

2002

University of Nevada, Las Vegas Transmutation Research Program Annual Report 2001

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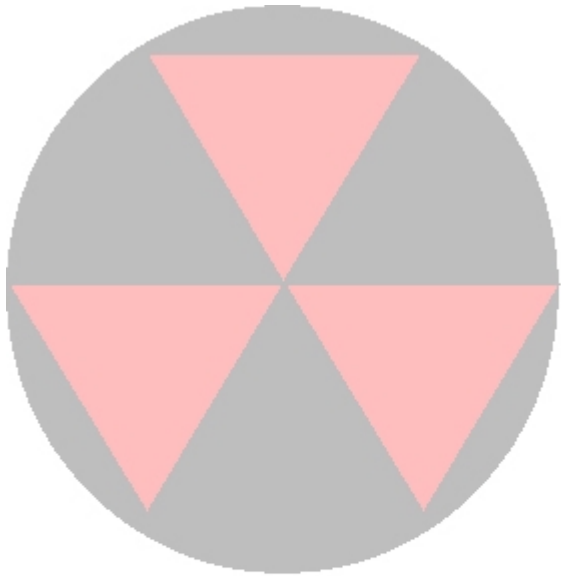
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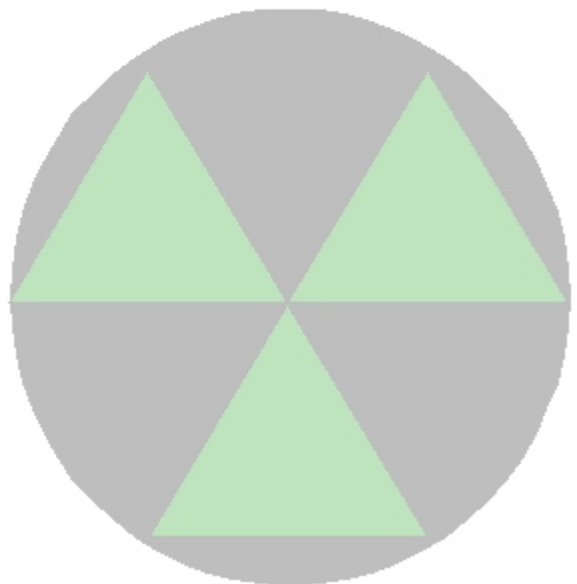
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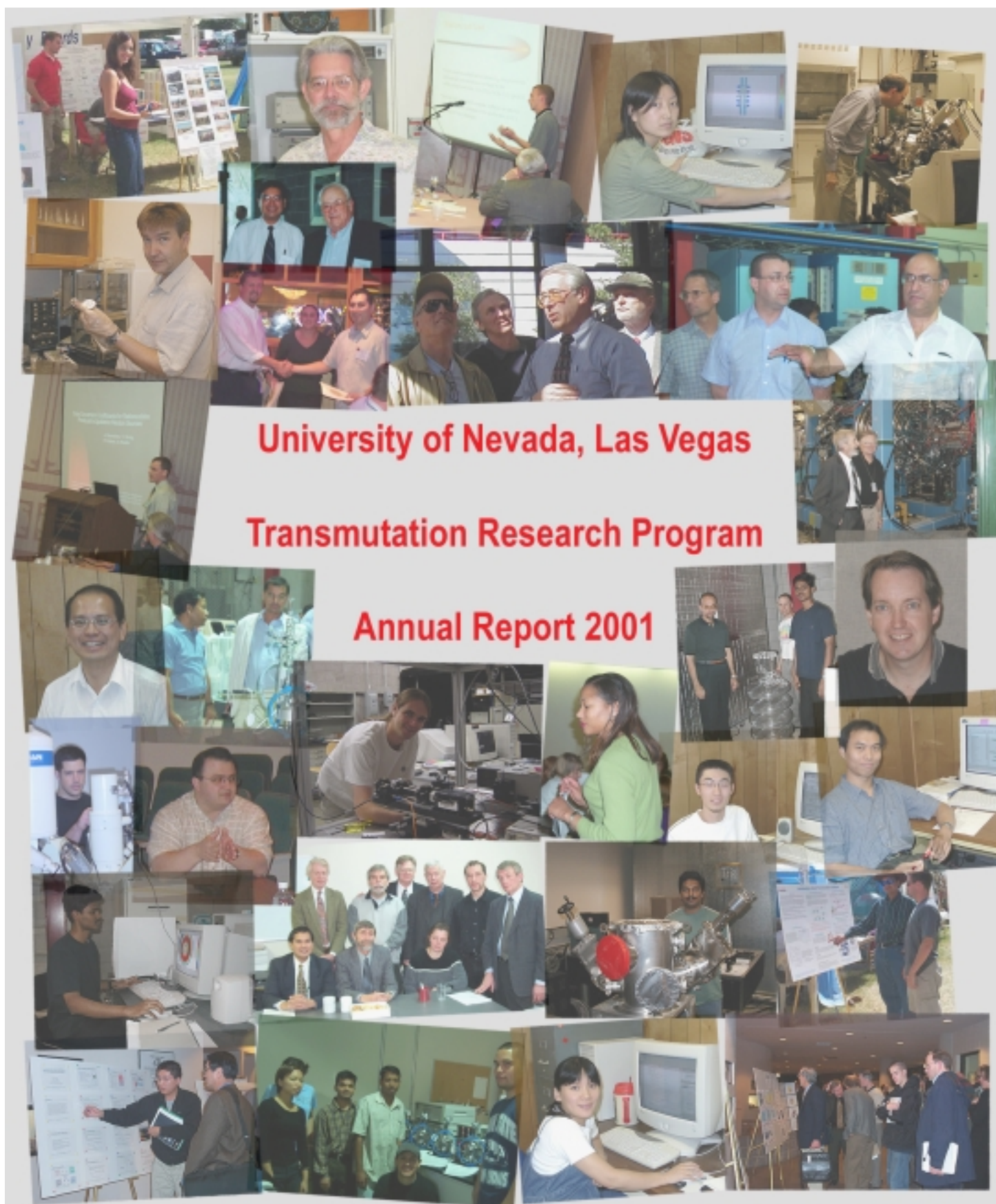
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University of Nevada, Las Vegas
Transmutation Research Program
Annual Report 2001





University of Nevada, Las Vegas

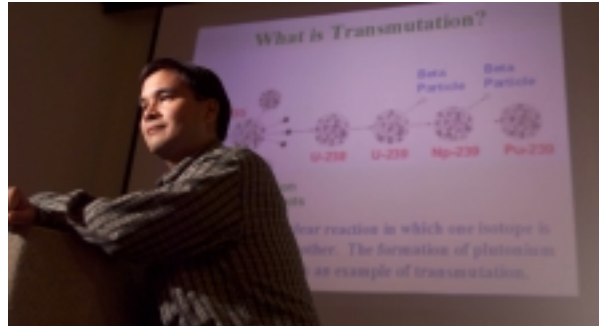
Transmutation Research Program

Annual Report 2001

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Letter from the Director



Anthony E. Hechanova, Ph.D.
Director, UNLV Transmutation Research Program



It is my great pleasure to present our first annual report, highlighting our program's foundation and achievements over the past, very active, year. Supporting this report are the many technical reports and scientific papers that have been generated over the past year, which can be found on our program's website at <http://aaa.nevada.edu>.

In our first year, the UNLV Transmutation Research Program grew from just a concept written down as part of a proposal into a solid, vibrant academic research program supporting 21 graduate assistantships in 6 academic departments across the UNLV scientific and engineering communities. The program also directly supports new research scientists that have come to UNLV as part of the program and provides undergraduate research opportunities (17 undergraduates were supported during our first year).

Through our collaborations with researchers from the national program, we were able to develop and initiate 12 research projects at UNLV. These projects, called *Tasks*, cover a broad spectrum of technologies supporting the national transmutation effort including spent fuel separations, advanced fuel fabrication, and accelerator, fast reactor and transmuter design. Given this diversity, we decided to change the name of the UNLV program from Advanced Accelerator Applications to the more general Transmutation Research Program.

In order to continue the growth and vitality of the research effort at UNLV, we needed to invest in our research infrastructure. We emphasized materials science and engineering capabilities in our enhancements to UNLV this year to build a foundation in areas that are in line with UNLV's strategic growth and our ability to address student-appropriate research in the transmutation program. The capstone of this effort this year was our procurement of a high resolution state-of-the-art Transmission Electron Microscope valued at over \$2 million.

Finally, I believe that through the TRP, we have established ourselves as the core university participant in transmutation research with active collaboration with Los Alamos, Argonne, Lawrence Berkeley and Oak Ridge National Laboratories, Idaho State University, Georgia Institute of Technology, Texas A&M, University of Florida, and the Khlopin Radium Institute in St. Petersburg, Russia. I am truly looking forward to great things for UNLV.

Sincerely,

Anthony E. Hechanova



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UNLV Transmutation Research

The UNLV Transmutation Research Program was established in March 2001 as part of the national Advanced Accelerator Applications program to develop the technologies necessary for the ecological and economical treatment of spent nuclear fuel.

The primary role of the UNLV program in the national effort is the training of graduate and undergraduate students in nuclear engineering and other related fields to support the augmentation of the U.S. human infrastructure for transmutation technologies.

The primary mechanism for this training is the direct involvement of the students in collaborative research supporting the national transmutation research and development program.



The audience was composed mostly of UNLV students at the American Nuclear Society Student Mini-conference's Accelerator Applications Topical Meeting in Reno, Nevada, November 10-12, 2001.



UNLV hosts the National AAA Quarterly Technical Review, January 15-16, 2002.



Students pose with DOE-NE Director William Magwood IV (fourth from right) and DOE-NE AAA Director John Herczeg (second from right) at a special workshop held for DOE-NE June 29, 2001.



TRP Director Anthony Hechanova with Nobel Laureate Burton Richter, chair of the NERAC Advanced Nuclear Transformation Technology Subcommittee, who gave a keynote lecture at UNLV.

To accomplish this role, UNLV has developed the TRP with the primary focus of supporting student research into transmutation and supporting technologies. This focus is realized through the student research component of the TRP, which is designed to operate as an internal research grant program supporting student research at UNLV.

Twelve independent student research tasks, supporting 25 graduate students and another 17 undergraduates, have been initiated in the first year of this program.

These research programs span the range of technology areas for transmutation, from the chemical separation of uranium from spent nuclear fuel, to the optimization of super-conducting components for proton accelerators, to the corrosion of materials exposed to lead-bismuth eutectic.

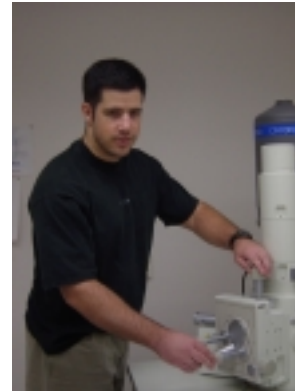
Program Overview

The student research component is supported by the infrastructure augmentation and the program support components. These components are responsible for all aspects of the program that are not directly related to the student research projects, such as hiring new faculty, bringing new research equipment to campus, assisting the development of new student research projects, coordinating with the national program, as well as the typical administrative details of a program of this size.

The primary goals of these components are to support the current University research efforts in transmutation technologies, to augment faculty and staff, and to increase research infrastructure necessary for the strategic growth of the UNLV research program.



