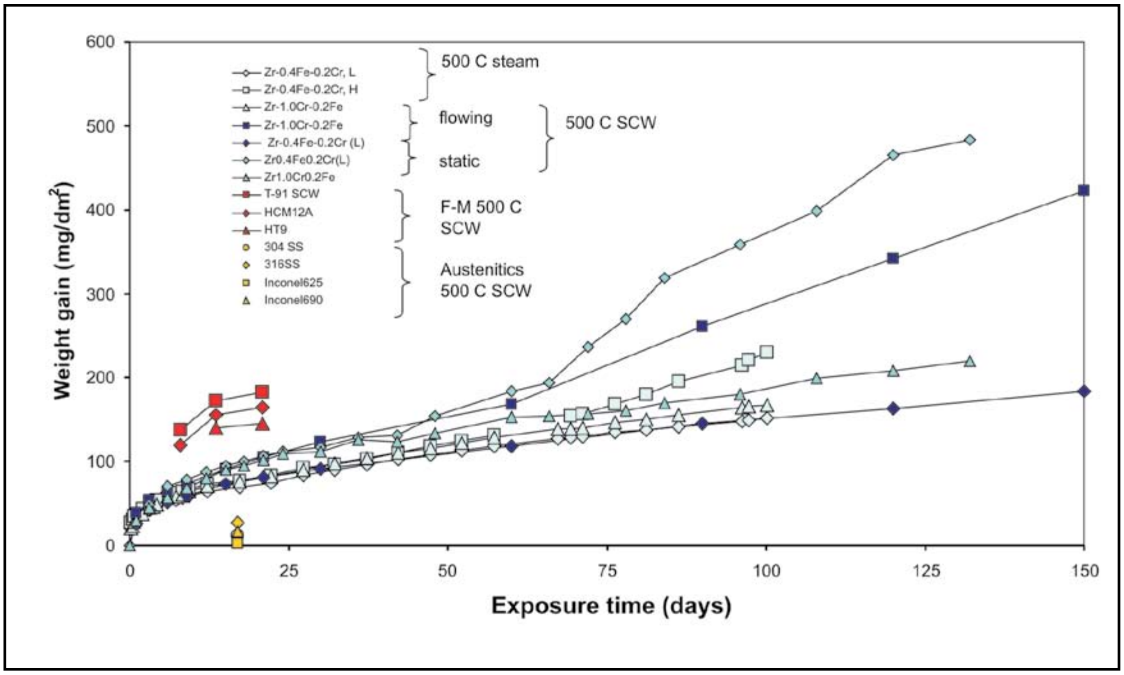

Figure 1. Weight gain versus exposure time for zirconium based model alloys tested in this program compared to ferritic-martensitic and austenitic alloys corrosion data from other programs.[1]

of blue) give very similar results. Results were consistent between static and dynamic autoclaves and showed a slightly higher rate in 500°C SCW as compared to 500°C steam. This suggests that static autoclave tests can be used to assess corrosion behavior at high temperature and that 500°C steam tests can be used as an effective screening test. For each alloy, the results were very reproducible from sample to sample and between laboratories. It is also clear that the corrosion rates for the best Zr alloys are higher than austenitic alloys and lower than ferritic-martensitic alloys.

These results also indicate that the alloy composition and microstructure are predominant in determining corrosion behavior. In general, the best alloys were from the ZrCrFe system (which also behaved the best in a 360°C water corrosion test). Higher alloying content improved corrosion resistance. The key to good corrosion resistance is to avoid breakaway corrosion and to maintain a stable, protective oxide. The onset of breakaway often occurs after long exposure times, which indicates that short exposure tests may be inadequate for determining corrosion behavior at high temperature.

To rationalize the differences in corrosion behavior, a concerted effort is underway to identify differences in oxide microstructure that cause the differences in corrosion behavior. The oxide layers in protective and non-protective oxides have been examined with a variety of techniques, including scanning and transmission electron microscopy. The samples have also been examined using synchrotron radiation diffraction to determine the phases present and the crystallographic texture of the oxide layer.

Using synchrotron radiation diffraction at the Advanced Photon Source (APS) at Argonne, with diffraction image plates, it is possible to obtain complete pole figures from thin oxide layers in a matter of a few hours. A series of samples taken from the corrosion testing in this program was examined at APS. Preliminary analysis shows that a fiber texture is better developed in the slower growing oxide than in the fast growing one. Similar pole figures were obtained for five poles of the monoclinic oxide phase (-111, 111, 200, 002 and -201) and for one pole of the tetragonal oxide phase (101) for the model alloy oxides created in this study, both for oxides formed at 500°C and at 360°C. The results are currently under analysis.

Microbeam synchrotron radiation diffraction examination of cross sectional samples of oxide layers at APS revealed the phases present, their crystallographic texture, and their orientation relationship to the matrix as a function of distance from the oxide-metal interface with a resolution of 0.2 microns. Figure 2 shows an example of a series of diffraction patterns taken from one of the model alloys in this study. Similar series were taken of most other alloys in this program, both at 360 and at 500°C. Successive diffraction patterns are obtained by placing the beam at different locations in the oxide layer in 0.2 micron intervals. The dotted line indicates the location of the oxide-metal

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1 G. S. Was and T. R. Allen, "Time, Temperature, and Dissolved Oxygen Dependence of Oxidation in Austenitic and Ferritic-Martensitic Alloys in Supercritical Water," International Congress on Advances in Nuclear Power Plants, Seoul, Korea, 2005.

G. S. Was, S. Teysseyre, and J. McKinley, "Corrosion and Stress Corrosion Cracking of Iron and Ni Base Austenitic Alloys in Supercritical Water," Corrosion 2004, New Orleans, 2004, NACE International, paper # 4492.

Y. H. Jeong, et al., "Corrosion of zirconium based fuel cladding alloys in supercritical water," Proceedings of the 12th International Conference on Environmental Degradation of Materials in Nuclear Systems—Water Reactors, TMS, 2005 interface. Although the results are under analysis, it is possible to discern small hydride peaks ahead of the oxide-metal interface, as well as a different structure near the oxide-metal interface from that of the bulk metal and the bulk oxide [especially around the (200) family monoclinic oxide peaks at 29 two-theta]. This indicates that the newly formed oxide has a different structure than the rest of the oxide layer. Such detailed structural information should yield clues about the oxide layer growth. Researchers expect that these oxide-metal interface structures will be different from alloy to alloy, helping explain the difference in corrosion behavior among these alloys.

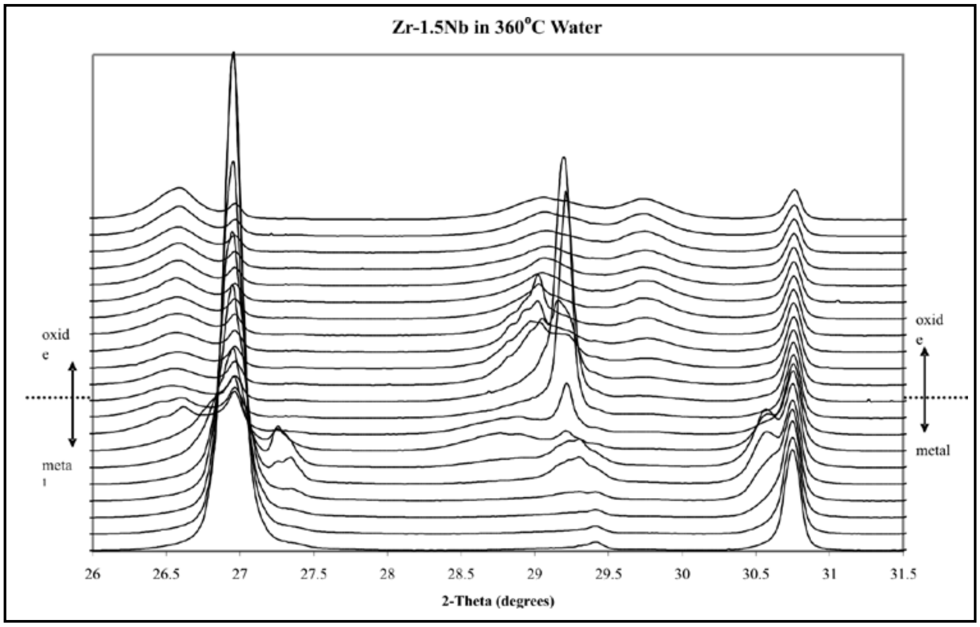

Figure 2. A series of diffraction patterns (intensity versus two-theta diffraction angle) obtained from a cross-sectional sample of Zr-1.5Nb oxide layer, using microbeam synchrotron radiation diffraction by placing the beam at different locations across the oxide-metal interface.

Planned Activities

The research team received a no-cost extension until July 31, 2006. This will allow them to perform more detailed analysis on the reasons for the different behaviors observed for the model alloys, thus paving the way for the design of better alloys for higher burnup. They also expect to have completed an initial assessment of the corrosion behavior of Zr-based alloys in high-temperature water. It is expected that the final report will contain an assessment of the behavior of Zr alloy in uniform corrosion in supercritical water and an assessment of the reasons for the differentiated behavior of different model alloys in low-temperature water.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Development of Structural Materials to Enable the Electrochemical Reduction of Spent Oxide Nuclear Fuel in a Molten Salt Electrolyte

PI (U.S.): C. T. Snyder, Argonne National Laboratory

PI (Korea): J. Hur, Korea Atomic Energy Institute (KAERI)

Collaborator: University of Illinois, Chicago

Project Number: 2003-024-K

Project Start Date: March 2003

Project End Date: December 2005

Research Objectives

The objective of this ANL and KAERI-led collaborative project was to develop advanced structural materials for use in a new technology that would enable the electrolytic reduction of spent nuclear fuel in a molten salt electrolyte. The effort included selecting and testing commercial alloys and ceramics as well as engineering and testing customized materials systems. The principal objectives of this project were 1) to assess and select candidate materials for service in the electrolyte reduction process and 2) to develop new candidate material systems (e.g., functional barrier coatings) for service in the electrochemical reduction process vessel.

Coating Technique	Bond Coating	Surface Coating	Vendor
Plasma Spray	Ni	None	Vartech, Inc. Idaho Falls, ID
	Ni-20Cr	None	Vartech, Inc. Idaho Falls, ID
	Ni-20Al	None	State University of New York at Stony Brook Stony Brook, NY
	Ni-22Cr-10Al-1.0 Y	None	State University of New York at Stony Brook Stony Brook, NY
	Ni	Y_2O_3	State University of New York at Stony Brook Stony Brook, NY
	Ni	$MgZrO_3$	State University of New York at Stony Brook Stony Brook, NY
	Ni	ZrO_2-13 Y_2O_3	State University of New York at Stony Brook Stony Brook, NY
	Ni	ZrO_2-13 Y_2O_3	State University of New York at Stony Brook Stony Brook, NY
PVD	None	AlTiN*	Balzer Tool Company Elgin, IL
	None	TiAlN*	National Coating Technology Northbrook, IL

The metal listed first for AlTiN and TiAlN has the greater concentration, resulting in differing material properties.

Table 1. Coating composition.

Research Progress

Research progress in 2005 began with corrosion testing of coated sample coupons. Eight coatings were applied by plasma spraying and two coatings were applied by physical vapor deposition (PVD). Of these 10 samples, four coatings were plasma-sprayed with a double layer, while the remaining six coatings consisted of a single layer. The double layer consisted of a nickel bond coat applied to the base alloy and a topcoat applied to the nickel layer, as shown in Table 1. The coated coupons were evaluated using the same test conditions as the metal alloys. The corrosion tests were performed for nine days at 675°C using 3 percent Li_2O in LiCl molten salt mixture, with a 10 percent O_2 in argon gas mixture flowing at 3 mL/min. These conditions best represent the expected environment during operation. During this initial evaluation of coatings, 316L stainless steel coupons were used as the metal substrate due to cost considerations and lack of immediate availability of nickel superalloy coupons.

Complete coatings analyses comprised evaluating each coating after corrosion testing and reporting on performance and corrosion protection. All coatings were sectioned after washing, placed on sample mounts, and examined by metallography and scanning electron microscopy (SEM). In addition, energy dispersive X-ray spectroscopy (EDS) and X-ray diffraction were utilized as necessary to adequately assess corrosion products.

Post-corrosion test results from the plasma spray technique are summarized below:

Nickel Coating. Microscopic evaluation of the post-corrosion nickel coating revealed a highly porous layer with partial detachment from the underlying stainless steel. The separation appeared to have been a result of the extensive corrosion of the nickel-stainless steel interface which extended into the SS substrate regardless of whether the nickel coating was attached or not.

Ni-20% Cr Coating. Post-corrosion examination revealed almost complete coating detachment from most of the surface of the sample offering minimal protection to the underlying SS substrate. The cause of the coating layer separation appeared to be the result of preferential corrosion at the Ni-20Cr-316L SS interface while the Ni-20Cr coating itself showed little effect. In addition, the corrosion extended into the 316L stainless steel substrate beneath the Ni-20Cr-316L SS interface.

Ni-20% Al Coating. Macroscopic post-corrosion examination of the coupon revealed that most of the coating was destroyed and corrosion was present in the underlying metal alloy. Even the few areas where the coating remained attached showed severe intergranular corrosion in the stainless steel substrate.

Ni-22% Cr-10% Al-1% Y. The post-corrosion coating appeared extremely porous and had almost entirely separated from the metal substrate. It is likely that the significant porosity in the remaining coating was generated by corrosion. In some areas, the porosity allowed severe localized corrosion of the 316L SS.