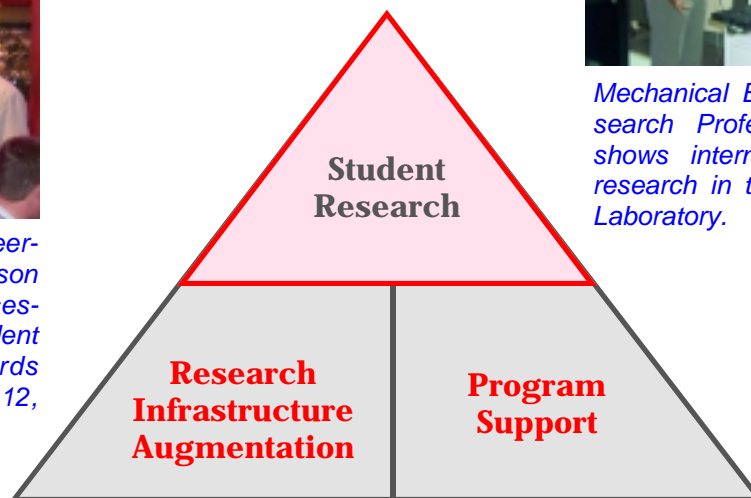
UNLV Mechanical Engineering Graduate Student Jason Viggato (right) wins best session paper at ANS Student Mini-Conference Awards Banquet, November 12, 2001.



UNLV Physics Graduate Student Dan Koury in the Electron Microanalysis and Imaging Laboratory.



Mechanical Engineering Associate Research Professor Ajit Roy (far left) shows international visiting scientists research in the Materials Performance Laboratory.



UNLV Transmutation Research Program Components

Through the infrastructure augmentation component, this year, the TRP supported the continued operation of the Electron Microanalysis and Imaging Laboratory (EMIL), enabled the development of a new Materials Performance Laboratory (MPL), and supported the addition of three Ph.D. researchers to the University faculty.

The program support component sponsored a number of workshops and meetings this year between University researchers and scientists from our National Laboratory partners and the international community for the development of transmutation technologies, as well as sponsoring the participation of UNLV students and faculty in the Accelerator Applications Topical Meeting at the American Nuclear Society winter conference.

Transmutation at a Glance

Introduction

Over 20% of the electricity generated in the U.S. is provided by nuclear power reactors. It is estimated that the amount of used nuclear fuel in the U.S. will reach 140,000 tons by the end of the operational period of current reactors.

Many countries take different approaches to the management and recycling of used nuclear reactor fuel. The U.S. is pursuing a strategy of waste management that would place used nuclear fuel in deep geologic repositories for a long time, separating it from the biosphere and allowing the radioactive isotopes of the waste to decay to more stable progeny.

Transmutation is an alternative waste management strategy undergoing research and development in the U.S. The new national program was authorized by Congress to begin in fiscal year 2001. The goals of the national program are to:

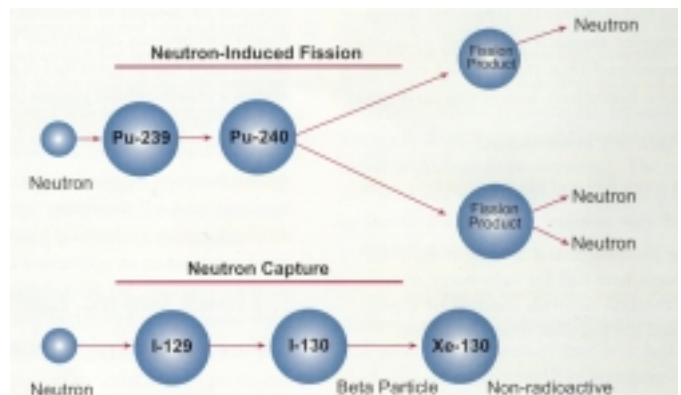
- Develop and demonstrate transmutation of civilian used nuclear fuel,
- Provide a test bed to conduct nuclear fuel science and materials engineering research and development,
- Provide capability of producing tritium for the nation's nuclear stockpile, and
- Provide capability of producing other isotopes for civilian and defense needs.

The transmutation concept could provide a dramatic shift in the U.S. waste management strategy by lessening the inventory of residual radioactivity, allowing recycling of fuel, providing optimization of final waste forms, and potentially removing much of the material from Nevada.

What is Nuclear Transmutation?

For centuries, alchemists have been trying to transform elements into other elements, primarily lead into gold. With modern nuclear science, we can finally accomplish this. Scientists are using nuclear transmutation to change one isotope into another more favorable isotope by changing its nuclear structure. This process is aimed at plutonium, other actinides, and long-lived fission products.

Transmutation can be done with two different processes: neutron-induced fission or neutron capture. Both processes start with the target nucleus absorbing an incident neutron. After the neutron is absorbed by the target nucleus, the nucleus can fission (splitting of the nucleus) or go through another nuclear transmutation process such as radioactive decay. Both processes lead to the same final result: transmutation of waste. These processes are illustrated in the figure below.

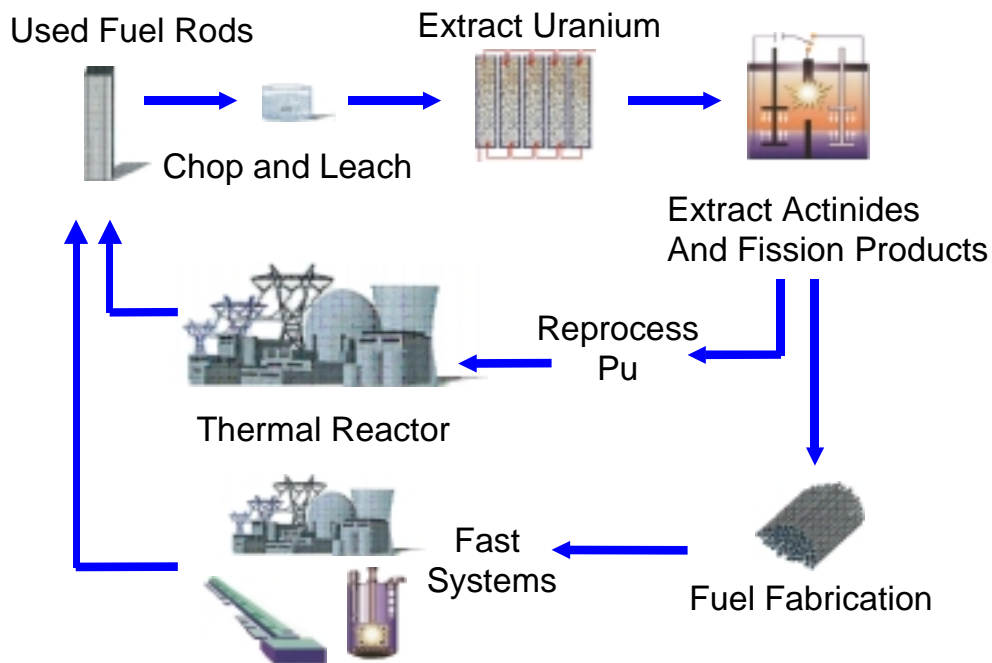


This picture illustrates how neutrons are used to transmute actinides and fission products.

Neutron-Induced Fission (Top): a neutron is captured by a fissile actinide (e.g. Plutonium-239) and is induced to split (or fission).

Neutron Capture (Bottom): a neutron is captured by a nucleus (e.g. Iodine-129). A new nucleus is produced, I-130, which decays into Xenon-130 which is a stable isotope (i.e., not radioactive). This decay process is complete within a few days.

Multi-tier Transmutation Concept



The above figure shows how used nuclear fuel could be managed under a multi-tiered transmutation strategy. In the first tier, plutonium would be recycled from used fuel and transmuted in a new advanced thermal reactor. In the second tier, remaining long-lived radioactive isotopes would be transmuted using a fast spectrum reactor and/or accelerator-driven system.

REDUCE, REUSE, RECYCLE, RESEARCH

Benefits from Transmuting Nuclear Waste

Many benefits are obtained from transmutation of nuclear waste. Some of them are:

- (1) The initial amount of high-level radioactive waste will be reduced.
- (2) The radiotoxicity of the residual waste will be reduced such that it could be less radioactive after 300 years than direct disposal of used nuclear fuel after 100,000 years.
- (3) Usable energy is produced by destroying hazardous components of used nuclear fuel. Plutonium and other isotopes can be continuously recycled.

(4) Someday other isotopes, such as uranium, may be reused. It is possible that other isotopes separated from waste could have a useful purpose in medicine and industry.

(5) The accelerator process will provide a powerful proton source that could be used in medical therapy and to produce isotopes for a variety of applications such as: medical isotopes, industrial isotopes and research isotopes.

Task 1

Design and Analysis of a Process for Melt Casting Metallic Fuel Pins Incorporating Volatile Actinides

Y. Chen, D.W. Pepper, and R. Clarksean

BACKGROUND

The Transmutation Research Program requires the incorporation of non-fertile actinides into the fuel matrix for the transmuter blanket. One of three currently proposed candidate matrices for the transmuter blanket is a metallic alloy fuel matrix. Metallic fuels are an outstanding candidate for a transmutation fuel due to excellent irradiation performance and ease of fabrication. However, including a volatile constituent during fabrication of these fuel pins presents a challenge.

High vapor pressure actinides, particularly americium, are susceptible to rapid vaporization and transport using traditional metal fuel casting processes. As a result, only a fraction of the desired charge is incorporated into the fuel pins. This proves unacceptable from a materials accountability standpoint and fails to meet the objective of including these actinides in the fuel for transmutation.

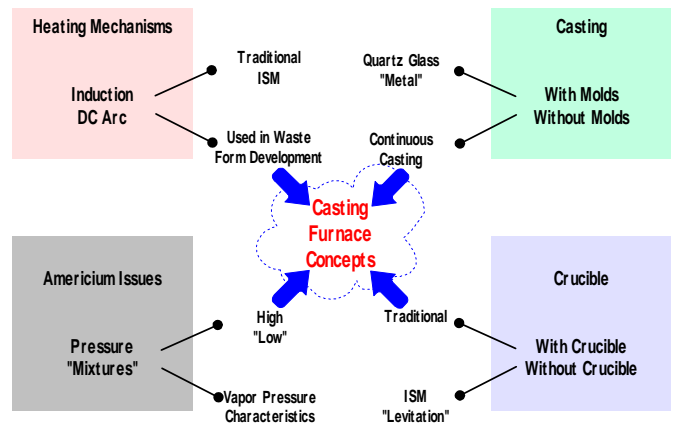
The goal of this project is to model and investigate the casting processes for metallic fuels to help design a process that minimizes the loss of the volatile actinide elements, such as americium, from the fuel.

OBJECTIVES

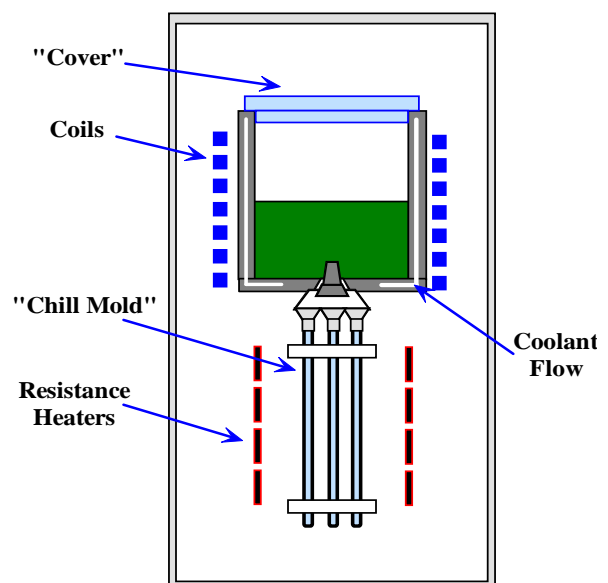
Three research objectives were defined for year one. The first objective was to document volatile actinide transport properties and issues. Using this information, the project was to then develop a parametric model for volatile actinide transport during casting, and then use that model to evaluate the various melt casting technologies. Based on the results of this work, the research group, along with their collaborators from ANL-West, were to select the melt-casting process(es) most suitable for the casting of metallic fuel pins containing volatile actinide elements.

ACCOMPLISHMENTS

The following illustration outlines the mechanisms and furnace options evaluated in the design process:



As a result of considering these variables, the conceptual design of the next generation metallic casting furnace has been proposed. The furnace concept uses an induction skull melter (ISM), covered crucible region, chill molds, and resistance heaters to control the preheating of the molds. The induction skull melting technique, shown below, allows for the control of americium transport as well as the length of the fuel pins that can be cast.



The proposed process theoretically achieves great melting efficiencies and minimizes potential contamination during the melting processes. The crucible cover selected controls the transport of americium from the melt. Resistance heaters control preheating of the molds and insure that the melt will flow into the molds. Chill molds permit proper geometric control. The melt will then flow into the molds either by gravity or through pressurization.

Additionally, the models needed to analyze the performance of the ISM and other furnace designs are being developed. Currently, the model of the furnace system consists of the following components: the casting rod model, the induction heating model, and the mass transfer model. The casting rod heat transfer model considers the flow of the melt into a chill mold. The induction heating model assists in determining the amount of heating produced by the system. Finally, the mass transfer model considers transport within the melt, vaporization at the interface, and transport in the gas phase. The modeling work in the first year focused on the development of these models and examined the possibility of modeling the thermal field within the furnace using a heat transfer code. The development of these models has been completed.

CONTINUED PROGRESS AND FUTURE GOALS

The successful incorporation of volatile actinides in metallic fuel pins requires further research and collaboration over the next two phases of this research. Continued model benchmarking and evaluation includes applying heat transfer and fluid mechanic effects. Activities of Am in molten U-Am and Pu-Am will be calculated and the controlling steps of the mass transfer process will also be studied. The final phase of this research involves a joint effort between UNLV and Argonne National Laboratory to demonstrate the acceptable use of the new furnace in a simulated remote environment. This includes the design and modification/fabrication of a small test furnace for remote operation.

HIGHLIGHTS

- Travel to Argonne National Laboratory to discuss issues related to casting process selection as well as modeling and research efforts prior to submitting the final report.
- A stipend research assistantship for a M.S. graduate student in the Mechanical Engineering department. M.S. granted in May 2002.
- Two research papers were submitted to the International Mechanical Engineering Congress and Exposition and the International Congress on Advanced Nuclear Power Plants related to metallic fuel pins furnace design.
- Four presentations were given at the following workshops/conferences: American Nuclear Society Winter Conference (Reno 2001); ANL Transmuter Fuel Development Workshop (Idaho, November, 2001); International Youth Nuclear Congress 2002 (Korea); and a TRP seminar (October 2001).



Xiaolong Wu received his M.S. in Mechanical Engineering May 2002.

Research Staff

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 Darrell W. Pepper, Dean, UNLV College of Engineering
 Randy Clarksean, Adjunct Professor, Mechanical Engineering Department

Students

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 Paul Lawson, Undergraduate Student

Collaborators

Mitchell K. Meyer, Leader of Fabrication Development Group, Nuclear Technology Division, Argonne National Laboratory
 Steven L. Hayes, Manager of Fuels & Reactor Materials Section, Nuclear Technology Division, Argonne National Laboratory

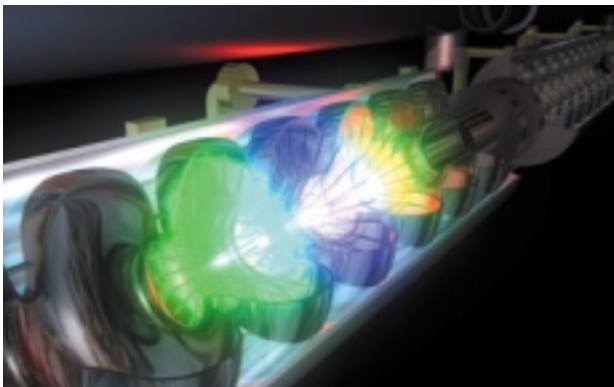
Task 2

Modeling, Fabrication, and Optimization of Niobium Cavities

R.A. Schill, Jr., M.B. Trabia, and Y. Chen

GOAL AND BACKGROUND

All technologies for the transmutation of nuclear waste require a large source of neutrons. One of the principal methods of generating these neutrons is by using a particle accelerator to bombard a heavy metal target. One of the more promising designs for particle accelerators for transmutation systems is the Superconducting Radio Frequency (RF) high-current linear accelerator (linac). The power supplies for these systems have three major components: niobium cavities, power couplers, and cryomodules. This research project will develop models to predict the behavior and performance of the niobium cavities, which will then be used to design and optimize the superconducting structures.



Picture of a niobium cavity for superconducting systems

A phenomenon known as “multipacting” limits the maximum amount of energy and power that the niobium cavity can store. This phenomenon occurs when energy needed to accelerate electrons is “stolen” from the cavity. As a result, power available to accelerate the proton or other particles is decreased. Therefore, the overall performance of the accelerator is reduced, or additional energy must be put into the system to accelerate the particle. To make the problem worse, the energy “stolen” by these electrons eventually turns into heat. This also negatively impacts accelerator performance.

One potential cause of multipacting is the presence of chemical products or foreign particles on the surface of a niobium cavity. To address this potential source of multipacting, the cavity walls are polished after manufacturing using chemical etching and high pressure rinsing. These cavities are not easy to manufacture, however, and may have unusual shapes and sizes that complicate this processing step. Researchers at Los Alamos National Laboratory propose using a baffle to improve uniformity in the etching process. The baffle is inserted inside the cavity to help di-

rect the etching fluid toward the walls of the cavity to produce a cavity with maximum surface quality and minimal multipacting losses. While a number of designs for this technique have been identified, the cavities are difficult to manufacture and result in a heterogeneous surface etch which damages grain structure.

The UNLV research group, working with collaborators from Los Alamos National Laboratory, is studying this problem and working toward techniques to optimize the design of these superconducting cavities. This is expected to have a direct impact on the performance of the large superconducting particle accelerators required for Accelerator-Driven Systems to transmute nuclear waste.

OBJECTIVES

The overall goal of this research project is to develop a stronger understanding of the multipacting phenomenon, and to use this understanding to optimize the design of niobium cavities to minimize or eliminate this parasitic phenomenon. To achieve this goal, the research team established the following objectives for the first year of this program:

- to study the effect of multipacting on niobium cavities with single and multiple cells;
- to improve the uniformity of surface finish in chemical etching;
- to investigate the relationship between the shape and surface condition of the cell and its performance; and,
- to provide a systematic approach for improving the performance of the niobium cavities.

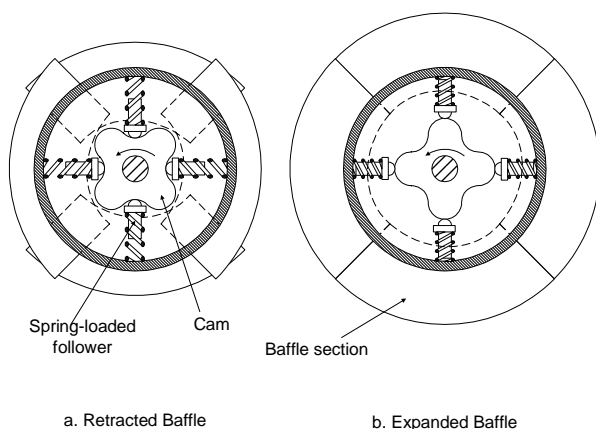
ACCOMPLISHMENTS

To address this problem, the research group began three simultaneous research tracks: a multipacting study, a computational fluid dynamics study (CFD), and an optimization study. These tracks worked on the problem in parallel, exchanging information and models as they were developed.

The multipacting track utilized commercial codes, a research code, and numerical analysis programs developed at UNLV to investigate particle tracking and multipacting. Ms. Myong Holl, a Mechanical Engineering undergraduate student, learned the suite of commercial codes purchased and assisted in simulating multipacting studies. Limitations in the research code were identified and addressed with the author of the code in person. Modifications made in the research code permitted examination of localized secondary

electron emission and impacting over the cavity surface. The commercial and research codes failed to track individual emitted particles. Therefore, a scheme that identifies potential multipacting locations was developed. Additionally, confidence in the validity of the codes was established through examining RF field resonance and particle tracking. A numerical analysis program that was developed permitted investigators to draw a single cell elliptic niobium cavity as well as a five-cell cavity. LANL's five-cell elliptic cavity was then modeled. Multiple codes written by the research team augmented the commercial and research codes and enhanced computer capabilities.

The CFD track provided a means to evaluate the current chemical etching process. During this study, the accuracy of the software used as a modeling tool was verified. Software variables were adjusted as needed. A finite element model for the proposed five-cell niobium cavity with a baffle was developed and a parametric study of the problem was conducted. This involved altering the variables that describe the geometry and location of the baffle subject to the constraint imposed by the cavity. Findings indicated that no scenario improved the performance index of the proposed baffle design. Through the optimization study, a modified design using an expanding baffle was developed. Although the results were deemed satisfactory (flow circulation was eliminated, and flow is closer to the surface of the cavity), mathematical steps were taken to improve the modified baffle design. The algorithm reached a solution after numerous function evaluations. The possible design for an expanding baffle and, thus, the velocity field for the optimized modified baffle design is depicted below.



HIGHLIGHTS

- S. Subramanian, Q. Xue, M. Trabia, Y. Chen, and R. Schill, "Modeling and Optimization of the Chemical Etching Process in Niobium Cavities" accepted for publication in the International Congress on Advanced Nuclear Power Plants (ICAPP).
- M.S. Thesis, "CFD Simulation of Niobium Cavity Etching Process," Qin Xue, August 2002.
- Dr. Stan Humphries, author of the RF Trak research code, presented a seminar in March 2002.
- Travel to Los Alamos National Laboratory established positive working relations with LANL colleagues and assisted in understanding the concerns and interests of LANL relative to this research.

Professor Trabia, Professor Schill, and graduate student S. Subramanian with a model of a cavity.



CONTINUED PROGRESS AND FUTURE GOALS

Future work involves modifying the models to bin the five-cell geometry and implement statistical analyses into code. In order to determine some of the parameters necessary for the modeling work, it will be necessary to perform some experiments on the nature of multipacting, and the properties of the niobium cavities in regards to this phenomenon. To support these experiments, some refurbishment of an existing vacuum system needs to be performed in the next proposal period. These modifications will allow the study of secondary emission properties of a Los Alamos surface treated niobium target being bombarded by electrons from an electron gun. The results of this work will be incorporated into the system models, which can then be used for another iteration of the cavity design and optimization work.