Ni Bond + Y_2O_3 Coating. The post-corrosion coating appeared dense and brittle and several deep cracks were evident. In general, there still appeared to be mostly continuous bonding between the yttria top coat and the Ni bond coat, however, there were small areas of discontinuity and porosity. The nickel layer, however, appeared to be almost completely separated from the base alloy. This may be a consequence of poor and/or no metallurgical bonding between the Ni layer and the stainless steel substrate due to the application process, or mismatched coefficients of thermal expansion. Since there was evidence of corrosion scale in some areas of the interface, it was most likely that the detachment was due to preferential corrosion in this area. Fractures noted in the yttria outer coating may have provided a pathway to the nickel layer and allowed the molten salt and oxygen to contact this interior interface. The fissures present in the Y_2O_3 coating contained remnants of the chloride salt and, based on contrast with the surrounding area on SEM micrographs and later confirmation by energy dispersive x-ray spectroscopy (EDS), the residue was found to contain chlorine. Subsequent thermal stress may have contributed to additional fractures in the coating.

Ni bond + $MgZrO_3$ coating. The coating appeared porous and brittle but there was significantly less fissuring and cracking than the Y_2O_3 coating. Corrosion was noted at the Ni-316L SS interface with greater porosity and deeper penetration into the microstructure of the 316L SS substrate. Some of the pores contained fragments of material and EDS analysis of these oxide fragments indicated they were rich in Fe and Ni. The Ni-$MgZrO_3$ interface was also porous and there appeared to be an oxide film formed between the ceramic outer coating and the Ni bond coat.

Ni Bond + ZrO_2-13 Y_2O_3. The test coupon coating that was submerged in the molten salt appeared extremely fractured while the coating remained adherent to the substrate metal on that portion of the coupon not submerged in the salt. The coating and Ni bond coat from the bottom portion of the sample fell away during the wash procedure, exposing the underlying metal substrate and corrosion debris at the surface of the exposed metal. The sample was examined using greater magnification to look at detail of both interfaces. It appeared that the majority of the corrosion had occurred at the Ni bond coat-316L SS interface, but the stainless steel substrate in the areas where cracks in the ceramic outer coating occurred showed corrosion effects as well. It is likely the cracks allowed direct contact of molten salt with the underlying metal substrate.

Ni bond + High Density ZrO_2-13 Y_2O_3. The coating remained intact after corrosion testing and no significant solids were obtained after washing. However, when examined under magnification, cracks extended through the thickness of the top coat which allowed the molten salt to contact the underlying Ni bond coat-metal substrate bond causing extensive corrosion to most of this interface. There appeared to be continuous bonding between the ceramic topcoat and the Ni bond metal. A cross section of the coupon showing the cracks in the outer coating and both interfaces is shown in Figure 1. An EDS analysis of the ceramic coating indicated the presence of oxygen, zirconium, and yttrium, with concentrations of 51.67 weight, 9.98 weight, and 38.35 weight percent, respectively. In the case of the Ni bond coat, the EDS results indicate a composition of 93.33 weight percent of Ni and small fractions of oxygen, carbon, and aluminum.

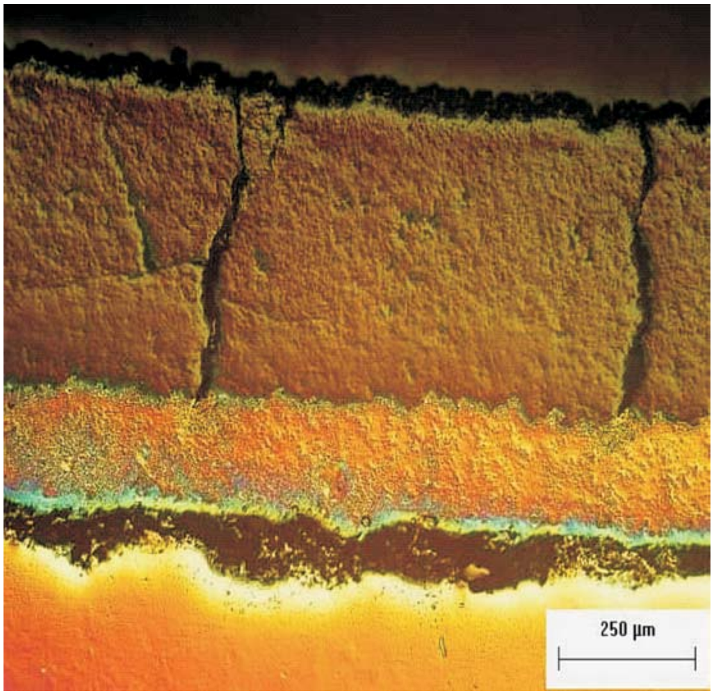

Figure 1. Optical micrograph of coupon # 8 cross section showing fractures through the entire thickness of the outer coating and extensive corrosion along the Ni bond coat-316L SS substrate interface.

Post-corrosion test results from the plasma vapor deposition (PVD) coating technique is listed below for each of the two material types. It should be noted that stoichiometery is shifted toward the first-listed metal and, as a result, each coating has differing physical properties. The exact stoichiometery and processing methods are proprietary.

AlTiN (PVD coating). In general, the post-corrosion coupon showed significant corrosion and no evidence of the PVD AlTiN coating was found. Corrosion products and salt deposits were the only findings on the surface of the coupon. The salt was removed during washing in de-ionized water leaving the corrosion products exposed on the surface. Evaluation of the cross section at higher magnification showed that the coating was definitely not present and the layer attached to the coupon was corrosion scale. At the interface of the corrosion scale with the base metal alloy, significant intergranular corrosion was observed.

TiAlN (PVD coating). The post-corrosion appearance was similar to that of the AlTiN coating. With the exception of a few spots in the area of the coupon immersed into the molten salt, no evidence of the coating was found. Only a few corrosion products and salt deposits were observed on the surface and there was no significant amount of solids collected after washing. Evaluation of the cross section at higher magnification is shown in Figure 2 and

Location	Element (wt. %)			
	O	Cr	Fe	Ni
1 (base metal)	---	27.3	62.3	7.8
2 (light gray oxide strip next to metal)	24.4	---	61.1	13.9
3 (Layered structure)	55.7	---	21.3	12.0
4 (white precipitates in layered structure)	---	78.3	9.2	10.6
5 (white precipitates decorating grain boundary)	---	77.7	8.7	12.4

Table 2. EDS spot locations. Elemental analysis results.

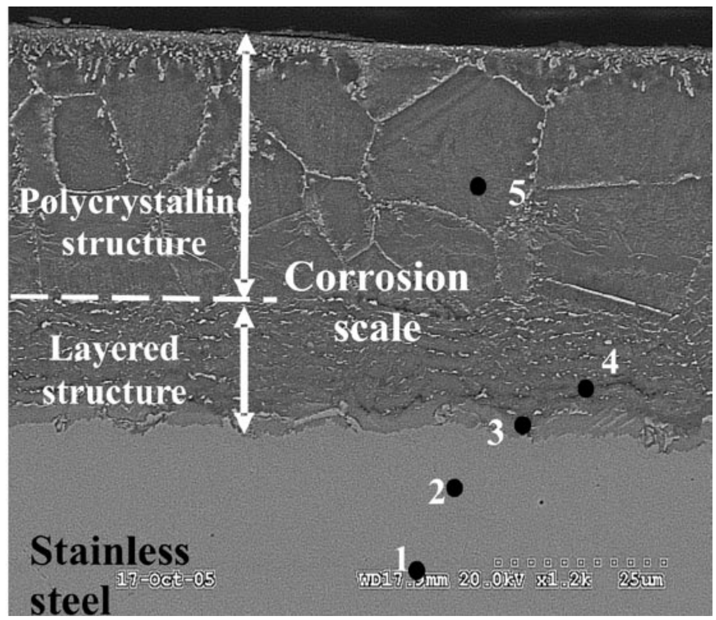

Figure 2. SEM micrograph of coupon # 10 after etching showing the stainless steel and the attached corrosion scale.

revealed a corrosion layer about 80 μm thick attached to the metal substrate surface. The layer appears to be free of defects and have a dual morphology. The top half of the scale is denser and appears to have a polycrystalline structure while the scale adjacent to the stainless steel is amorphous. There is a uniform corrosion front advancing into the stainless steel and no deep localized areas of penetration or intergranular corrosion.

The post-corrosion coupon was later etched with a solution (1:1:1 HCl, HNO_3, deionized H_2O) to reveal the microstructure of the stainless steel. Cavities observed on the scale near the stainless steel suggest that these might have been portions of the metal substrate before conversion to oxides in the scale. EDS spot analyses showed no traces of Al, Ti, or N found near the stainless steel or in the corrosion scale. The elemental analysis results are shown in Table 2, corresponding to the locations identified on Figure 2.

Functional Barrier Coatings. Complete coatings analyses comprised evaluating each coating after corrosion testing and reporting on performance and corrosion protection. All coatings were sectioned after washing, placed on sample mounts, and examined by metallography and SEM. In addition, EDS and X-ray diffraction were utilized as necessary to adequately assess corrosion products. In general, corrosion attack for most of the coated coupons occurred at the substrate-topcoat or Ni bondcoat-substrate interface, resulting in partial or complete coating separation and loss of protection. It was noted that interface adherence between the nickel bondcoat and the topcoat in selected coupons appeared intact for those topcoats containing yttria and zirconia. The most adherent interface appeared to be the nickel bondcoat and the high-density ZrO_2-$13Y_2O_3$ topcoat.

As mentioned previously, pre-corrosion SEM micrographs were performed at INL and are generally at lower magnifications. Any additional analyses, such as X-ray diffraction and EDS, were not performed. More detailed studies are needed before any inferences can be made regarding coating form and structure after the actual deposition on the 316L SS. As such, the pre-corrosion work should be treated as preliminary results.

The ceramic coatings containing zirconia, especially those of higher density, together with Inconel MA 754, Haynes 214, and Haynes HR 160 as substrate alloys, appeared to provide the most corrosion-resistant material system.

Planned Activities

This project was completed on December 31, 2005.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Screening of Gas-Cooled Reactor Thermal-Hydraulic and Safety Analysis Tools and Experiment Database

PI (U.S.): T.Y.C. Wei, Argonne National Laboratory

PI (Korea): W.J. Lee, Korea Atomic Energy Research Institute (KAERI)

Collaborators: Idaho National Laboratory

Project Number: 2004-001-K

Project Start Date: June 2004

Project End Date: May 2007

Research Objectives

This research project supports development of the Very-High-Temperature Reactor (VHTR), one of six reactor technologies under the Generation IV International Forum (GIF). The Department of Energy selected this system to demonstrate the production of hydrogen in conjunction with emission-free electricity. The Korean Ministry of Science and Technology (MOST) also selected the Pebble Bed Reactor (PBR) and Prismatic Modular Reactor (PMR) technologies for further evaluation under their Nuclear Hydrogen Development and Demonstration (NHDD) Project.

This project addresses the thermal-hydraulic and safety analysis capabilities that are to be used in the reactor plant analysis/auditing workscope. Specific objectives of this research are 1) development of a formal qualification framework, 2) initial filtering of the existing databases, and 3) preliminary screening of tools for use in thermal-hydraulics and safety analyses.

Research Progress

Researchers completed work to qualify the methodology. The "top-down" and "bottom-up" qualification methodology has been adapted specifically to the analysis requirements of the gas-cooled reactors designs and the systems that will be analyzed in this I-NERI effort. In particular, the software tools that have been shown to be applicable to the systems under consideration will be compared to the projected system's analysis needs and requirements.

Since this project will use existing software and numerical models for the most part, it will focus on defining and performing adequacy evaluation and acceptance testing, i.e., qualification methodology of the selected software. The elements of the adequacy evaluation and acceptance testing are shown in Figure 1. This adequacy evaluation is a time-honored procedure that has become commonly accepted in the international community as well as the domestic community. The procedure was recently used to determine the adequacy of the tools to calculate the transient behavior of the Westinghouse AP600 advanced reactor system. The methodology has been adapted specifically to the analysis requirements of the gas-cooled reactor designs.

For the Phenomena Identification and Ranking Tables (PIRT) task, the researchers have abstracted the main determinants of phenomenology from the list of duty cycle, design basis, and beyond design basis events to be analyzed in the safety report. The team generated this list in a manner to avoid excluding any possible event. Having listed these event classes, they then examined the key features that describe the reactor's operating regime. They generated tables that provide the values of these features for all classes of duty cycle, design basis, and beyond design basis events. Other tables rearrange this information to show the event classes that fall under each unique set of values for the regime features, and provide a tentative list of the phenomena in the gas reactor, both expected and hypothetical. Researchers developed potential design issues associated with each. A draft list of component classes that align with these key instances of phenomena are also given in the tables.

Researchers linked together all of these tables in an effort to identify the major thermal-hydraulic phenomena modeling required for the development and validation of thermal-hydraulic analysis tools of the VHTR. They have developed preliminary PIRTs for two reference VHTR designs: 1) 600 MW_{th} GT-MHR for the representative prismatic modular reactor (PMR) and 2) 400 MW_{th} PBMR for the representative pebble bed reactor (PBR).