Research Staff

Robert A. Schill, Jr., Co-Principal Investigator, Associate Professor, Department of Electrical and Computer Engineering
 Mohamed B. Trabia, Co-Principal Investigator, Chair, Mechanical Engineering Department
 Yitong Chen, Assistant Director, UNLV Nevada Center for Advanced Computational Methods

Students

Qin Xue, Satishkumar Subramanian, and Anoop George, Graduate Students
 Myong Holl and Greg Loll, Undergraduate Students

Collaborators

K.C. Dominic Chan, Project Leader, SCRF Engineering Development and Demonstration, Los Alamos National Laboratory
 Tsuyoshi Tajima, Team Leader, Accelerator Physics & Engineering, LANSCE-1, Los Alamos National Laboratory

Task 3

Corrosion of Steel by Lead Bismuth Eutectic

J.W. Farley, D.L. Perry, and A. Johnson

BACKGROUND

Materials for transmuter systems need to be able to tolerate high neutron fluxes, great temperatures, and chemical corrosion. For lead bismuth eutectic (LBE) systems, there is an additional challenge in that the corrosive behaviors of materials in LBE are not well understood. Additionally, the database for materials performance in LBE is poor. Most of the available information has come from the Russian programs. These programs focused on the engineering requirements of the LBE systems and not on the corrosion chemistry and mechanisms. As such, these studies do not provide adequate insight with regards to the interactions between LBE, steels, and the corrosion process.

This research program will analyze various steel samples that have been exposed to LBE as part of the national program to develop LBE and transmutation technologies. This information will be paramount in developing engineering efforts to control, avoid, and/or minimize the effect of corrosion of steels by LBE in transmuter and LBE systems. Additionally, this program provides UNLV researchers with hands-on experience that will be crucial in developing the UNLV LBE program, supporting the University's mission with the ISTC target complex, and the future development of additional facilities to examine LBE systems.

OBJECTIVES

The research group plans to test the hypothesis that oxygen in lead and bismuth corroborates the corrosion processes between lead bismuth eutectic, steels, and other system components by examining the evidence left in the corroded layers of the exposed steel samples. Data will provide the elemental composition of the samples and the spatial distribution of elements, both before and after corrosion. This should allow researchers to determine the chemical species present and their spatial heterogeneity, the chemical reactions occurring in the LBE/steel system, and the dependence of the chemical reactions upon composition, temperature, and time. During this work, the program also plans:

- To elucidate the mechanism(s) and kinetics of corrosion in LBE/steels, which have not been studied in detail;
- To determine the signature of chemical species in samples of steels previously in intimate contact with LBE;
- To determine the forms of solid oxides from corrosion products and lead and bismuth; and,
- To measure the different responses of different kinds of steels to LBE.

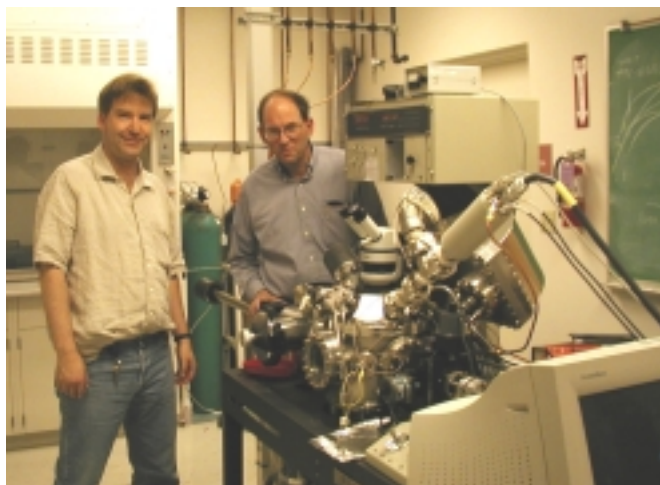
ACCOMPLISHMENTS

Numerous techniques have been employed for the analysis and characterization of samples. Four techniques, Electron Probe Microanalysis, Micro-Raman, X-ray photoelectron/Auger spectroscopy (XPS/Auger), and powder X-ray diffraction, employ laboratory instruments available at UNLV. One technique, which makes use of the X-ray fluorescence microprobe, requires use of the Advanced Light Source (ALS) at Lawrence Berkley National Laboratory (LBNL).

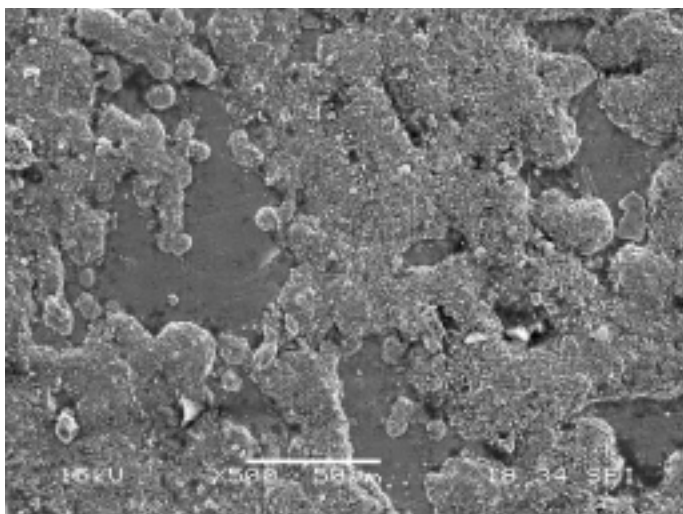
Several of these techniques examined those samples of stainless steel exposed to LBE in experiments conducted by the Russians. Los Alamos National Laboratory provided the samples to UNLV (through a contract with IPPE, Russia). Samples not exposed to LBE were also analyzed. Verification of the Russian sample analysis was completed in addition to the other analyses.

Graduate student Dan Koury found important differences with regards to oxygen and chromium in LBE corroded samples and fresh samples. An oxide layer, 1 micron thick, covered some areas while other areas were not covered. Additionally, it was observed that, while oxygen was present in LBE exposed samples, oxygen was absent from samples that were not exposed to LBE.

Sputter depth profiling was performed on the steel samples exposed to LBE at a Russian laboratory. Removing the outer layer of contamination via sputtering permits analysis of material further down in the sample. Preliminary analyses done at UNLV on the XPS resulted in a plot of elemental abundance as a function of depth at one location on the steel-LBE sample.



Professors Johnson and Farley with the XPS.



SEM of 316 steel sample exposed to LBE for 2000 hours at 450 C. EDAX analysis was performed on different, highly localized areas. A quick glance shows that some areas are covered with corrosion.

CONTINUED PROGRESS AND FUTURE GOALS

Evaluations of the fate of metal components following LBE exposure will be investigated. This should determine if metal components were dissolved into the LBE or left behind at the base of the corrosion layer as the corrosion layer grew. Advantages and disadvantages of sputtering at grazing incidence and at normal incidence have been identified, and will be used to direct future XPS investigations.

Additionally, a plethora of data (primarily XPS data) is currently being analyzed and provides enough material for at least one or two more scientific papers. Data acquisition from Laser Raman Spectroscopy, which will allow researchers to determine chemical species, is scheduled to begin after June 2002.

The results of this work are being presented to the scientific community. Currently, Allen Johnson plans to present at the 2002 AVS meeting in Denver (November 2002), and Dale Perry presents findings at the FACCS meeting in Boston, November 2002.

HIGHLIGHTS

- Completion of a M.S. graduate thesis by Dan Koury in August 2002.
- Student visits to national laboratories: Graduate students Dan Koury and Brian Hosterman to LANL, and undergraduate student Denise Parsons to ALS/LBNL.
- A new XPS facility was installed.
- The presentation of findings from EDAX and XPS at the 2001 Winter meeting of the American Nuclear Society in Reno, NV by graduate student, Dan Koury.
- A peer reviewed and revised conference paper was submitted to the Journal of Nuclear Materials and accepted for publication in 2002.
- Dan Koury presented findings with regards to oxygen and chromium content in samples to a delegation from DOE headquarters.
- A graduate project initiated by Brian Hosterman, who joined the research group in Fall 2001, examines LBE samples using the laser Raman system at UNLV. Data collection began in June 2002.
- Participation by undergraduate student, Denise Parsons, who brings experience from work carried out at the Nevada Test Site and the Yucca Mountain Project.



Brian Hosterman, Dan Koury, and Prof. Farley take a break from the ANS meeting in Reno, November 2001.

Research Staff

John Farley, Principal Investigator, Professor, Department of Physics

Dale Perry, Lawrence Berkeley National Laboratory, Adjunct Professor, UNLV Department of Physics

Allen Johnson, Assistant Professor, Department of Chemistry

Students

Dan Koury and Brian Hosterman, Graduate Students

Denise Parsons, Undergraduate Student

Collaborators

Ning Li, LBE Project Leader, Los Alamos National Laboratory

Task 4

Hydrogen-Induced Embrittlement of Candidate Target Materials for Applications in Spallation-Neutron-Target Systems

A. Roy, B.J. O'Toole, Z. Wang, and D.W. Hatchett

GOAL AND BACKGROUND

Spallation-neutron-sources, such as those under investigation for use in accelerator-driven transmutation systems, generate neutrons through the collision of high-energy protons, or charged hydrogen atoms, with heavy metal targets such as lead. As a result, these systems also tend to deposit a significant amount of hydrogen in the materials of the transmuter target and superstructure. This can result in accelerated corrosion and changes in the properties of the exposed materials. Of particular importance is a phenomenon called hydrogen embrittlement, in which materials lose their ductility (ability to deform under stress) and become brittle (more susceptible to fracture) after reacting with hydrogen. Given the extreme temperature ranges and large quantities of hydrogen expected in the accelerator-driven transmutation systems, these phenomena are of particular importance to the transmutation program.

This research program will examine the effects of hydrogen on hydrogen embrittlement, environment-induced stress corrosion cracking (SCC), and other hydrogen induced/enhanced corrosion phenomena in target materials. The UNLV research group will also examine the effectiveness of various surface and heat treatments in minimizing the impact of these phenomena in candidate materials. It is hoped that establishing a baseline performance of these materials in a hydrogen rich environment (analogous to the expected in-proton-beam environment of the target systems) will pave the way for conducting in-proton-beam radiation experiments and eventually support the materials qualification needed for facility design and operation.

OBJECTIVES

The principal research objective of the UNLV research program is to examine the phenomena of hydrogen embrittlement, stress corrosion cracking, and other hydrogen induced/enhanced corrosion phenomena in candidate materials for use in a spallation-neutron-source. Working with the national program, stainless steel alloys HT-9, EP-823, and EP-422 have been selected as the candidate materials for investigation at this time.

The research group plans to examine these phenomena with the following methodology. Tensile specimens under constant load and slow-strain-rate (SSR) conditions will be used to evaluate alloy susceptibility to stress corrosion cracking and hydrogen embrittlement in environments of interest. Optical microscopy and scanning electron microscopy will be used to evaluate the extent and morphology of cracking of these alloys. The concentration of hydrogen

resulting from cathodic charging will be analyzed using secondary ion mass spectrometry (SIMS). Attempts will be made to correlate the resultant cracking parameters to the microstructures for the different stainless steels and heat treatments. Further, the localized corrosion behavior of these alloys is being evaluated by electrochemical polarization techniques.

RESEARCH ACCOMPLISHMENTS

The first major challenge facing the UNLV research group was to bring the capabilities to perform the proposed work to the University. This was accomplished through the establishment of the Materials Performance Laboratory (MPL), a materials performance user facility, at UNLV. Capabilities of this facility include the ability to conduct thermal treatments, metallographic evaluation, sample preparation, mechanical testing, and corrosion studies involving aqueous environments at elevated and ambient temperatures.

Once the experimental facilities became available, the sample stock materials for the initial experimental campaign were prepared. The material stock was then subjected to various thermal treatments at UNLV before the sample specimens were prepared. One set of each material stock was heat treated to produce quenched and tempered metallurgical microstructures typical of martensitic stainless steels. These heat-treated materials were sent to a different off-site facility to machine tensile specimens for evaluation of their ambient temperature mechanical properties and their susceptibility to SCC/HE in aqueous environments of interest. Simultaneously, efforts are well underway to machine small cylindrical specimens to perform electrochemical polarization experiments. Evaluation of the SCC behavior has now been well established and analysis of the tensile specimens machined from heat-treated bars is now underway.

Data quantifying the percent chemical composition for three heats of each metallurgic alloy was acquired for 14 different elements. Additionally, the ambient temperature mechanical properties of one alloy (EP-823) were tested. Constant-load SCC tests of that same alloy are currently in progress.

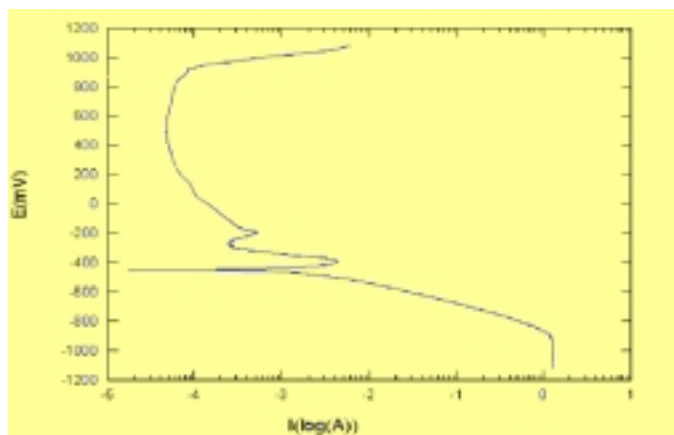
The experimental setups for constant-load SCC testing and electrochemical polarization studies are shown on the next page. A typical calibration curve showing potentiodynamic polarization behavior of Type 430 ferritic steel in 1N sulfuric acid solution at 30°C follows.



Constant-Load SCC Test Setup



Electrochemical Polarization Test Setup



Potentiodynamic Polarization Curve for Type 430 Ferritic Stainless Steel in 1N H₂SO₄ Solution at 30°C, Scan Rate: 0.166 mV/sec (ASTM G 5).

HIGHLIGHTS

- Two graduate students are currently working towards M.S. and Ph.D. degrees – Mark Jones and Md. Kamal Hossain, respectively. The “prospectus of thesis” is currently being developed for both students.
- Four technical papers are being written based on results from this research. These papers will be presented at the annual conferences of the “Electrochemical Society” and “NACE International”.

CONTINUED PROGRESS AND FUTURE GOALS

The testing campaign for all three types of martensitic stainless steels will continue. The testing campaign includes performing heat treatments on the remaining formulations of all three test materials, performing localized corrosion testing using electrochemical techniques, performing metallurgical evaluations (including microstructural characterizations), and conducting failure analyses using the Scanning Electron Microscope. Data and results will be prepared for technical and scientific presentations for both presentations and publications.

Additionally, tests involving slow-strain rate units and electrochemical equipment are being performed to establish the testing techniques and related parameters. It is anticipated that all testing techniques will be standardized prior to their implementation in MPL.



MPL weekly student and staff meeting.

Research Staff

Ajit Roy, Co-Principal Investigator, Associate Research Professor, Mechanical Engineering Department
 Brendan O'Toole, Co-Principal Investigator, Assistant Professor, Mechanical Engineering Department
 Zhiyong Wang, Assistant Professor, Mechanical Engineering Department
 David Hatchett, Assistant Professor, Department of Chemistry

Students

Raymond Kozak, Mark Jones, and Mohammad Kamal Hossain, Graduate Students
 Aaron Tippetts, Undergraduate Student

Collaborators

Ning Li, LBE Project Leader, Los Alamos National Laboratory

Task 5

Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics

S. Moujaes and Y. Chen

GOAL AND BACKGROUND

Many of the international efforts to develop transmutation technology, including the U.S., Russian, and European scientific communities, have determined that lead bismuth eutectic (LBE) is a potential material for use as both a spallation target and a coolant. To exploit this potential, a more thorough understanding of the effect and rates of corrosion on steels, particularly non-Russian alloys, inside the LBE systems is required. Properly controlling the oxygen content in LBE systems has been observed to drastically reduce the corrosion of structural steels in LBE. However, the transport of oxygen and formation of corrosion products is not well understood; thus, their interaction, variation, corrosion, and precipitation along the flow path requires further characterization.

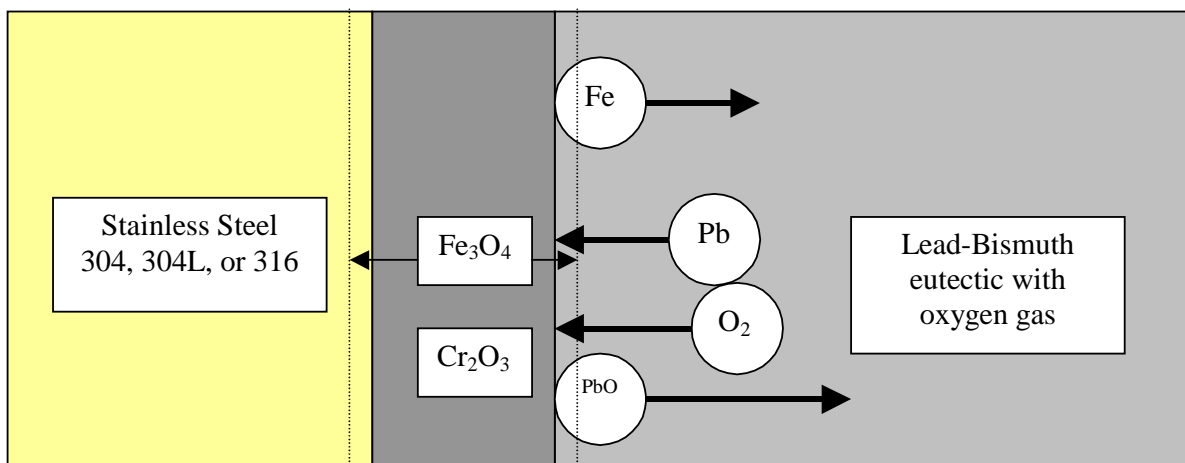
Direct testing, although absolutely essential, can be relatively expensive, time consuming, and inadequate to predict system corrosion performance beyond test conditions. The proposed work combines chemical kinetics and hydrodynamics in target and test-loop lead bismuth eutectic (LBE) systems to model system corrosion effects. This approach will result in a predictive tool that can be validated with corrosion test data used to systematically design tests and interpret the results. It also provides guidance for optimizing LBE system designs. Initial steps include developing predictive tools necessary to determine oxygen levels and corrosion products through computational fluid dynamics (CFD) modeling. Finally, invaluable information will be acquired by incorporating results from CFD modeling with kinetic information highlighting the corrosion process between LBE and structural materials.

OBJECTIVES AND RESEARCH METHODS

The UNLV researchers have broken down their effort into three phases. Phase I simulates the corrosion process and phenomena occurring at the tube walls for a number of loop conditions. Phase II numerically simulates the effect of corrosion on components placed in the loop at predetermined ports. Phase III involves experimental testing of Phase II objectives. The experimental data acquired regarding corrosion effects will be compared with numerical simulations and used to benchmark the models. Variables to be analyzed include the distribution of LBE stream velocity, temperature, oxygen, and corrosion product concentrations close to the substrate. This will support the calculation of corrosion and precipitation rates in the entire system.

Using CFD coupled with chemical kinetics assists the researchers in obtaining reliable data for the experimental design. This will also serve to establish a predictive capability in the United States. Coupled with knowledge regarding the reaction chemistry and kinetics of potential corrosion rates, these codes can be used with reasonable confidence after proper validation, to investigate the behavior of new components exposed to LBE and oxygen.

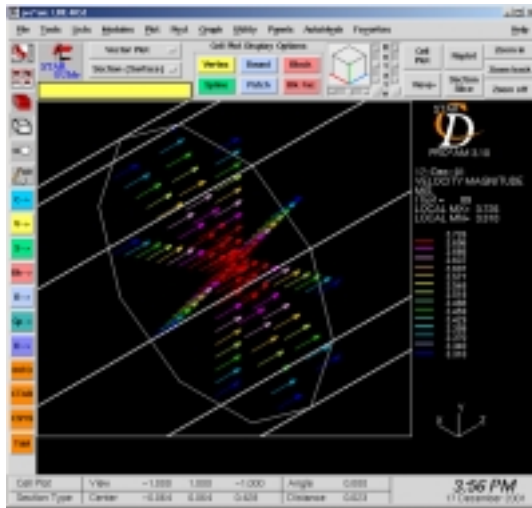
The most difficult challenge facing this work involves overcoming and developing an efficient numerical model with the correct chemistry reaction rates for use in different components of a typical LBE flow loop. Anticipated obstacles, progress, and research methods require intimate communications with Los Alamos National Laboratory scientists. This ensures that the research objectives are appropriately focused on the Transmutation Research Program needs.



Schematics of corrosion processes between the metal surface and the liquid metal.

RESEARCH ACCOMPLISHMENTS

An intensive and ongoing literature search has provided limited information about the LBE system, especially with regards to chemical kinetic and thermodynamic data. However, researchers have been able to glean some insight regarding the corrosion mechanism on the material surface from the open literature. With this insight, researchers are attempting to determine what mechanisms foster the corrosion process. Potential scenarios include differentiating whether they are a function of kinetics, diffusion, or multiple mechanisms.



Velocity profile along a cross section of the pipe.

The transport of oxygen and corrosion products as well as their interaction and variation of corrosion and/or precipitation along the flow path are not well understood. Past experimental studies monitored corrosion history of specimens in one test loop over several thousand hours. This showed that corrosion occurs at higher temperatures but precipitation occurs at intermediate temperature. The model developed by the UNLV research team has confirmed that the temperature distribution in an LBE system is important for understanding the corrosion process in the system.

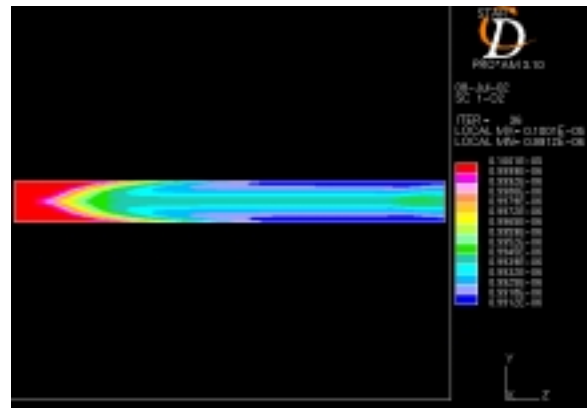
Thermal data for the species have been obtained from LANL. Thermal constants of lead, required for running the code, have been calculated and the input data for calculating these constants have been obtained. Effort is being made to calculate the transport data for each of the species involved in the reactions.

Finally, various codes are analyzing the fluid flow and the reactions taking place in the flow and on the surface. Two sections from the test loop have been chosen for the analysis. Lead and oxygen are allowed to flow through the

HIGHLIGHTS

- A student was sent to the CD-Adapco at its Plymouth, Michigan training facility to receive the fundamental training on how to run the commercial code (STAR-CD)
- Presentation of "Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics" by Kanthi Dasika at the International Youth Nuclear Congress 2002 in Daejeon, Korea April 16-20, 2001
- Presentation by C. Wu and K. Dasika at the ANS Student Mini-Conference in Reno, Nevada, November 2001 "Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics"
- Presentation of a paper "Numerical Modeling of Lead Oxidation in Controlled Lead Bismuth Eutectic Systems: Chemical Kinetics and Hydrodynamic Effects" by Chao Wu at the ICAPP/ANS Conference in Hollywood, Florida, June 2002

system and the liquid lead reacts with oxygen. The walls are defined as made of stainless steel and the surface reactions between iron and oxygen have been considered.