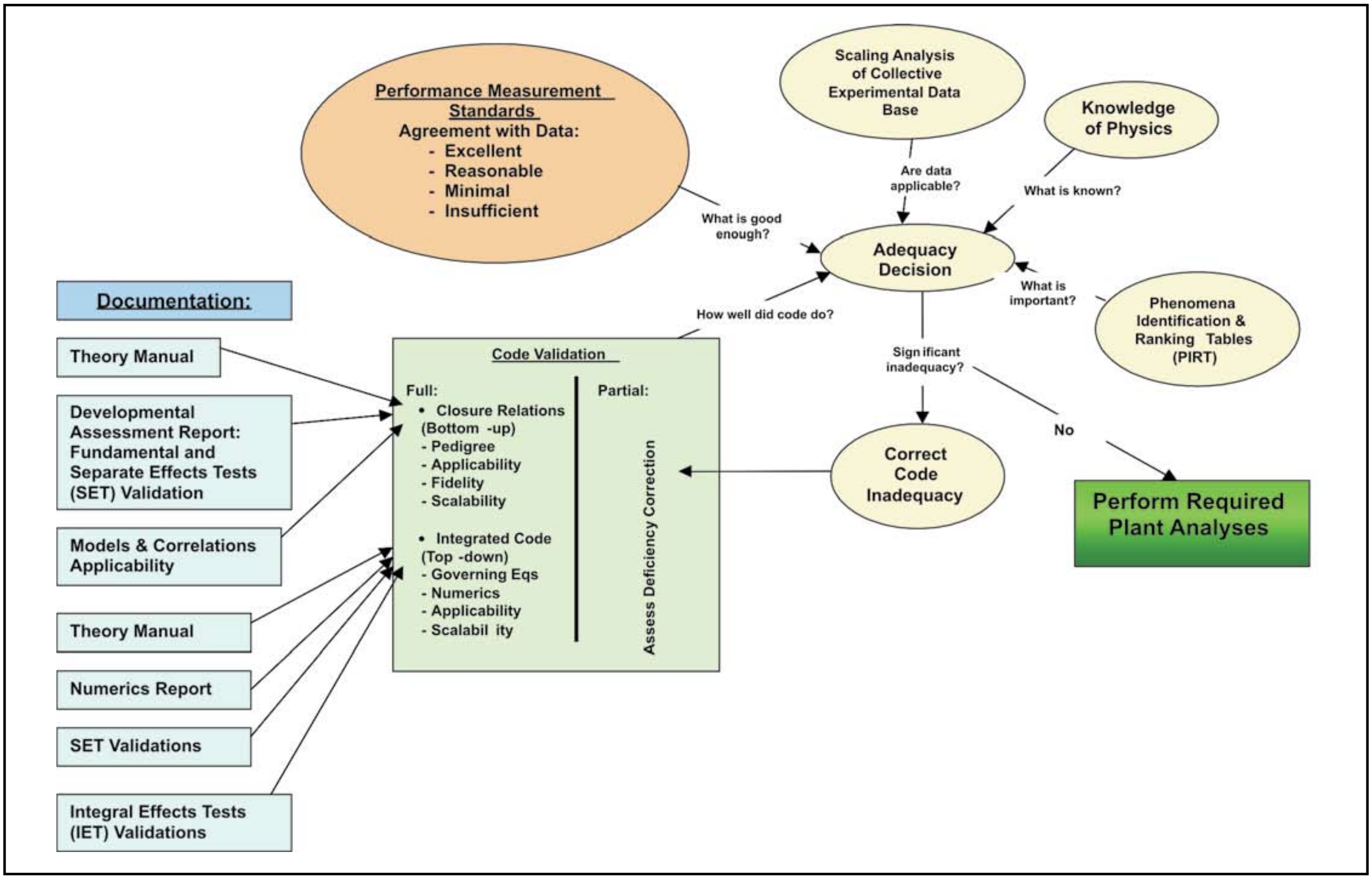

Figure 1. VHTH system design software - elements of adequacy evaluation & acceptance testing practices.

The preliminary PIRTs focus on three highly ranked event scenarios: 1) high-pressure conduction cooling initiated by loss of flow and simultaneous failure of shutdown cooling system, 2) low-pressure conduction cooling initiated by loss of coolant with air-ingress, and 3) load changes including normal operation conditions. In the first two events, a normal reactor shutdown (scram) occurs. Each scenario is subdivided into several time phases reflecting the major thermal-hydraulic characteristics and processes of the event. For each phase, each component of the reference designs is examined to identify the various phenomena. The phenomena were then ranked by separate expert panel groups in Korea and the U.S. with respect to their influence on the selected primary criteria, both safety and non-safety. The Korean experts from KAERI, academia, and industries employed the Analytical Hierarchical Process (AHP) technique. A single consensus ranking was established following a meeting between the two research teams.

The PIRTs generated in this study may also be used to identify the experimental database and further experiment needs as well as qualify the capability of existing analysis tools.

Planned Activities

Following are the remaining tasks for this I-NERI project:

- Perform initial scaling analyses
- Screen the applicability of the existing experimental data base
- Perform scoping calculations

Completion of these tasks is expected to result in identification of the following:

- The systems codes to be used
- The weaknesses or gaps in the code models for representing thermal-hydraulic phenomena expected to occur in the VHTR, both during normal operation and upset conditions
- The models that need to be developed and the supporting experiments
- The semi-scale experiments needed for validating the models

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Investigation of Heat Transfer in Supercritical Fluids for Application to the Generation IV Supercritical Water-Cooled Reactor (SCWR)

PI (U.S.): J. R. Wolf, Idaho National Laboratory

PI (Korea): Y.Y. Bae, Korea Atomic Energy Research Institute (KAERI)

Collaborators: Rensselaer Polytechnic Institute

Project Number: 2004-002-K

Project Start Date: October 2004

Project End Date: September 2007

Research Objectives

Because of the lack of phase change in the supercritical water reactor (SCWR) core, these reactors cannot use design criteria based on critical heat flux, unlike light water reactors (LWRs). The commonly accepted practice is to specify cladding temperature limits that must be met during different transient events. However, little information exists about heat transfer to supercritical water in a reactor environment.

The objectives of this project are: 1) to address the issues associated with measuring heat transfer to supercritical water at prototypical SCWR conditions and 2) to develop tools to predict SCWR thermal transients. In addition to using supercritical water as an experimental medium, researchers will also use surrogate fluids such as CO_2 at supercritical conditions. These alternative fluids will provide valuable insight into the physical phenomena that may be present. Because of their lower critical temperatures and pressures, they can significantly reduce the cost and time to complete the experimental program.

Research Progress

A primary objective of the U.S. effort is to design and construct a bundle test section for installation in the Benson facility supercritical water test loop in Erlangen, Germany.

The research team held a meeting with European and Korean partners to identify requirements and interfaces for the test section. Participants agreed on the basic design concept for the test section. The completed test section design will include four heater rods simulating a section of SCWR fuel bundle, along with channels for moderator flow. The design will be flexible to accept a solid moderator rod, as is planned for the Korean SCWR system. The test section for the Benson Loop supercritical loop is shown in Figure 1 and technical requirements are shown in Table 1.

In 2005, Rensselaer Polytechnic Institute joined the project as a U.S. collaborator. Their efforts over the next few years will focus on developing and applying their NPHASE computational fluid dynamics code to supercritical water analysis.

Korean partners have completed the construction of a CO_2 test facility, which is currently undergoing commissioning to reduce electrical noise and tune the facility. The team initiated testing with the 4.4 mm diameter tube and data collection is underway. They have completed numerical simulation of flow through the 4.4 mm tube and provided information to other members of the team in order to set boundary conditions for additional tests. They have also begun the numerical simulation of CO_2 flow through an 8 mm diameter annular passage that they expect to conclude before the start of single rod testing.

Planned Activities

Researchers will complete the final design of the Benson Loop supercritical water heat transfer test section and begin its fabrication. Fabrication is not expected to be completed until fiscal year 2007. They will apply the NPHASE code for analysis of existing single-tube supercritical water heat transfer experiments as well as begin a scaling study to link analytical test results from surrogate fluid experiments, such as the Koreans are performing, to test data from actual supercritical water experiments.

Researchers will continue their single-rod supercritical CO_2 heat transfer and pressure drop experiments. They have initiated procurement of a single-rod test section, and expect to conduct testing with this section in the first half of 2006. They will also initiate fabrication of a supercritical CO_2 four-rod test section in order to have a direct counterpart to the four-rod supercritical water test facility at INL.

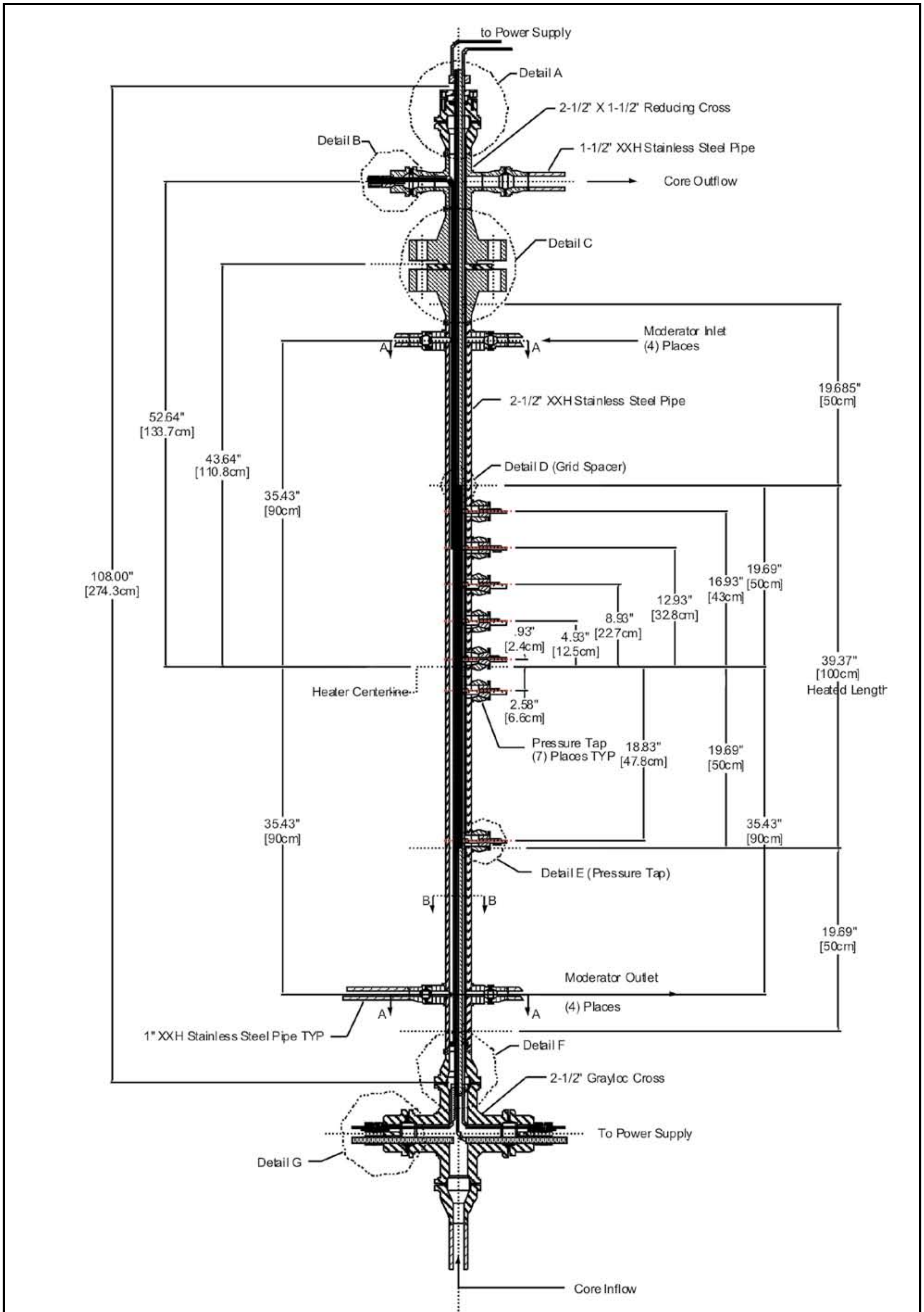

Figure 1. Benson loop supercritical water test section.

Bundle geometry	2x2, square tube insert
Maximum Pressure	25 MPa = 3,625 psia
Test section water inlet temperature (enthalpy window) both for coolant and moderator (individually chosen); two independent moderator flows	280 to 488°C
Maximum test section water outlet temperature	550°C
Maximum test section power flux	1,500 kW/m^2
Heater rod diameter	10 mm or equivalent
Heater rod heated length	1 m
Inlet length (unheated)	0.5m
Outlet length (unheated)	0.5m
Number of spacer grids	3 (at least)
Range of Coolant Mass flux	200 – 1,000 $kg/(m^2s)$
Number of heater rods	4 (one replaceable dummy rod (square))
Rod spacing to diameter ratio (pitch)	1.15
Direct or indirect heated rods	To be decided

Table 1. SCWR Benson loop test section requirements.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Development of Advanced Suite of Deterministic Codes for VHTR Physics Analysis

PI (U.S.): T. A. Taiwo, Argonne National Laboratory

PI (Korea): K. S. Kim, Korea Atomic Energy Research Institute (KAERI)

Collaborators: Seoul National University (SNU)

Project Number: 2004-003-K

Project Start Date: October 2003

Project End Date: September 2006

Research Objectives

The objective of this project is to develop an advanced suite of deterministic computer codes for use in Very High Temperature Reactor (VHTR) design and licensing. Researchers will investigate the capabilities of currently available physics analysis tools, focusing on VHTR modeling requirements. Based on this assessment, they will identify required enhancements to the lattice physics, whole-core, and fuel cycle modeling capabilities. They intend to implement these enhancements by developing an advanced suite of codes based on the conventional two-step lattice and whole-core calculational approach, as applied to block-type VHTR designs. In parallel, the project will seek to adapt the 3-D whole-core transport code DeCART, developed for light water reactor (LWR) applications under a previous I-NERI project, for VHTR analysis. This code eliminates the approximations and laborious multi-group constant generation needed for the two-step approach by representing local heterogeneity explicitly without homogenization. Other code features include using a multigroup cross-section library directly without group condensation and incorporating pin-wise thermal-hydraulic feedback. The team will perform necessary verification and validation tests of the new suite of codes using appropriately defined benchmark problems and available experimental data.