Variation of concentration of oxygen along the pipe.

CONTINUED PROGRESS AND FUTURE GOALS

The next step in the modeling process is to perform a parametric study examining the impacts of velocities and temperatures of the fluids on the corrosion rates. From this analysis, researchers hope to help decipher the most appropriate temperatures, velocities and concentrations of each of the species in the test loop for the minimization of corrosion.

Research Staff

Samir Moujaes, Principal Investigator, Associate Research Professor, Mechanical Engineering Department
Yitong Chen, Assistant Director, UNLV Nevada Center for Advanced Computational Methods

Students

Chao Wu and Kanthi Dasika, Graduate Students

Collaborators

Ning Li, LBE Project Leader, Los Alamos National Laboratory

Task 6

Neutron Multiplicity Measurements of Target/Blanket Materials

C.D. Hull and W.H. Johnson

GOAL AND BACKGROUND

The number of neutrons available from any transmutation system is the critical parameter in determining how quickly material can be transmuted. This means that maximizing neutron production while utilizing minimal power provides the most efficient transmutation system. For spallation neutron systems, neutron production and neutron use of the system may be determined using the MCNPX code package.

The LAHET Code system (LCS), part of the MCNPX package, provides simulation capabilities for a variety of particles in the higher energy regimes (which is the primary difference between the MCNPX package and the traditional MCNP package). Currently, the uncertainty associated with the neutron fluxes calculated using LCS for neutron proliferation simulation is 10-12% at the 95% confidence level. This uncertainty is thought to be due to the leakage of high-energy neutrons and protons, or multiple scattering, in the radial directions of thick targets. This uncertainty is unacceptable for most nuclear systems, and would result in significant limits on the operation of an accelerator-driven transmutation system.

One of the best methods for reducing uncertainty in modeling is to benchmark theoretical models, such as MCNPX (and the LAHET code within), against experimental observations. Unfortunately, the measurements of neutron production per unit volume necessary to validate and benchmark the code calculations for these source term volumes are lacking.

This research project plans to develop the technologies and experimental plans needed to address this data need. Initially, it involves the development of nuclear transport models and the acquisition of nuclear instrumentation necessary to perform neutron multiplicity measurements. By measuring neutron leakage from targets with various diameters, empirical measurements can be compared between detector systems and the MCNPX predictions. Additionally, precision position sensitive measurements of the source term volume for neutron production will permit systematic determination of major uncertainties in the LCS. This allows the performance of very low uncertainty measurements in the few percent range at the 95% confidence level. Finally, the acquisition of neutron multiplicity measurements on a variety of targets over a range of energies further validates and benchmarks the LCS.

Two neutron detector systems will be designed, fabricated, and deployed to collect experimental data in support of this effort. The first detector system uses ^3He (helium) gas tubes. Systems of this type have been used for many years. The second detector system is based on ^6Li (lithium) glass fibers. This newer, solid-state technology uses neutron sensitive scintillating glass fibers as detector elements.

The two detector systems have been designed to measure the neutron multiplicity of large, complex lead and lead-bismuth targets.

OBJECTIVES

To begin developing the database necessary for the validation and benchmarking of the LAHET component of the MCNPX code suite, the UNLV research program has set forth the following objectives. First, the current MCNPX suite will be used to develop models of multi-element neutron detector systems. These models of the detector systems will be incorporated into the design of detailed models for the entire detector-target system. These models will first be used to help design the irradiation experiments, and then will be used to model the behavior of the system. Irradiation experiments corresponding to the detector-target system models will be performed, and measurements of the neutron leakage from the targets will be acquired. High spatial resolution and position sensitive measurements of the source term volume will also be acquired. The results of the experimental campaign will be compared with the simulated system to evaluate the performance of the MCNPX model. This database will also be made available to the code designers to allow them to benchmark the LAHET component of the MCNPX code.

RESEARCH ACCOMPLISHMENTS

Nuclear transport code models and calculations of neutron detection efficiency at various positions in the target-detector assembly were completed and interpreted prior to developing designs of the neutron detection systems needed to perform multiplicity measurements.

Colleagues at the Khlopin Radium Institute (KRI) finished preliminary nuclear transport codes using customized code developed by KRI researchers. These modeling efforts were coordinated with U.S. researchers and results indicate neutron production efficiencies of approximately 13%-19% in a lead target of 40 cm diameter and 1 m in length bombarded with a pulsed 1 GeV proton beam. These results are extremely simplified and represent only a "first cut" at the transport code models.

Numerical models performed at the Harry Reid Center using MCNPX Code were initiated following MCNPX training in January 2002 at UNLV. Dean Curtis, an undergraduate computer science student at UNLV, assisted with MCNPX model development for both the Russian ^3He and the American neutron glass fiber detector systems. Mr. Curtis assisted with the configuration and operation of the PC systems that will execute transport codes and archive modeling results. Mr. Curtis also collaborates with LAN-SCE and UNLV's Mechanical Engineering department to further refine and augment modeling efforts.

KRI colleagues completed preliminary geometric models for the ^3He detector configuration. Carter Hull and Tom Ward approved one of the three models submitted by KRI. Completion of the model for the neutron glass fiber detector prototype permitted the initiation of detector design and fabrication studies. The ^3He target monitoring system, designed for U.S. laboratory needs and experimentation protocols, is in the final design and initial fabrication stages. It is suitable for prolonged, unattended operation. Data can be accessed via telecommunication lines such as direct cabling, modem, and high speed intranet/internet. Dr. Hull and Dr. Ward plan to approve the final design in Russia at KRI sometime after June 2002.

Researchers completed the American glass fiber detector prototype. It is ready to be tested in upcoming target experiments at LANSCE. Various limitations warrant that the experimental detector system not have the spatial resolution required for the actual target and blanket system. However, the proof-of-principle data provided will be invaluable.

FUTURE WORK AND GOALS

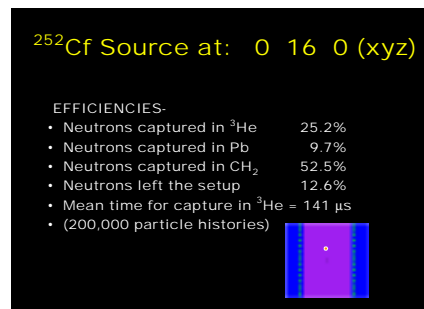
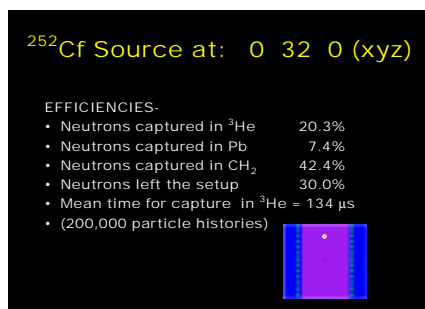
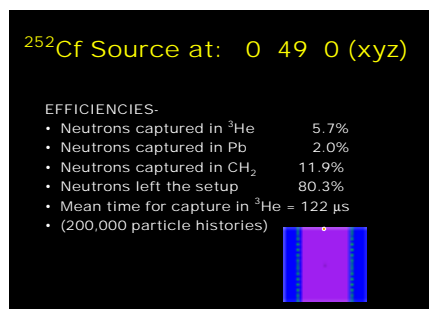
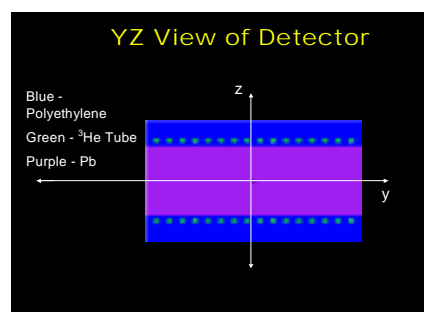
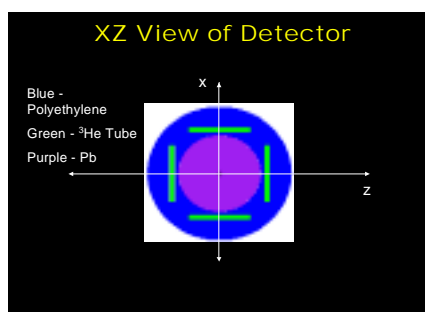
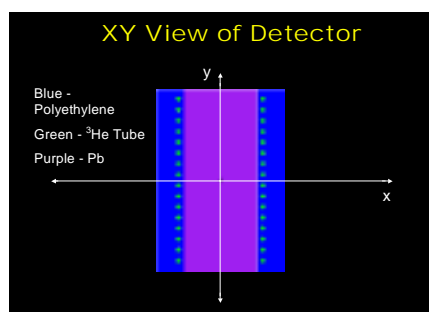
Work in year two and subsequent work includes many tasks:

- refinement of MCNPX models of detector systems (various targets and beam energies);

- completion and modification of the glass fiber neutron detection system;
- integration and testing of the neutron fiber detector and electronics;
- acquisition of initial neutron multiplicity measurements; comparison of models with measurement results;
- review and modification of codes if indicated; and,
- review and validation of the data.

Project results will be submitted for publication in peer reviewed journals. Other goals include additional graduate research projects to refine these initial models and to perform neutron-multiplicity measurements on a variety of targets over a range of energies. These measurements are essential in validating and benchmarking the LCS modeling results of target materials. The neutron leakage measurements will provide a systematic set off precision data that will enable direct comparison with code calculations. These sets of measurements will enable the transmutation program to reduce the uncertainty and risk of design engineering and operation of the sub-critical multiplier system.

Future work may include measurements at the accelerator at Brookhaven National Lab. This accelerator produces beams of pions, kaons, and protons of appropriate energies that could be used to test the codes.



MCNPX Model of Target-Detector System

Research Staff

Carter D. Hull, Principal Investigator, Research Scientist, Harry Reid Center for Environmental Studies
William H. Johnson, Assistant Professor, Department of Health Physics

Students

Steven J. Curtis, Graduate Student. Dean Curtis, Undergraduate Student.

Collaborators

Michael Todosow, Division Head, Nuclear Science and Technology Division, Brookhaven National Laboratory
Eric J. Pitcher, Lujan Center, Los Alamos National Laboratory
Thomas Ward, Science Adviser, U.S. Department of Energy Consultant

Task 7

Development of Dose Conversion Coefficients for Radionuclides Produced in Spallation Neutron Sources

P.W. Patton and M.J. Rudin

GOAL AND BACKGROUND

Ensuring the safety of workers at accelerator-driven nuclear facilities is paramount before these systems can be deployed for nuclear transmutation or any other mission. Spallation neutron sources produce as many as 660 rare radionuclides in either the target or blanket during the spallation process that are not addressed in current radiation protection standards. This research program seeks to address this problem through the generation of internal and external dose coefficients (DCs) for these “new” isotopes. This effort supports not only graduate students at UNLV, but also establishes a research consortium with representatives from several universities and national laboratories.

Dose coefficients are used by radiation safety personnel to determine the radiation dose incurred to a tissue or organ system from a given exposure. To ensure worker safety and limit exposure to radionuclides, these parameters are often expressed in terms of Annual Limits on Intake (ALIs) and Derived Air Concentrations (DACs). Results from this study will produce ALIs and DACs for those rare radionuclides created by current technology that are not included in FGR 11 (Federal Guidance Report No. 11). Additionally, DCs developed will augment radiological data in Publications 68 and 72 of the International Commission on Radiological Protection (ICRP), contributing to the safe operation of accelerator-driven nuclear systems in the United States and abroad.

OBJECTIVES

For the first year of this effort, the UNLV research team set out four objectives. First, the university and laboratory consortium had to be established. This consortium was tasked with helping to determine the methodology for determining the dose coefficients, and to ensure that the resulting DCs will be of use to the national programs developing accelerator-driven nuclear systems (such as the SNS or an accelerator-driven transmutation system) and to the health physics community as a whole. The second goal of this program was to determine a methodology and then prioritize the radionuclides so that the research effort would address the most significant radionuclides first. Working with the Georgia Institute of Technology, the UNLV team then needed to formalize the developed methodologies, and ensure that they are reproducible. The final objective for the first year of this program was to use the developed methodologies to begin generating dose coefficients.

RESEARCH ACCOMPLISHMENTS

The research consortium, consisting of university participation from the Georgia Institute of Technology, Idaho State University, Texas A&M University, University of Florida, UNLV, and Tbilisi State University in Tbilisi, Republic of Georgia was established. This core group of university partners was supplemented by representatives from Department of Energy Laboratories at Los Alamos National Laboratory (LANL) and Oak Ridge National Laboratory (ORNL). From this consortium, a working group was formed to implement the goals and objectives underlining consortium efforts.

The Dose Coefficient Working Group (DC Working Group) directs project activities, prioritized radionuclides that will be considered in this project, developed the methodologies to determine internal and external DCs, and coordinates informational exchange among participants. The DC Working Group met for the first time in Las Vegas in January 2002 and formulated an action plan for the rest of the project.

The DC Working Group developed a draft methodology to determine internal and external DCs. Radiological data was acquired from a nuclear physics database developed at Brookhaven National Laboratory. This data included decay modes, decay energy levels, and radiation energies and intensities. The data was downloaded to an input file for execution in the Dose Calculation (DCAL) program developed by ORNL. Formatting problems encountered while incorporating input files in the DCAL program are currently being addressed.

A prototype methodology to determine dose conversion coefficients for short-lived radionuclides produced in spallation neutron sources was developed by a Georgia Tech graduate student, Mr. Omar Wooten, and Tony Andrade of Los Alamos National Laboratory. Mr. Wooten put radiological data in a format that could be read by DCAL. He determined DCs for 3-4 radionuclides using this method. However, several “bugs” resided in the developed methodology and require refinement before utilization in the UNLV DC project. Mr. John Shanahan of UNLV and Mr. Wooten have been working closely together to troubleshoot computer-programming glitches and further develop the internal DC methodology.

The Working Group prioritized a group of radionuclides for DC determination. These radioisotopes were selected for prioritization because researchers expect their release following air emission or activation of a mercury target after a long irradiation period. The prioritized list was further refined to include only radionuclides with a half-life

greater than 1 minute. 120 radionuclides were identified in the priority group. These radionuclides were then assigned to the various members and groups participating in quantifying DCs. To provide a quality check on the adopted methodology, some radioisotopes were assigned to more than one team. The metabolic models and data from ICRP 30 and 66 will be used for evaluating the dose coefficients, permitting the use of the best technology available while maintaining consistency with current standards.

For consistency with Federal Guidance Report No. 11, dose coefficients will be evaluated for the following target tissues of “reference man”: gonads, breast, lung, red marrow, bone surface, thyroid, and remainder of body. Additionally, the total committed effective dose equivalent (total dose incurred based on radiation type and organ type in a 50 year time frame) will be calculated. From these calculations, the ALIs and DACs can be determined.

To educate participants on the methodology used to generate internal and external dose coefficients for these select radionuclides, UNLV hosted a student workshop in May 2002 in Las Vegas. Students from UNLV, Idaho State University, Georgia Institute of Technology, along with professional staff from Tbilisi State University in Tbilisi, Georgia, attended the workshop. Dr. Keith Eckerman, the new DOE project collaborator, also attended. Following the student workshop, the DC Working Group held its second meeting. Dr. Mark Rudin of UNLV and Dr. Richard Brey of Idaho State University joined participants from the student workshop. The group developed an outline of project tasks for the remainder of the fiscal year.

Individuals and groups represented at the working group meeting will generate input batch files for the following radionuclides: ^{201}Au , ^{61}Co , ^{131}Ce , ^{194}Pb , $^{183\text{m}}\text{Os}$, and ^{41}Ar . Students reviewed the files during the Annual Health Physics Meeting in Tampa, FL in June 2002. Additionally, Adam Arnt of ISU wrote a DC methodology that was modified at the Health Physics Meeting student workshop. Mr. Shanahan is developing a final draft outline of the DC methodology by August 2002. An additional Working Group meeting will be held at UNLV in August or September 2002. Further modifications to this code will facilitate its use for calculating dose coefficients.

HIGHLIGHTS

- The research consortium, including Georgia Institute of Technology, Idaho State University, Texas A&M University, University of Florida, UNLV, Los Alamos National Laboratory (LANL), Oak Ridge National Laboratory (ORNL), and Tbilisi State University in Tbilisi, Republic of Georgia, was established.
- A student workshop was hosted at UNLV to train graduate students from participating universities on the methodology of generating dose coefficients.
- Researchers presented the “Development of Dose Conversion Coefficients for Radionuclides Produced in Spallation Neutron Sources” at the 47th Annual Bioassay, Analytical, and Environmental Radiochemistry Conference, Las Vegas in November 2001 and at the American Nuclear Society Winter Meeting, Student Mini-Conference in Reno, NV November 2001.
- “Development of Dose Conversion Coefficients for Radionuclides Produced in Spallation Neutron Sources” was presented as a poster at the Annual Meeting of the Health Physics Society, Tampa, FL June 2002.

CONTINUED PROGRESS AND FUTURE GOALS

In the second year of the project, researchers plan to expand the number of participants in the DC Working Group. Work will continue to refine and optimize the DC methodology, with a primary focus on reproducibility. The determination of internal and external dose coefficients will continue, expanding the effort to include more radioisotopes.

For FY02, the Dose Coefficient research group plans to generate DCs for approximately 86 radionuclides that could be created from spallation neutron sources. The group also plans to generate results that will be considered for inclusion in a future report from the International Commission on Radiation Protection (ICRP). It is also expected that this work will be presented and published at selected professional meetings and publications.

Research Staff

Phillip W. Patton, Principal Investigator, Assistant Professor, Department of Health Physics
Mark Rudin, Chair, Department of Health Physics

Students

John Shanahan and Yayun Song, Graduate Students

Collaborators

Keith F. Eckerman, Oak Ridge National Laboratory
Faculty and Graduate Students from Idaho State University, Georgia Institute of Technology, Texas A&M University, and University of Florida

Task 8

Development of a Systems Engineering Model of the Chemical Separations Process

Y. Chen, D.W. Pepper, and R. Clarksean

GOAL AND BACKGROUND

Chemical separations processes and technologies are the corner stone of any strategy to reprocess or transmute used nuclear fuel. For the transmutation effort, the actinides, along with iodine and technetium, are the primary targets for partitioning. In the direct disposal waste management strategy currently envisioned, these elements are the primary components of the predicted risk to the public. Even if reprocessing the plutonium as reactor fuel does not come to pass, the removal of transuranics and long-lived fission products from discharged fuel dramatically decreases the toxic nature of the spent fuel significantly.

This research project proposes the development of a comprehensive systems engineering model of the chemical separations processes required for the transmutation program, with the goal of performing a system-wide evaluation and optimization of overall system deployment options. Systems analysis makes it possible to present decision-makers with concise evaluations of system options and their characteristic features. As the sophistication level of the systems engineering model is increased, it becomes possible to make relative comparisons of process options with regard to waste generation, proliferation resistance, throughput capabilities, facility requirements, and cost. Establishing confidence in the models gives the decision-making process greater objectivity and technical credibility.

OBJECTIVES

The first year of this research project was focused on studying and analyzing the process of developing a systems engineering model for the chemical separations processes. Specific research objectives include the following tasks:

- Developing a framework and environment for a systems engineering analysis of the chemical separations system for the program;
- Establishing a baseline systems engineering model from which modifications and improvements can be made; and,
- Refining the existing computer program that gives a detailed examination of the uranium extraction process, a critical component of the overall scheme.

Developing a systems engineering model involves establishing project goals and needs, defining all unit operations, and selecting the commercial software packages/environments to be evaluated. A basic system model must first be developed. As part of this effort, the UNLV research team will refine Argonne National Laboratory's code, the Argonne Model for Universal Solvent Extraction, or AMUSE, which provides a baseline approach to the integrated analysis of the materials separations process.

AMUSE analyzes the uranium extraction process along with other related solvent extraction processes. It defines many of the process streams that are integral to the systems engineering model. Improving and streamlining AMUSE involves reviewing/analyzing code structure, examining other possible implementations, defining first year software activities, developing a verification plan, and modifying/improving the software. Combining the above tasks ensures that calculations made in AMUSE are accurately transferred to the overall systems model. Additional modules will be developed to model pyro-chemical process operations not treated by AMUSE.

CURRENT ACTIVITIES AND ACCOMPLISHMENTS

A number of software products are being evaluated for use in the systems engineering modeling project. These include iSIGHT, MATLAB, LBNL, SPARK (systems tool), ASPEN process modeling tool, Easy 5 (Boeing), Visual Basic/Visual C/C+ and others. Criteria for selecting one of these products includes the following: the ability to interact with a wide range of existing simulation tools written in a number of different languages and forms; the ability for the user to seek out and determine all input values and assumptions for each simulation package; the potential for integration over a disperse network system; the need for a drag and drop approach to adding additional components to the process; a simple process to transfer data between components; and, an ability to optimize individual processes or the complete system.

Preparation for system engineering development included specialized training. AMUSE code training was held in October for students, and a WebX training and informational conference for iSIGHT was held from 9-11:20 a.m. on December 14.

Once the software project has been selected, student training begins. The complete process will be defined within the selected software environment over the next several months. Attendance at the Argonne National Laboratory Transmuter Fuel Development Workshop made it clear that the product must be capable of analyzing a wide range of processes quickly and easily. Additionally, it is clear that developing a systems engineering model of the complete process proves quite valuable in assessing many of the proposed concepts.

The AMUSE code is currently being studied and analyzed. The interface of AMUSE has been designed using Visual Basic. The mass balance interface code has been designed and developed. The UREX visual Basic interface and design and implementation is still in progress. A software interlace model of the uranium extraction process is being written in visual basic.

To date, the system engineering model will be coupled with the graphical interface AMUSE code, MATLAB, and iSIGHT.