Research Progress

Researchers assessed existing computational tools that can be used in the neutronics design and analysis of VHTRs, focusing on their static and depletion analysis capabilities. They have identified neutronics characteristics to be simulated in the core models along with Monte Carlo and deterministic capabilities for their representation. For the two candidate designs of gas-cooled high-temperature reactors that are being considered internationally (pebble-bed and prismatic-block types), researchers found that the double heterogeneity arising from using coated fuel particles (CFPs) in fuel elements should be properly represented in the core physics codes. Results show that this effect could be as large as 15 percent $\Delta k/k$. They also found that the effect arising from the use of an annular core design was significant, with large power peaks at the interfaces between the core and reflectors. These power peaks must be properly modeled in order to accurately predict core temperature distributions and peaks. In addition, neutron streaming arising from the design choices (pebble-bed and associated voids and hollow coolant holes in the prismatic-type core) also requires appropriate models, as the effect could result in errors in k_{eff} as large as 4 percent $\Delta k/k$, if not properly represented.

Researchers have extensively investigated the applicability of existing physics codes to VHTR analyses, including the performance of various lattice codes that can be used in generating cross sections for VHTR studies. Detailed assessment of WIMS8, DRAGON, and HELIOS codes were performed by analyzing VHTR fuel element designs and benchmarks. In order to use the HELIOS code, which is not capable of modeling coated fuel particles explicitly (as are WIMS8 and DRAGON), researchers developed an indirect method, dubbed the "reactivity-equivalent physical transformation (RPT) procedure." RPT captures the self-shielding effect of randomly distributed fuel particles by representing a fuel region as an equivalent cell of two homogeneous zones. Additional work is required to validate and verify these codes for VHTR applications and to upgrade them for routine use in future design studies.

An assessment of whole-core diffusion and transport codes showed that a number of well-established deterministic tools are applicable to VHTR analyses, with some level of modeling improvement. Based on these assessments, two separate code systems have been selected for the conventional two-step core analysis procedure:

- WIMS8 and DRAGON for generating multigroup cross sections and DIF3D/REBUS-3 for whole-core physics and fuel cycle analyses
- HELIOS lattice code and the MASTER whole-core analysis code

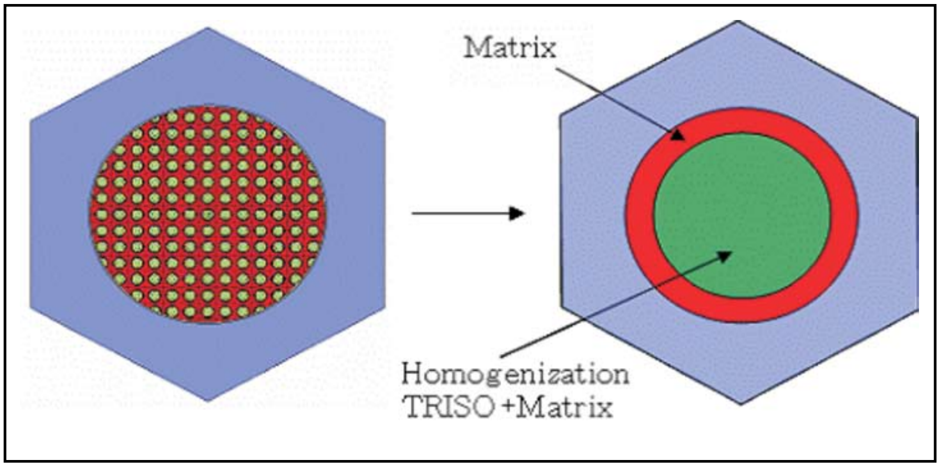

Figure 1. The RPT homogenization method.

Researchers have already completed the initial modifications needed to make these code suites applicable to VHTR analysis and performed preliminary verification tests. The results indicated that these code suites are working properly and provide reasonably accurate solutions compared to high-fidelity Monte Carlo solutions. Additional improvements of these code systems are being made to enhance the solution accuracy and to automate the links among different codes.

The project team has also evaluated existing data in order to create benchmark problems that could be used for code validation. For example, researchers evaluated data available in the open literature for High-Temperature Engineering Test Reactor (HTTR) start-up experiments. From this, they developed Monte Carlo (MCNP) and deterministic models to analyze four critical configurations attained along the path to full-core loading. The results showed a significant difference (1.8 percent $\Delta k/k$) between the core criticality calculated by the MCNP code and experimental measurements. That is, the deterministic codes resulted in larger differences of 2.3–3.4 percent $\Delta k/k$. These discrepancies are consistent with those reported during an HTTR experiment evaluation effort previously organized by the International Atomic Energy Agency (IAEA). The magnitude of these differences is attributed to the incomplete specification of the HTTR core configuration (e.g., impurities and nitrogen in graphite, design data uncertainties, etc.), uncertainties in nuclear data, and approximations inherent in the code solution methods (primarily for the deterministic codes). Due to the incomplete data, it is not possible at this stage to conclusively determine the major contributors to the discrepancies.

Planned Activities

Currently, the DeCART code can handle only rectangular fuel elements. Researchers are extending its geometry-handling capability to include hexagonal fuel elements. They will implement the modular hexagonal ray tracing scheme proposed recently for efficient ray tracing, and will incorporate an adaptive resonance calculation feature applicable to VHTR analysis in order to provide an effective thermal feedback scheme. Once the DeCART code is equipped with the features of the double heterogeneity treatment and hexagonal geometry handling, it can be used for three-dimensional whole-core transport calculation as well as group constant generation.

The whole-core transport calculation capability of DeCART provides a means to assess the errors in nodal diffusion theory solutions caused by the modeling issues such as fuel/reflector coupling and neutron streaming. Taking the DeCART solution as the reference, researchers will assess the accuracy of the nodal solutions for non-uniform temperature conditions, for which whole-core Monte Carlo solutions are impractical. For a consistent comparison, the same cross section library will be used in both the two-step and direct calculations. This assessment would direct the additional improvements required for the nodal methods. Researchers will verify the resulting suite of deterministic codes, both lattice and whole-core solution schemes, against multi-group Monte Carlo solutions using pre-calculated multi-group cross sections.

After all the improvements and the extensions are completed, the overall accuracy of the suite of codes will be quantified by analyzing the HTTR startup experiments again, along with additional validation tests using other available experiment data.

Development of Voloxidation Process for Treatment of LWR Spent Fuel

PIs (U.S.): B.R. Westphal/K.L. Howden, Idaho National Laboratory

PI (Korea): J.J. Park, Korea Atomic Energy Research Institute (KAERI)

Collaborators: Oak Ridge National Laboratory

Project Number: 2004-004-K

Project Start Date: June 2004

Project End Date: April 2007

Research Objectives

This research project is developing a head-end fuel treatment process, known as voloxidation, as part of the Advanced Fuel Cycle Initiative. Voloxidation involves oxidizing uranium oxide fuel at high temperatures using either air or oxygen. When used as a head-end step for aqueous or pyrochemical treatment processes of spent nuclear fuel, voloxidation provides three important advantages. First, it may be used to separate the fuel from the cladding, which could simplify process flow sheets by excluding the cladding constituents from the fuel constituents. Segregation of cladding may also generate less high-level waste. Second, voloxidation decreases fuel particle size, as a result of the oxidation cycle, which may increase the efficiencies of downstream dissolution processes. Third, voloxidation treatment may remove problematic constituents from the fuel prior to downstream treatment operations. Gaseous fission products such as cesium-137, krypton-85, xenon-133, technetium-99, carbon-14, and tritium (^{3}H) may be removed prior to fuel dissolution, thus simplifying the process flow sheets and yielding more flexible waste treatment operations.

The objective of this research is to develop a voloxidation process for light water reactor (LWR) spent fuel, which provides a means of separating fuel from the cladding, reduces particle size, and removes volatile fission products. This project focuses on process development in three general areas:

- Measurement and assessment of the release behavior of volatile and semi-volatile fission products from the voloxidation process
- Assessment of techniques to trap and recover gaseous fission products
- Development of process cycles to optimize fuel cladding separation and fuel particle size

Research Progress

Researchers are developing analytical techniques to assess fission gas release. By analyzing previous data, they have identified improvements in analytical measurement methods for determining volatile fission product releases. They have researched volatile and semi-volatile fission products that are expected to be released from a voloxidizer along with the optimal techniques for analysis. In another task, researchers are conducting hot experiments on fission gases released during voloxidation using irradiated spent oxide fuels. They performed 13 experiments with spent fuel to study the effects of operating conditions such as temperature, pressure, and oxidative gas on fission product removal. The results of fission gas release experiments using spent fuel show that ^{14}C and ^{85}Kr can be completely removed.

The research team has completed the development of unit processes. This subtask included a literature review and experimental results on feasible trapping methods for gaseous fission products such as cesium, rubidium, cadmium, technetium, carbon-14, iodine, and krypton. The most promising trapping method for each gaseous fission product was selected based on process reliability, simplicity, decontamination factor, availability, and disposal. Researchers are currently designing an off-gas treatment system for a hot cell environment so that they can begin testing irradiated spent fuels. Figures 1 and 2 present schematics of the off-gas treatment system.

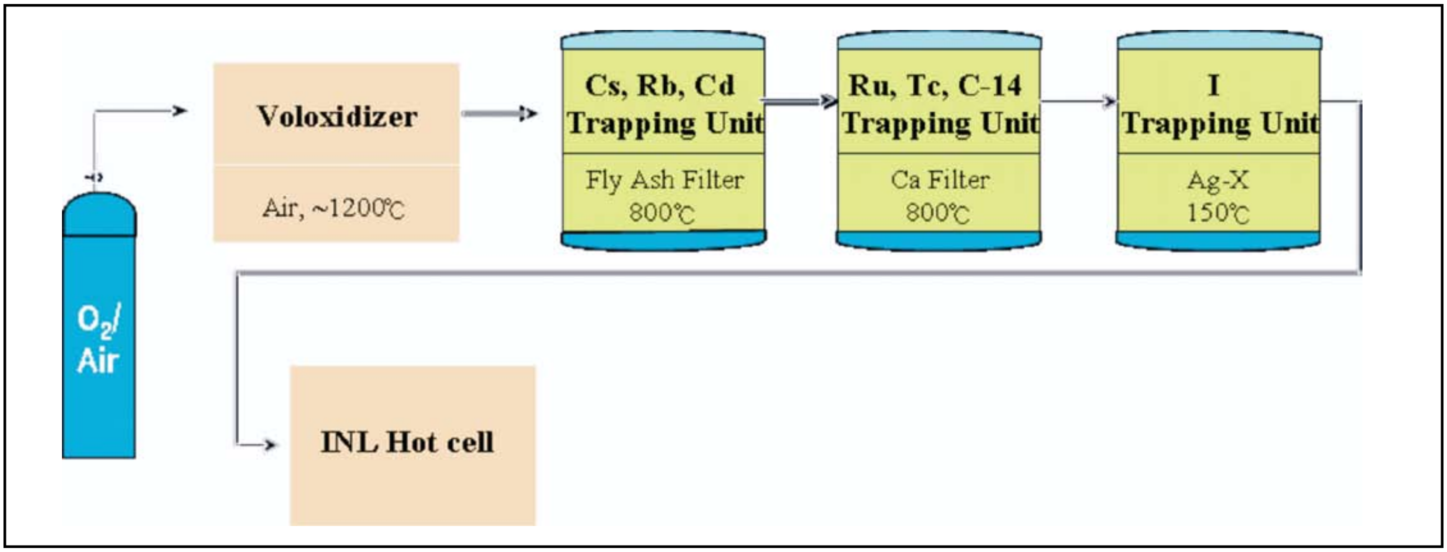

Figure 1. Schematic of off-gas treatment system.

The team has completed the design of equipment for process testing that is capable of high-temperature oxygen atmospheres. This includes the design of components such as off-gas collection, inlet and outlet flow lines, flow and temperature instrumentation, and on-line monitoring instruments. They conducted experiments with this equipment and irradiated spent oxide fuel in order to develop process parameters to optimize particle size and decladding techniques.

Planned Activities

Researchers will issue a final report on the development of optimal analytical methods and equipment to assess fission gas release during the next year. The report will cover improvements for the analysis of tritium, carbon-14, and iodine, specifically the sorption and extraction techniques related to the measurement of these fission products. Hot experiments with spent oxide fuels are ongoing at both INL and KAERI to determine the effects of operating parameters on the removal of volatile fission products. Both programs have slightly differing process goals, which mean that the particular fission products of interest differ as do the conditions necessary to achieve removal. Despite these differences, the test programs are complementary and provide the opportunity for validating the research.

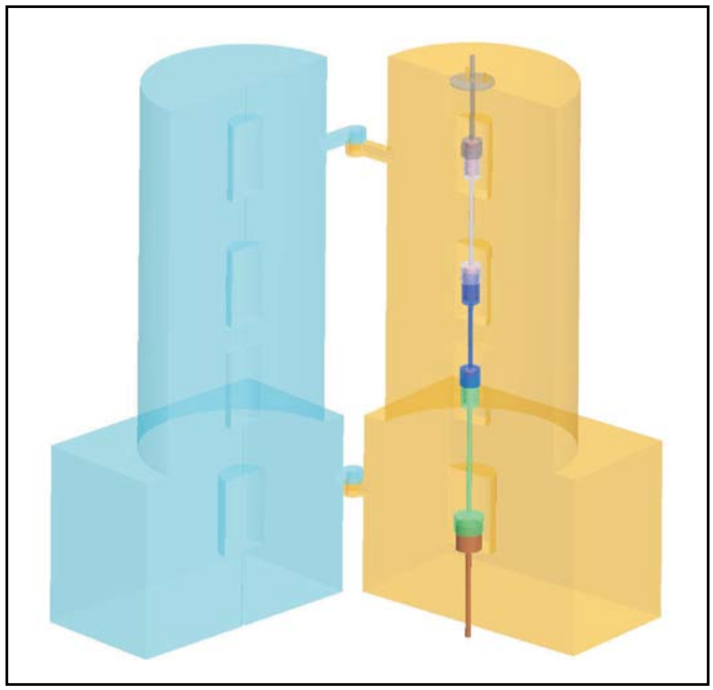

Figure 2. Voloxidation furnace with off-gas treatment system assembly.

The team will also pursue fabrication, installation, and testing of the off-gas treatment system during the remaining period of the project. The off-gas treatment system will be attached to a new furnace capable of operating in a hot cell environment to test irradiated LWR fuels. Following testing, researchers will measure and evaluate the trapping efficiencies for fission products of interest based on previously accumulated data.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Development and Test of Cladding Materials for Lead-Alloy Cooled Transmutation Reactors

PI (U.S.): N. Li, Los Alamos National Laboratory (LANL)

PI (Korea): T. Song, Korea Atomic Energy Research Institute (KAERI)

Collaborators: Seoul National University (SNU)

Project Number: 2004-005-K

Project Start Date: June 2004

Project End Date: May 2007

Research Objectives

The objective of this research project is to develop and establish accurate and reproducible methods for measuring the fuel cladding corrosion rate and corrosion product redistribution in lead-alloy flow loops under conditions approximating those of transmutation reactors. Researchers are exploring both subcritical and critical systems in support of the Advanced Fuel Cycle Initiative (AFCI) and Generation IV lead-alloy-cooled fast reactor (LFR) program. In addition, they will test selected new cladding materials, including silicon and chromium-containing alloys to identify suitable candidates and to define directions for innovative and evolutionary cladding material developments. They will also develop internationally acceptable procedures for measuring corrosion rates by conducting tests with a set of controlled materials. Materials and test conditions will be defined by the collaborating organizations. The research team will incorporate improved oxygen sensors and accurate flow meter and coolant chemistry monitoring techniques into the process. They will systematically construct data sets to characterize the effects of chemical and metallurgical variables on corrosion resistance in transmutation reactor environments. Researchers will consider the overall objective satisfactorily achieved when all three laboratories consistently reproduce test results on candidate cladding materials, including those new Si- and Cr-containing alloys, over a range of coolant conditions.

Research Progress

Researchers are obtaining corrosion data from lead-alloy corrosion loops operated by each collaborating institution, as shown in Figure 1. LANL operates a lead-bismuth loop called DELTA (DEvelopment of Lead-alloy Technology and Applications) which has two test sections operating between temperatures of 400°C and 550°C. Typical flow rate is 2 m/s and the heaters require 65 kW of electrical power. The sample holder accommodates up to 186 samples.

Seoul National University (SNU) completed the construction of the HELIOS (Heavy Eutectic liquid metal Loop for Investigation of Operability and Safety) lead-bismuth test loop and started operation in May 2005. The main objectives of operability and safety tests using HELIOS are focused on the thermo-hydraulics and material corrosion issues. The maximum flow velocity is designed to be 2 m/s, and core inlet and outlet temperatures are 300°C and 400°C, respectively.

KAERI finished welding their Pb-Bi loop, but operation is delayed until April 2006 due to financial issues. The Pb-Bi loop is isothermal, with design flow velocity in the test loop about 2 m/s at temperatures of 450-550°C. The charging volume of the lead-bismuth eutectic (LBE) in the circulation loop is around 0.03 m^3. KAERI has finished the design of a second loop for liquid lead. The design objective of the Pb loop is to achieve a minimum temperature in the cold section of 450°C and a maximum temperature in the hot part of 600°C. Differential temperatures can be 50, 100, or 150°C. The system has 30 heating rods, each 1.35 m in length. Cooling is done by room temperature air. To enhance the cooling capacity, the air cooling duct is designed so that both the inner and outer surfaces are contacted by hot Pb.

The research team has selected several materials for common testing by all three laboratories: ferritic-martensitic alloys T91 and HT9 and austenitic stainless steel 316L. They established a common test condition of 450°C for these tests, along with 10^{-6} weight percent oxygen concentration, 2 m/s flow velocity, and 1,000 hours exposure time. For their individual test programs, LANL is interested in obtaining corrosion data for a wide range of temperatures, while KAERI will focus on higher temperatures and SNU on relatively low-temperature data.

The 1,000 hr corrosion test program at the DELTA facility included over 20 different materials immersed in the flowing LBE for 333, 667, and 1,000 hours at 450°C. LBE flow velocity was about 1.2 m/s, and the targeted oxygen concentration 10^{-6} weight percent. They also completed another test, including surface-treated steels (shot-peened 316L and HT-9, and aluminized 316L), at nominal test conditions of 520°C, 1.2 m/s LBE flow velocity, and oxygen concentration ranging from 10^{-5} –10^{-8} weight percent. The test durations were 133, 267, and 400 hours. Figure 2 shows the results of these tests.

Figure 1. Lead-alloy loops developed by LANL, KAERI, and SNU.

Researchers developed the oxygen sensor which is needed to measure the oxygen content in the lead-alloy system. The design is based on the general oxidation-reduction electrochemical reaction through an oxygen ion conductor made of yttria stabilized zirconia (YSZ) ceramic. The cell contains layers of metal and metal oxide configured as: (A/AO)|YSZ|(B/BO), where A and B denote metal, and AO and BO mean their oxides. Various combination of A and B can exist. In LBE research, (Bi/Bi_2O_3)|YSZ|(Pb/PbO) is widely used. As shown in Figure 3, the oxygen sensor incorporates a unique technology for metal-to-ceramic joints, using an electromagnetic force to join the metal and ceramic mechanically. To enhance sealing, the final feed-through to the outside was spot-welded with Ceramaseal, with the ceramic insulation

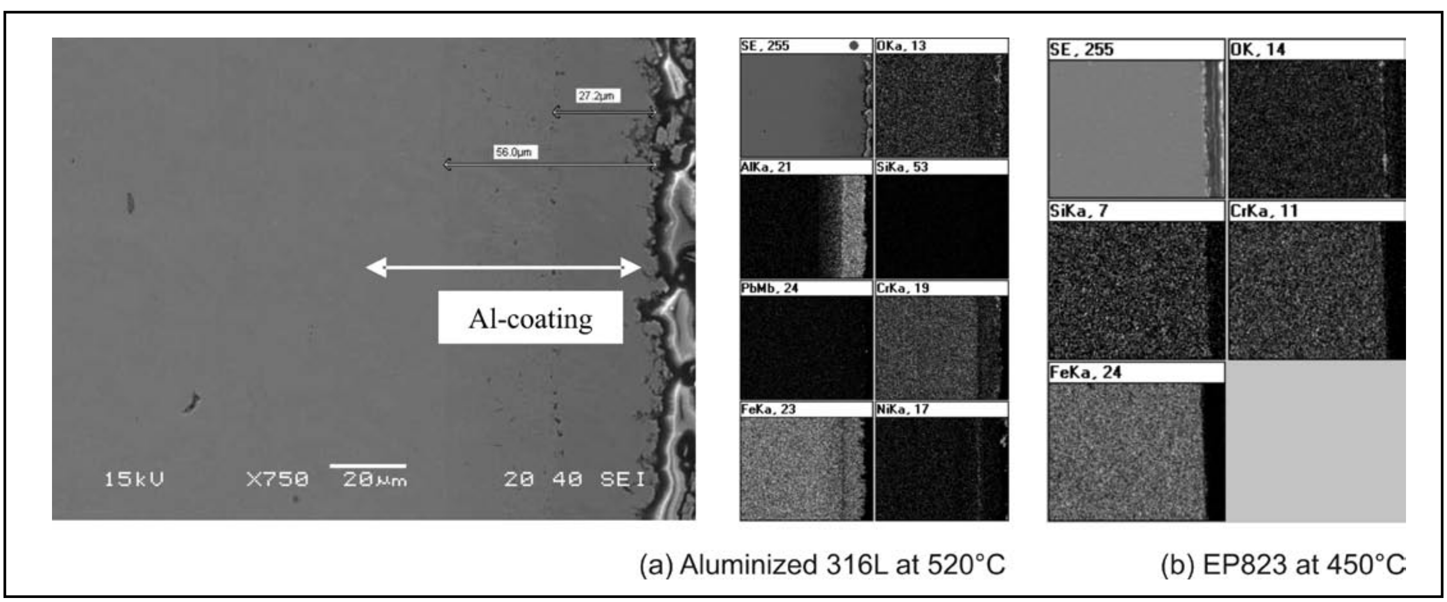

Figure 2. Test results from the LANL DELTA loop at 450 and 520°C.

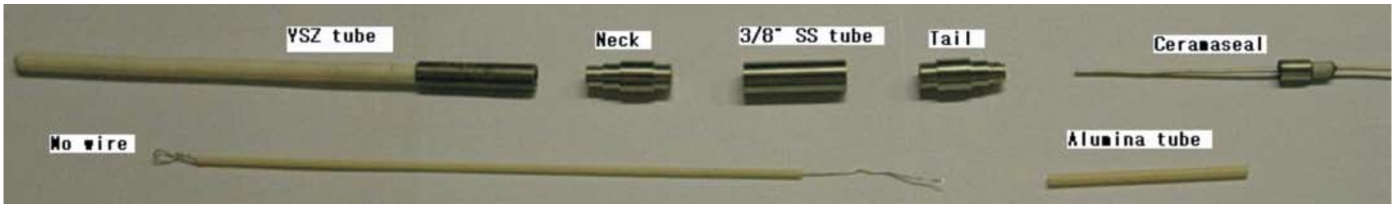

Figure 3. Description of oxygen sensor parts before assembling.

inserted between the wire and the outer annular tube. The researchers produced a pilot sensor having Bi/Bi_2O_3 as the reference materials.

Researchers established a strategy for the sensor calibration method. Based on the Ellingham diagram, they expect that the oxygen concentration in LBE remains constant while a specific metal specimen is oxidized. Therefore, if the DC potential between metal specimens is measured at a constant current condition, a sudden change of potential will occur when the metal surface is oxidized. At that moment, the YSZ signal will be the oxygen activity for the oxidation of the specific metal. Researchers tested the first oxygen sensor and the result is shown in Figure 4.

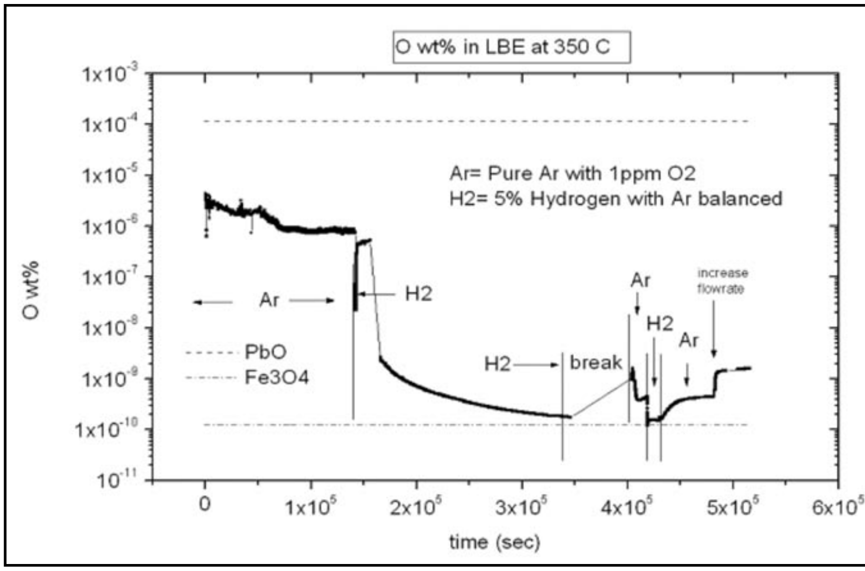

Figure 4. Oxygen concentration in LBE under change of the environmental gas.

Researchers initiated a sustained effort to establish a kinetic model of corrosion in oxygen-controlled LBE/Pb and have gradually incorporated the key features of surface oxidation, scale removal by liquid metal flow, mass transfer, and deposition of corrosion products. With scattered test data, wide-ranging conditions, a scarcity of test results for durations longer than several thousand hours (especially in flow loops), and different approaches to analysis and interpretation, it is imperative that a comprehensive model is developed and benchmarked for more uniform reporting, analysis, and interpretation. Such a model would be necessary to predict long-term corrosion behavior that would be costly and time-consuming to obtain through direct measurement.

The kinetic modeling of mass transfer processes in flowing liquid metal in non-isothermal loops successfully captured the effects of oxygen concentration, the non-uniform distribution of corrosion and deposition (e.g., the "down-stream" effects), the transient to steady state, and the effects of corrosion product build-up in closed loops. This finding cautions the use of data obtained from test loops (and by extension technological systems) built with materials of similar corrosion resistance to the test materials for the following reasons:

- Because the corrosion rate depends on the global (loop) conditions of temperature and flow distribution, using local conditions to describe corrosion can lead to inaccurate conclusions. For instance, corrosion rate can vary substantially in an isothermal section of a non-isothermal test loop, and the rate measured at some intermediate temperature (a typical use of loops to measure corrosion at different temperatures) can be quantitatively or even qualitatively different from that at the same temperature but in a different configuration.
- In static testing, due to limited mass transfer in the liquid metals and the changing corrosion product concentration, long-term corrosion may not be measured at all (see next discussions).

After incorporating the effects of oxide growth and corrosion through the protective oxides, the corrosion can be modeled as the composite of two processes: oxidation of steels (following a predominantly parabolic law) and scale removal through the oxides (linear in time, where the rate depends on global conditions). In a simplified version (not considering alloy composition effects and spatially heterogeneous effects), the observed/measurable effects are:

- The oxide thickness grows parabolicaly in the early time, while the rate constant may be computed based on Wagner's theory.
- The scale removal effect begins to manifest most prominently in the weight changes of the materials: weight increase due to oxidation peaks in relatively short time (a few hundred hours at 500°C with LBE flowing at 2 m/s), then starts to decrease, eventually approaching the long-term corrosion rate (in longer than several thousand hours under the aforementioned conditions). The effect on oxide thickness is little in the same time period.
- Over the long run, the oxide growth will be balanced by the scale removal and approach a limiting thickness. If the oxide stays structurally stable (against spallation), then a constant long-term corrosion rate may be attained.
- Static testing cannot measure long-term corrosion rate in flowing heavy liquid metal coolant (HLMC) systems. However, due to the ease of such testing, it is very valuable as a means to screen materials with suitable oxide growth and stability, and protective coatings.

Planned Activities

LANL will continue to perform corrosion testing using their DELTA Pb-Bi loop. They will perform a series of relatively short (up to a few hundred hours) tests to measure the oxidation and scale removal rate constants. They will also screen and select the most promising candidates for medium-to-long term (6,000 hrs or longer) testing.

KAERI will complete the construction of their Pb and Pb-Bi loops and begin performing corrosion tests at relatively higher temperatures.

SNU will obtain Pb-Bi corrosion data using the HELIOS loop. Researchers will benchmark the data and test conditions of common samples and share other data. The on-line corrosion monitoring method will be established and applied to the samples in the loops.

SNU developed oxygen sensors though subtask 2.1. Researchers will calibrate the oxygen sensors to convert output voltage to real oxygen contents in lead-alloy, comparing measured calibration data with the theoretical predictions. They will also develop calibration procedures using a static cell. Those developed sensors will be used in the loops and long-term stability will be examined.

The corrosion and precipitation model developed by LANL will be applied to the loops to predict dissolution and precipitation. Then, researchers will measure corrosion products to compare the theoretical prediction with actual corrosion and precipitation patterns. They will also design and construct a test facility for embrittlement research.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Alternative Methods for Treatment of TRISO Fuels

PI (U.S.): C. T. Snyder, Argonne National Laboratory

PI (Korea): E. Kim, Korea Atomic Energy Institute (KAERI)

Collaborators: None

Project Number: 2004-006-K

Project Start Date: May 2004

Project End Date: December 2005

Research Objectives

Current methods in treating spent tri-isotropic (TRISO) coated fuel particles call for dry mechanical crushing and/or grinding using a crusher assembly and an attritor grinding mill for breaching the outer pyrolytic carbon and silicon carbide layers of the fuel particle. This project explores alternative methods of breaching the protective layers and investigates new separation methods for the resulting fines and fuel.

The Advanced Fuel Cycle Initiative (AFCI) and the KAERI Advanced Spent Fuel Conditioning Process (ACP) are developing strategies for separating and transmuting the transuranic elements (plutonium, neptunium, americium, and curium) and long-lived technicium and iodine fission products (^{99}Tc and ^{129}I) contained in spent nuclear fuel. Most of the high-level radiotoxic material of nuclear waste destined for direct disposal is in long-lived fission products and the transuranics that can be transmuted, recycled, and/or disposed in smaller volume. TRISO-coated fuel particles from High Temperature Gas Reactors (HTGR) is part of this inventory. The TRISO fuel consists of a microspherical kernel of uranium oxide approximately 600 µm in diameter; a low-density, porous pyrolytic carbon buffer layer approximately 60 µm thick adjacent to the fuel kernel; an isotropic PyC layer approximately 35 µm thick followed by a silicon carbide layer approximately 35 µm thick; and a final PyC layer approximately 45 µm thick. Coated fuel particles are mixed with a graphite matrix and sintered to form a fuel compact. Fuel compacts are contained in a fuel rod approximately 35 mm in diameter and 600 mm in length. The rods are inserted into vertical holes made in a graphite block and, when placed into the HTGR, helium gas coolant flows through gaps between the holes and the rods.

Research Progress

Researchers have begun investigating promising technologies for breaching the TRISO coating for this study. Several methods under consideration are listed below, ranked in order of effectiveness:

- Radio Frequency Induction
- Microwave
- Ultrasound
- Laser

Each of these techniques uses various methods of interaction with the coating material to cause rapid heating to induce breaching of the fuel kernel. The interaction induces thermal stress cracking and debonding in the coating layers by thermal expansion of residual internal gas which ruptures the coating layers. These methods may be combined with a subsequent quenching to enhance stress on the material properties.

Promising separation technologies under consideration for this study can be ranked in the following order:

- Fluidization separator
- Cyclone separator
- Electrostatic precipitation

Separation is carried out according to the differences in density or size of the particles. The fluidization separator is equipped with a vibrator for effective separation of breached particles from kernels.

The cyclone is simple, durable, and easy to maintain, as it has no moving parts. Cyclone separators use centrifugal forces generated by a rapidly spinning gas to separate solids. Larger particles migrate to the wall of the cyclone and proceed downward while the smaller particles tend to exit upwards with the overflow.

The electrostatic precipitator imparts an electrical charge to the particles passing through a high-intensity electrical field. The electrostatic precipitator can be used for collecting very fine powders from sub-microns up to 60 microns particle.

Planned Activities

Based on preliminary research, the project team has ranked breaching and separation methods according to their ability to effectively eliminate the pyrolytic and silicon carbon layers surrounding the fuel kernel in a TRISO particle. While they have evaluated these methods separately based on their own merits, they may also investigate a conceptual model that combines two or more of these techniques into a single process for breaching and separation.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Supercritical Carbon Dioxide Brayton Cycle Energy Conversion

PI: J. Sienicki, Argonne National Laboratory

Foreign Institution: S.O. Kim, Korea Atomic Energy Research Institute (KAERI)

Collaborators: None

Project Number: 2005-001-K

Project Start Date: October 2005

Project End Date: September 2008

Project Abstract

The objective of this project is to develop Supercritical Carbon Dioxide (S-CO_2) Brayton cycle energy conversion systems and evaluate their performance when coupled to Generation IV reactors. The S-CO_2 Brayton cycle is expected to provide improved conversion efficiencies at high temperatures. The plant has a smaller footprint, is less complex, and uses fewer components than a conventional design. Moreover, the high fluid density of S-CO_2 greatly reduces component sizes. For example, an S-CO_2 turbine for a 400 MW_t heat source may be no more than 1 meter in length and 1 to 1.5 meters in diameter. This substantially reduces the technical risks associated with developing reactors and energy conversion schemes that require much higher temperatures.

During this project, the Korea Atomic Energy Research Institute (KAERI) will develop S-CO_2 Brayton cycle energy conversion systems coupled with Very High Temperature Reactors (VHTR) and Sodium Fast Reactors (SFR). At the same time, Argonne National Laboratory (ANL) will advance development of an S-CO_2 Brayton cycle energy conversion system for coupling with Lead-Cooled Fast Reactors (LFRs).

The project team will develop a plant dynamics analysis computer code for the coupled S-CO_2 Brayton cycle/reactor systems. The code will be applied to investigate and develop control strategies during operational transients and postulated accidents. In addition, dynamic analyses of integrated plant transient behavior will be performed for specific control strategies. The team will also work with a commercial turbomachinery vendor to develop improved methodologies for turbomachinery modeling during normal and off-design performance.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Development of HyPEP, A Hydrogen Production Plant Efficiency Calculation Program

PI (U.S.): C. Oh, Idaho National Laboratory

PI (Korea): Y. J. Lee and W. J. Lee, Korea Atomic Energy Research Institute (KAERI)

Collaborators: R. Vilim, Argonne National Laboratory

Project Number: 2005-002-K

Project Start Date: October 2005

Project End Date: September 2008

Research Objectives

This research project will evaluate and optimize cycle efficiencies for producing hydrogen and electricity in a Very-High-Temperature Reactor (VHTR). Systems for producing electricity and hydrogen are complex and the calculations associated with optimizing these systems are intensive, involving a large number of operating parameter variations and many different system configurations. This research project will produce the HyPEP computer model, which is specifically designed to be an easy-to-use and fast-running tool for evaluating nuclear hydrogen and electricity production facilities. The HyPEP computer model accommodates flexible system layouts and its cost modeling capability makes it well-suited for system optimization.

Specific activities of this research are designed to develop the HyPEP model into a working tool, including 1) identifying major systems and components for modeling, 2) establishing system operating parameters and calculation scope, 3) establishing the overall calculation scheme, 4) developing component models, 5) developing cost and optimization models, and 6) verifying and validating the computer code. Once the HyPEP code is fully developed and validated, it will be used to execute calculations on candidate system configurations.

Research Progress

The research team began the first task of this project, which includes defining the scope of system modeling in HyPEP by identifying and hierarchically categorizing the major systems, components, and the operating parameters of the Nuclear Hydrogen Development and Demonstration (NHDD) facility and the Next Generation Nuclear Plant (NGNP). During the first three months, they evaluated and selected a programming language, set up the overall model/calculation requirements, and established the hierarchical system/component modeling system. The component hierarchy has been defined and the overview is shown in Figure 1. The results will form the basis of the plant modeling interface of HyPEP and help define the thermal-hydraulic processes and phenomena to consider.

Researchers have begun formulating the numerical solution scheme and established the following overall outline. The node-link-block is the basic fluid/heat flow network scheme:

- Node component handles chemical reactions for the high-temperature electrolysis and thermo-chemical systems. It represents thermal-hydraulic (T/H) volume with scalar properties (e.g., volume, mass, molar fraction, energy, pressure, temperature).
- Link component models flow between nodes and has such properties as mass flow rate, pressure drop, and the scalar properties of the donor-node.
- Block component represents the solid structures that conduct or generate heat and provides models for the solid-to-fluid boundaries where convection occurs.

The basic equations consider the steady-state mass and energy transport of reactive multi-species fluid mixtures. General thermo-dynamic table search routines have been written and are being tested. The routines are developed with options for user-added property tables.

Researchers have evaluated four programming languages: Visual C++, Visual Basic, Fortran, and Delphi. They have tentatively selected Delphi for the HyPEP development. Delphi is an object-oriented version of the PASCAL language and has versions for the .NET as well as the win32 environments. As HyPEP will have a strong hierarchical structure, the object-oriented program language was deemed to best suit the programming style. The language comparison is summarized in Table 1.

The team initiated development of the base algorithms for the graphical user interface (GUI). They have set up a basic "prototype windows form" to test GUI routines, which is shown in Figure 2. They have also written support routines to enable implementation of the GUI features, which are currently being tested. These routines facilitate on-screen manipulation of components.

Planned Activities

At the end of year 2006, it is expected that a working preliminary version (alpha version) of the HyPEP program will be produced. Major planned R&D activities are as follows:

- **Basic Equation Setup and Numerical Solution Development**. Researchers will set up steady state mass and energy conservation equations for Flow Network. A numerical solution scheme will be developed for flexible network topology. Ancillary routines to obtain T/H properties, heat transfer correlations, pressure drop correlations, etc., will be developed and coded. The numerical scheme will be coded to produce a preliminary working code, and verification and refinement are planned for the next fiscal year.

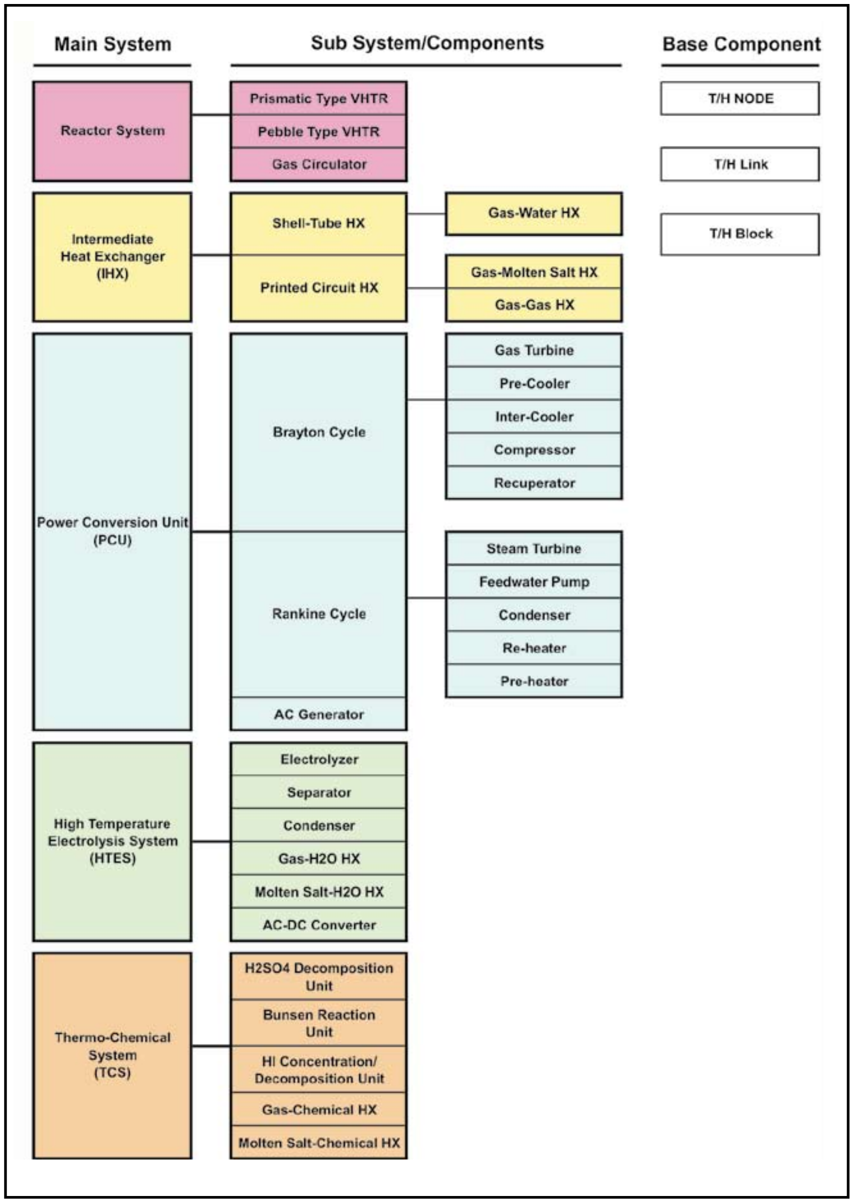

Figure 1. Hierarchical system/component of HyPEP.

Features/Comments	DELPHI	C#	Visual Basic	Fortran
Base Language	Pascal	C	Basic	Fortran
Win32 Version	Delphi2005	C++	MS Visual Basic	Compaq, Lahey etc.
NET Version Common Language Runtime	Delphi2005	MS C# Borland C# etc.	MS Visual Basic	Intel Fortran
OOPS Capability	Very Good	Very Good	Good	No
Structured Programming	Good	Good	Good	Poor
Body of ready-made scientific software	Small	Small	Small	Large
Code Reusability	Good	Good	Fair	Poor
Web Programming Capability	Good (ASPX, ActiveX))	Good	Good (ActiveX)	Poor
Integrated Development Environment	Good	Good	Good	Good
Rapid Application Development (RAD)	Good	Fair	Fair	Poor

Table 1. Comparison of major programming languages.

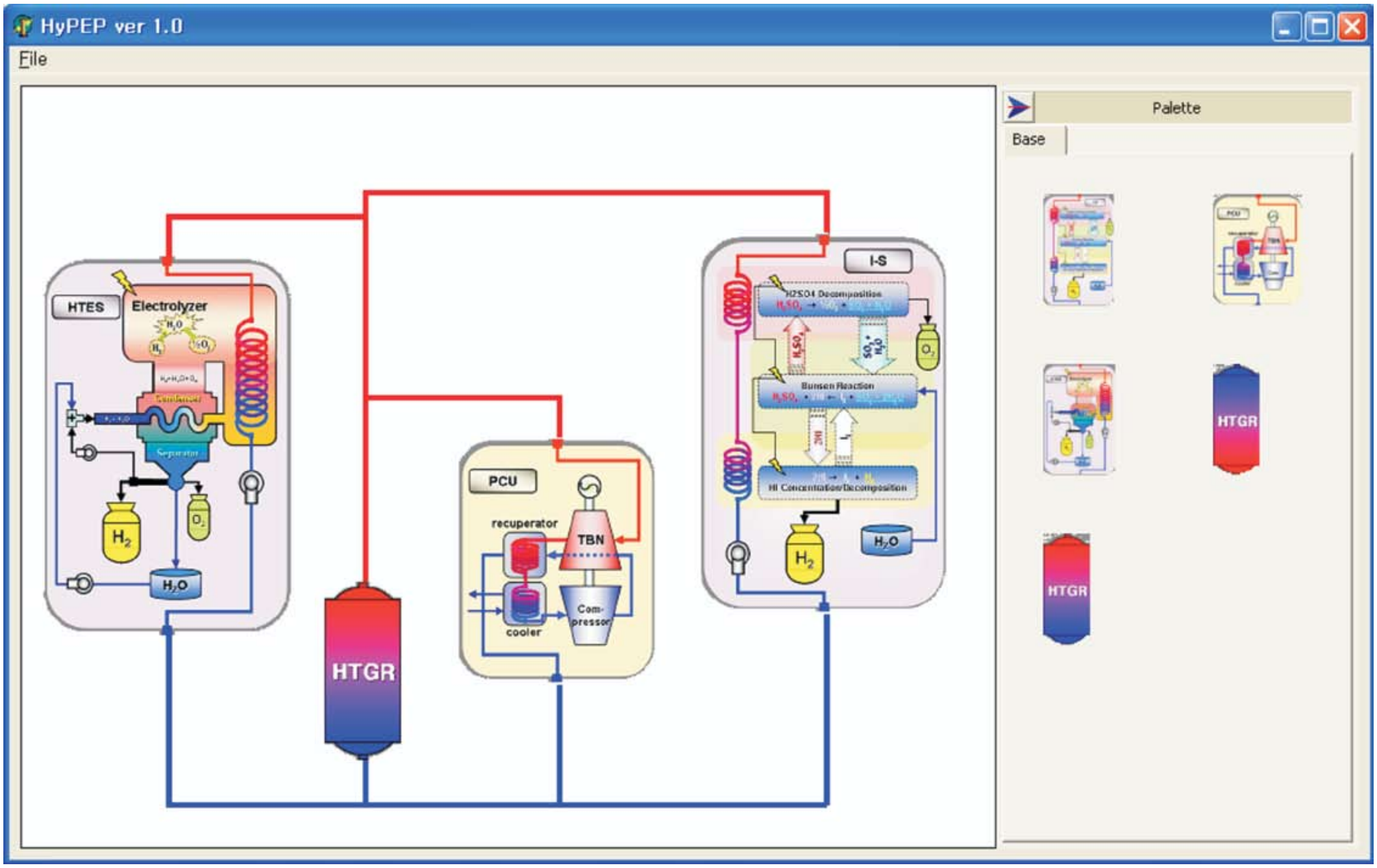

Figure 2. Screen capture of the "prototype windows form" for HyPEP GUI routine development.

- **GUI Development**. The main activity will be developing the object class definitions, which will also be used in numerical coding development. The GUI support routines for component generation and deletion, drag-drop, connection maintenance, flexible layout, etc., will be developed and coded.
- **Component Model Development**. Component specific models will be developed. The models to develop include:
    - VHTR and IHX model
    - Power conversion unit (PCU) T/H model (Brayton cycle and Rankine cycle)
    - HTES T/H model
    - Thermo-chemical model (I-S Cycle). The Node, Link, and Block components will be further developed. The template for the palette, on-screen input/output template for the components will be defined and developed
- **NHDD System Model & Preliminary Calculation**. With the interim version of the HyPEP, a simple NHDD System layout will be modeled and preliminary calculations will be carried out to confirm integrity of the numerical scheme and the ancillary routines.
- **Component Sizing Model Development**. Models will be developed to evaluate the component sizing. Because the model will basically rely on a database, the main task will be to collect and categorize a reliable database.
- **Cost Model Development**. Researchers will develop a simple model (based on database) to calculate the overnight construction cost and an algorithm to calculate simple interest.
- **HyPEP Verification & Validation**. HyPEP will be assessed against established codes such as HYSYS or ASPEN for the program verification and validation.
- **Development of System Optimization Method**. A calculation method/procedure will be developed for the optimization of a nuclear hydrogen production facility. The HyPEP program will be used as the main tool in the method.
- **System Integration**. All the sub-models in the VHTR with PCU and hydrogen plant will be integrated for steady-state analyses. This task includes transient analyses for the control system development.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Improvement of the Decay Heat Removal System for VHTR

PI (U.S): T.Y.C. Wei, Argonne National Laboratory

PI (Korea): Y. S. Sim, Korea Atomic Energy Research Institute (KAERI)

Collaborators: Idaho National Laboratory

Project Number: 2005-003-K

Project Start Date: October 2005

Project End Date: September 2008

Project Abstract

The objective of this project is to improve the performance of the reactor cavity cooling system (RCCS) of the Very-High Temperature Reactor (VHTR) design. The RCCS is a major component in safely and passively removing decay heat. Improving this system is an important step in licensing the VHTR. A beyond-design basis accident involving depressurization of the primary coolant system, accompanied by a loss of station electric power, is accommodated by passive conduction-radiation heat transfer from the reactor core to the vessel boundary, and then primarily by radiation from the vessel wall to the RCCS. Water-cooled and air-cooled RCCS concepts have been proposed that rely either on natural convection or gravity drain to discharge decay heat to the environment. The preliminary Phenomena Identification Ranking Tables (PIRTs) developed by Argonne National Laboratory (ANL), Idaho National Laboratory (INL), and the Korea Atomic Energy Research Institute (KAERI) under a separate I-NERI project have identified various phenomena that are important for these decay heat removal accident scenarios, and particularly to the RCCS.

Based on these findings, this cooperative project is aimed at the following three goals: 1) improving RCCS performance through a combination of well-focused experiments that provide data for model validation and design performance testing, 2) improving and validating the analysis methodology, and 3) improving the designs of innovative heat transfer concepts. Upon DOE approval, the ANL Natural Convection Shutdown Heat Removal Test Facility (NSTF) will be refurbished specifically for both the VHTR water- and air-cooled RCCS options in order to conduct experiments that can validate and improve the RCCS analysis tools. The coupled Fluent-RELAP analysis tool developed by INL will be used to analyze various RCCS design concepts. A radiation-enhanced heat transfer mechanism will be developed by KAERI. Validation studies will be carried out during the course of the project as the experiments are conducted. The integrated partnership between the U.S. and Korea could lead to a comprehensive validation program of these innovative design concepts, which will benefit both countries' VHTR programs.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Development of Head-end Pyrochemical Reduction Process for Advanced Oxide Fuels

PI: S. Herrmann, Idaho National Laboratory

Foreign Institution: K. Jung, Korea Atomic Energy Research Institute (KAERI)

Collaborators: None

Project Number: 2005-004-K

Project Start Date: October 2005

Project End Date: September 2008

Project Abstract

Pyroprocessing can be a very effective method for producing stable waste forms from the highly radioactive fission products found in spent nuclear fuel. This is of great interest to both the United States and the Republic of Korea (ROK) for the purpose of closing the fuel cycle for Generation IV fast reactors. However, pyroprocessing was originally developed for treating metal fuels, while the primary feed material for this process may be oxide spent fuel. A proposed solution to this problem is to develop a process for converting spent oxide fuel into a metallic form.

The United States and the ROK have been active in developing pyrochemical conversion methods for producing feed material that is compatible with pyroprocessing. Both countries favor this electrolytic reduction method, referred to as "oxide reduction." While significant advances have been made in oxide reduction over the last decade, including electrolytic reduction, a number of important technical issues need to be resolved in order to properly assess implementation of this technology.

This research project combines the expertise and unique capabilities of the Idaho National Laboratory and KAERI to make advances towards designing an economical, high-throughput oxide reduction process. The project will focus on two technical issues: 1) the effect of fission products and 2) process scalability.

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

11.0 U.S./OECD Collaboration

The U.S. and an international consortium under the auspices of the OECD-NEA signed a bilateral I-NERI Agreement in March 2002. The U.S./OECD-NEA collaboration has only one project, "Melt Coolability and Concrete Interaction Program," and the agreement specifies equal funding from the OECD-NEA and the U.S for a maximum of five years. The U.S. funding is provided by the U.S. Nuclear Regulatory Commission and the DOE, with DOE providing funding for the initial three-year period.

11.1 Work Scope

R&D topical areas for the U.S./OECD-NEA collaboration include:

- Resolving ex-vessel debris coolability issues through a program that focuses on providing both confirmatory evidence and test data for the coolability mechanisms identified in the Melt Attack and Coolability Experiments integral effects tests
- Addressing remaining uncertainties related to long-term, two-dimensional, molten core-concrete interaction under both wet and dry cavity conditions

11.2 Project Summaries

This project was completed in FY 2005. A summary of the completed project follows.

Directory of Project Summaries

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

Melt Coolability and Concrete Interaction (MCCI) Program

PI (U.S.): M. T. Farmer, Argonne National Laboratory

PI (International): Organization for Economic Cooperation and Development (OECD)

Collaborators: None

Project Number: 2002-001-N

Project Start Date: March 2002

Project End Date: December 2005

Research Objectives

Although extensive research has been conducted over the last several years in the areas of melt coolability and core-concrete interaction (MCCI), two important issues warrant further investigation. The first concerns the effectiveness of water in terminating a core-concrete interaction by flooding from above, thereby quenching the core debris and rendering it permanently coolable. The second issue concerns long-term two-dimensional concrete ablation by a prototypic core oxide melt.

The goal of the MCCI research program is to conduct reactor material experiments and associated analysis to achieve the following two technical objectives:

1) Resolve the ex-vessel debris coolability issue through confirmatory evidence and test data for those mechanisms identified in integral debris coolability experiments
2) Address remaining uncertainties related to long-term two-dimensional core-concrete interaction under both wet and dry cavity conditions

Achievement of these two objectives will lead to improved accident management guidelines for existing plants and better containment designs for future plants. In terms of meeting these objectives, the workscope for the fourth year of the program consisted of: 1) carrying out a large scale melt eruption test (MET) to provide separate effects data on the melt eruption cooling mechanism, 2) conducting a third large molten core-concrete interaction (CCI) experiment to provide data on 2-D cavity erosion behavior and debris coolability following late-phase cavity flooding, and 3) completing final program documentation.

Research Progress

Melt eruption testing focused on providing data on the melt entrainment coefficient under well-controlled experiment conditions. In particular, the experiment featured an inert basemat with remotely controlled gas sparging, since this is the most important parameter in determining the entrainment rate. A schematic of the MET facility is shown in Figure 1. Details of the test section design featuring the inert basemat are shown in Figure 2.

The first test during this year, MET-1, investigated the cooling behavior of a fully oxidized 400 kg PWR core melt containing 25 weight percent calcined siliceous concrete. Entrainment rate data obtained from this and other tests can be used directly in existing models to evaluate the effect of melt ejection on mitigation of the core-concrete interaction. As part of the overall workscope, researchers reviewed the reactor material database to provide a technical basis for model development and validation activities. The test results and information from the review indicated that the melt eruption database includes both siliceous and limestone/common sand concrete types. Melt eruption data were obtained for all tests (both integral and separate effects) conducted with limestone/common sand concrete. The entrainment coefficients for these tests were within the range in which this mechanism would contribute significantly to melt cooling and stabilization at plant scale. The review further indicated that no spontaneous eruptions occurred after cavity flooding for tests conducted with siliceous concrete. Modeling of this process indicated that the melt sparging rate from core-concrete interaction was the key parameter influencing the entrainment process. Thus, the reduced gas content for this concrete type may have been a key contributor to the

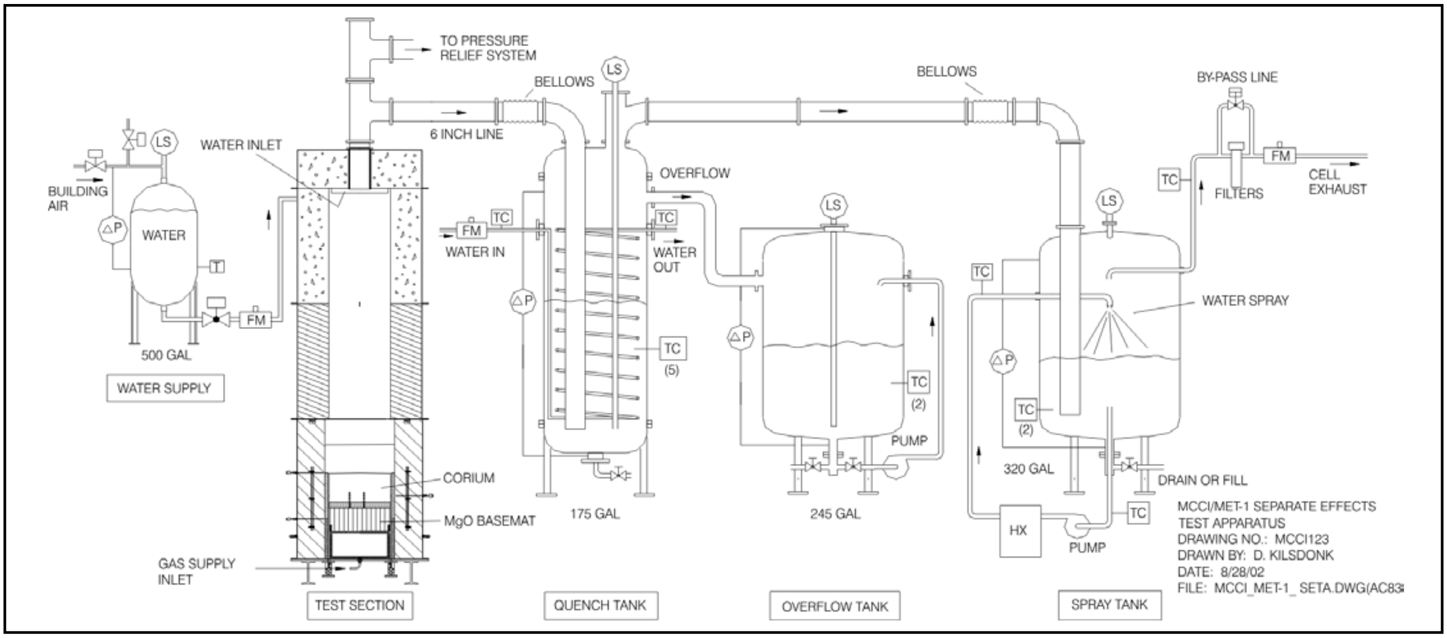

Figure 1. MET and CCI test facility.

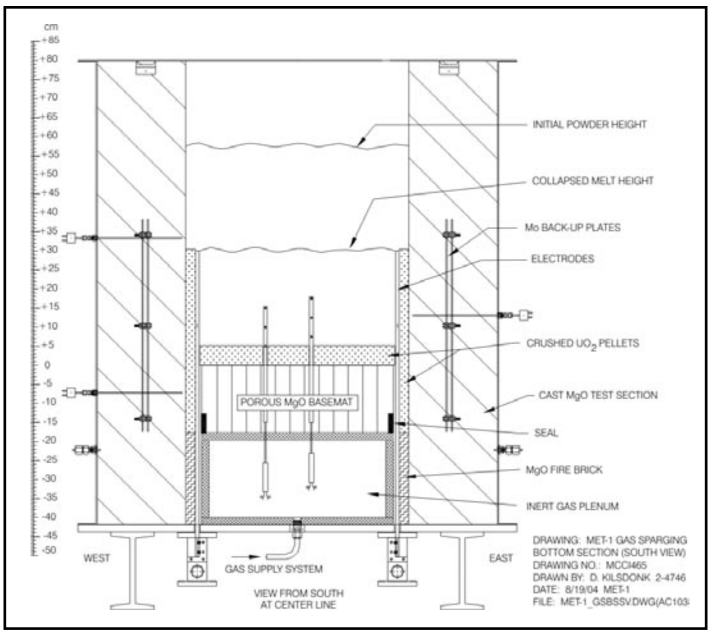

Figure 2. MET test section.

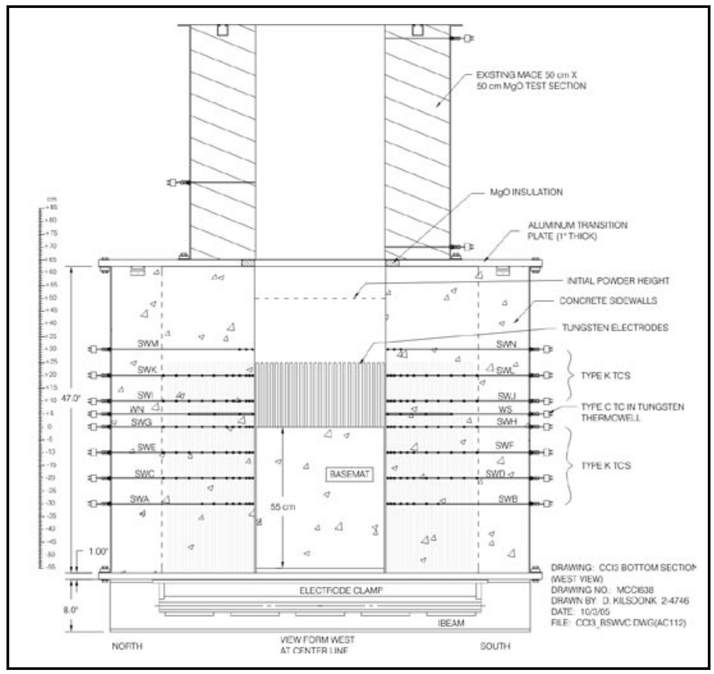

Figure 3. CCI test section.

lack of eruptions for these tests. The review also indicated that test occurrences (i.e., crust anchoring and early termination of power input) may have precluded eruptions from occurring in the tests with this concrete type.

The large-scale CCI tests were intended to provide data in several areas to support the overall project objectives, including: 1) lateral vs. axial power split during dry core-concrete interaction, 2) integral debris coolability data following late phase flooding, and 3) data regarding the nature and extent of the cooling transient following breach of the crust formed at the melt-water interface. In terms of this year's activities, the third core-concrete interaction test, CCI-3, investigated the interaction of a fully oxidized 400 kg PWR core melt, initially containing 8 weight percent calcined siliceous concrete, with a specially designed two-dimensional siliceous concrete test section that had an initial internal cross section of 50 x 50 cm.

A schematic of the 2-D concrete test section is shown in Figure 3. The core-concrete interaction results indicate that radial ablation is a key element of the overall cavity erosion process. A photograph showing the post-test debris configuration after removal of a test section sidewall is provided in Figure 4. Melt temperature data obtained during the test is provided in Figure 5. The researchers found that late-phase flooding causes a significant increase in the upward heat flux from the

Figure 4. CCI-3 post-test debris.

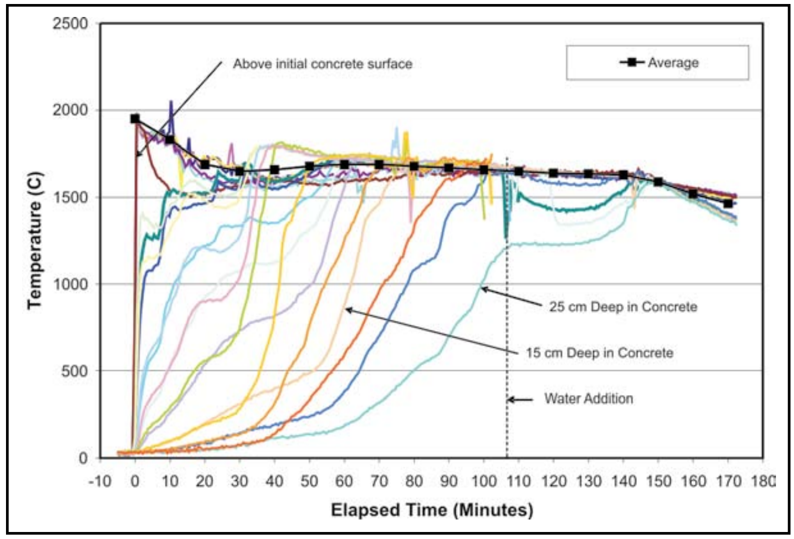

Figure 5. CCI-3 melt temperature data.

debris. Force measurements made during the crust loading sequence indicate that the crust material is structurally quite weak.

In terms of applicability to plant conditions, the tests carried out under this project have provided a significant amount of information for resolving the ex-vessel debris coolability issue and for reducing modeling uncertainties related to two-dimensional molten core-concrete interaction under both wet and dry cavity conditions. Furthermore, the tests provided both confirmatory evidence and test data for coolability mechanisms identified in earlier integral effect tests. This data forms the basis for developing and validating models of the various cavity erosion and debris cooling mechanisms. These models can be deployed in integral codes that are able to link the interrelated phenomenological effects to form the technical basis for extrapolating the results to plant conditions.

As part of the program, one such model was upgraded to include the experiment findings related to debris coolability. This model was used to scope out an approximate debris coolability envelope for the two concrete types that were evaluated as part of the program. The results[1] for limestone/common sand (LCS) concrete, shown in Figure 6, indicated that melt stabilization can be achieved over a fairly broad range of accident conditions as long as the cavity is flooded fairly soon after vessel breach. This concrete is typical of that used in many U.S. plants. For the same set of modeling assumptions, the results indicated that the melt is much less coolable when undergoing interaction with siliceous-type concrete.

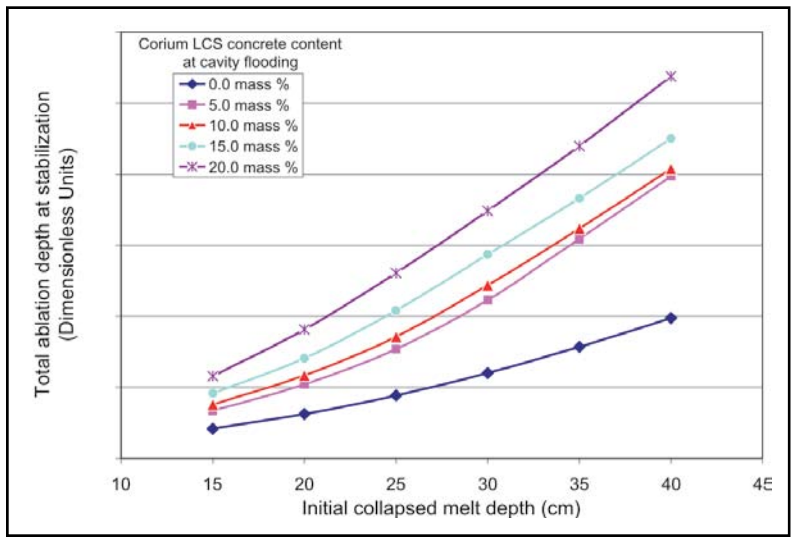

Figure 6. Coolability predictions for LCS concrete.

The research team published one journal article and four peer-reviewed conference papers[1-5], as well as 24 full-length technical reports, to document the results of this program.

Planned Activities

This I-NERI research project is complete. From an accident management viewpoint, the tests have shown that cavity flooding can be effective in mitigating the accident sequence, but the results indicate that the cooling mechanisms may not be sufficiently robust to fully quench and stabilize the full range of melt depths calculated for all accident sequences. Thus, the researchers have developed plans for a follow-on program to 1) further reduce modeling uncertainties in the cooling mechanisms and 2) investigate engineering counter-measures that can ensure that the

[1] Key data is protected by a proprietary agreement. Predicted ablation depths at stabilization are part of the protected information.

full range of melt depths can be quenched and thermally stabilized under all accident conditions. Such a program would be funded separately from this I-NERI project.

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