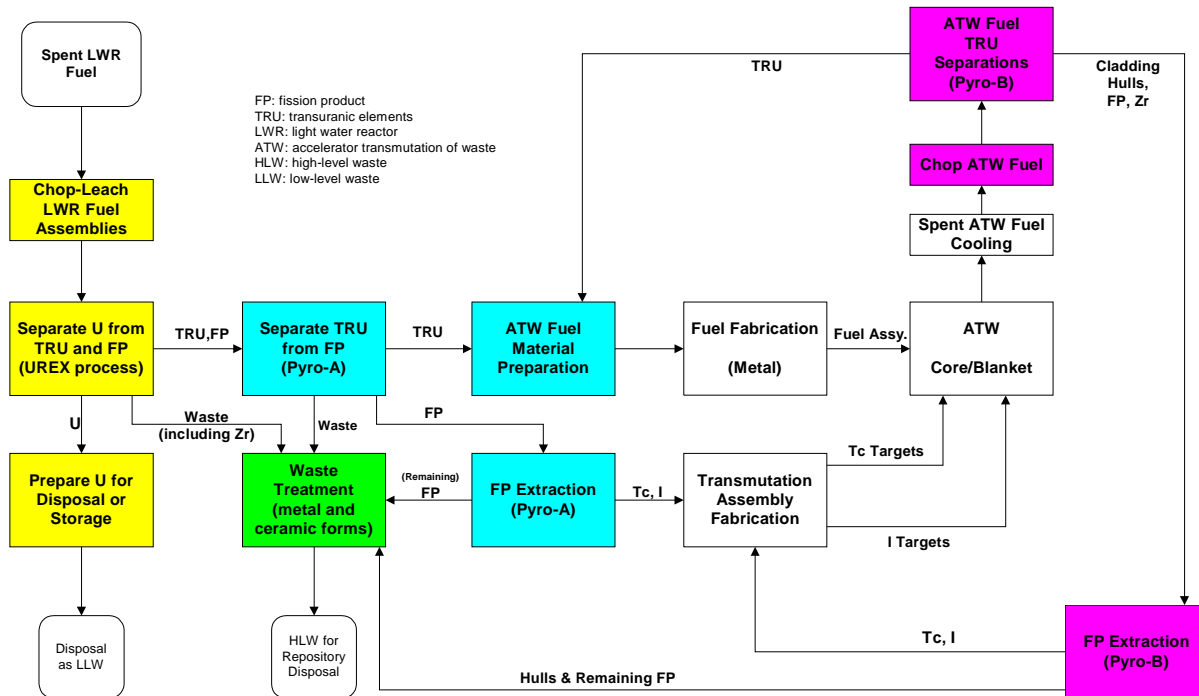
FUTURE PROGRESS AND GOALS

Work on revising the AMUSE code will continue. Since the AMUSE code analyzes chemical extraction processes, including uranium extraction, and defines many of the process streams integral to the systems engineering model, the calculations made in AMUSE need to be accurately transferred to the overall systems model. Additional modules will be created to expand the capabilities of the AMUSE code to address other solvent extraction processes, and new modules will be developed for analyzing the pyrochemical process operations. These modules will be refined as experiments are conducted.

This system model will then be used to analyze case studies and designs at ANL and UNLV to demonstrate the basic or advanced engineering system model. Additional analysis work conducted during this time will validate the engineering systems model efforts. It would also support the testing program associated with various models. Detailed modeling work will continue from year 1 to refine the existing models and to make detailed comparisons to the experimental test results. Finally, work will continue to optimize the AMUSE uranium extraction process.

HIGHLIGHTS

- Presentation of “Development of an Integrated System Engineering Interface for the Chemical Separations Process (AMUSE)” by Sridhar Munaga at the ANS Student Mini-Conference in Reno, Nevada, November 2001.
- Presentation of “Development of a Systems Engineering Model of the Chemical Separations Process” by Lijian Sun and Jianhong Li at the ANS Student Mini-Conference in Reno, Nevada, November 2001.
- Presentation of “Development of a Systems Engineering Model of the Chemical Separations Process” by Lijian Sun at the TRP Seminar at UNLV, Las Vegas, Nevada, April 2002.
- Conference paper entitled “Development of a Systems Engineering Model of the Chemical Separations Process” by L. Sun, J. Li, Y. Chen, R. Clarksean, D. Pepper, J. Laidler, and G. Vandergrift at the International Congress on Advanced Nuclear Power Plants/ANS, Hollywood, FL June 2002.



A block diagram of the current separations process as envisioned by Argonne National Laboratory researchers.

Research Staff

Yitong Chen, Principal Investigator, Assistant Director, UNLV Nevada Center for Advanced Computational Methods
Darrell W. Pepper, Dean, UNLV College of Engineering
Randy Clarksean, Adjunct Professor, Mechanical Engineering Department

Students

Lijian Sun, Sridhar Munaga, and Jianhong Li, Graduate Students
Yulien Chen, Undergraduate Student

Collaborators

James J. Laidler, Senior Scientist, Chemical Technology Division, Argonne National Laboratory
George F. Vandergrift, III, Senior Scientist, Chemical Technology Division, Argonne National Laboratory

Task 9

Design and Evaluation of Processes for Fuel Fabrication

G. Mauer

GOAL AND BACKGROUND

One of the primary concerns in selecting a fuel matrix for actinide-bearing fuels, such as those for transmutation systems, is fuel fabrication. Fuel fabrication technologies for the fabrication and re-fabrication processes must meet several technical considerations, such as minimizing secondary radioactive waste streams, economic viability, reasonable capital outlay, and must be easy to maintain over the transmuter core life cycle. Additionally, the fuel type chosen must be easily manufactured in a remote environment. The volatile behavior of americium during thermal processing further complicates these goals. Currently, the national program is investigating a number of candidate fuel matrices: metallic, ceramic, dispersion, nitride, and carbide/TRISO, just to name the leading candidates.

This project examines the manufacturing processes currently under consideration for these fuel types, as currently envisioned by the Argonne National Laboratory-West manufacturing group. Each fuel type requires developing a distinct remote fabrication process. Conceptual fuel fabrication processes for the fuel types will be developed in conjunction with ANL. This knowledge allows scientists to make an informed selection regarding which candidate fuels require further development and irradiation testing for a transmutation system.

OBJECTIVES AND RESEARCH METHODS

The first phase of the research effort devoted time to the analysis and assessment of the multiple steps required in the manufacture of different fuel types. Following collection of pertinent manufacturing and process-related information, a database was created to provide information on characterizing the design, operations, and cost implications of various fuel choices. Researchers anticipate that the fabrication processes for different fuel types would differ in terms of equipment types, throughput, and cost. Due to the interactive nature of the modeling and design of the fuel fabrication processes, close cooperation with the fabrication development group at ANL and other researchers is essential to the long-term success of this effort.

Conceptual modeling of a sample manufacturing process was performed by developing a 3-D model of a sample process, its flow of materials, and the equipment required to handle the material flow. These models aid in the identification of issues, costs, and impacts of each fuel type on the fuel manufacturing process and the transmuter fuel cycle. Detailed process models were developed after outlining preliminary requirements for large-scale fuel production in a remote environment for a network of transmutation systems. Realistic simulations permit the prediction, analysis, and elimination of potential problems. The dynamic system simulation detects inconsistencies and possible design flaws. It allows for timely modifications to previously unsuspected problem areas.

RESEARCH ACCOMPLISHMENTS

The UNLV research team achieved the following tasks during the first year of research:

- Survey of candidate transmutation fuels, coupled with a detailed evaluation of the identified fuel manufacturing processes following criteria established by the national fuel development program;
- Conceptual computer modeling of one manufacturing process allowing the identification of areas where automated processes are crucial to maintain the required throughput rates;
- Mr. Richard Silva, M.S. student, developed an initial work cell simulation with two robots. He will continue to develop detailed 3-D process simulation models for his thesis project; and,
- Mr. Jae-Kyu Lee, a Ph.D. student, developed a conceptual methodology for vision-based hot cell supervision and control.



Dual slave arm end effector in the UNLV Robotic Hot Cell Unit. The master is configured identically, and is guided by a human operator.

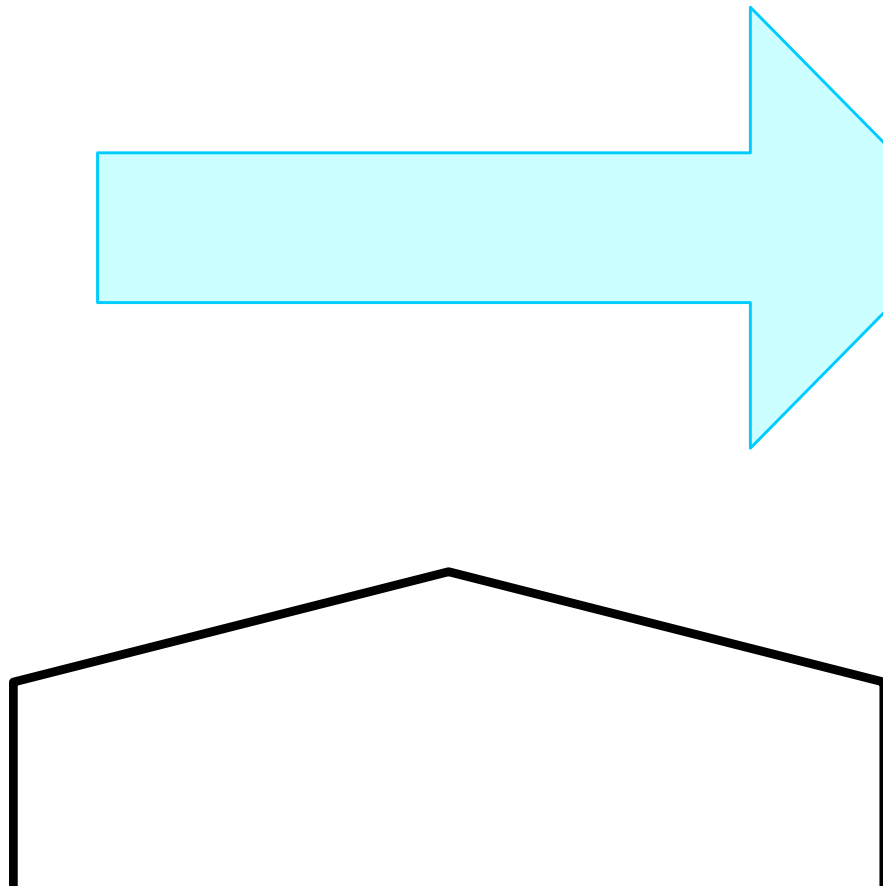
CONTINUED PROGRESS AND FUTURE GOALS

The second phase of the project involves the identification and analysis of remote manufacturing technologies required for efficient large-scale remote fuel fabrication. Process models developed in the project would be available to Transmutation Program personnel for a more accurate definition of the impact of fuel choice on the transmuter fuel cycle. In particular, the process models could better define relative process losses, waste generation, and capital cost for the three potential fuel types. These process models would allow the early identification of issues that may disqualify a fuel type for consideration in a transmutation system in the system specification process. Models will

HIGHLIGHTS

- A Transmutation Research Program seminar presentation by Mr. Jae-Kyu Lee, Ph.D student, and Dr. G. Mauer, P.I., entitled “Transmuter Fuel Fabrication Process.”
- Presentation of a paper entitled “Transmuter Fuel Fabrication Processes” by J.-K. Lee at the ANS Student Mini-Conference in Reno, Nevada, November 2001.

also allow more accurate definitions of requirements for automation.



Possible Configuration for Powder Processing (e.g. Oxide or Nitride Fuel) Fabrication Work Cell.

Research Staff

Georg Mauer, Principal Investigator, Professor, Mechanical Engineering Department

Students

Jae-Kyu Lee and Richard Silva, Graduate Students
Tim Atobalele, Undergraduate Student

Collaborators

Mitchell K. Meyer, Group Leader, Fabrication Development, Argonne National Laboratory
Yue Guan, Advanced Systems Technology and Management, Inc., Consultant to Argonne National Laboratory

Task 10

Development of a Mechanistic Understanding of High-Temperature Deformation of Alloy EP-823

A. Roy and B.J. O'Toole

GOAL AND BACKGROUND

Alloy EP-823 has been developed as a structural material for Lead Bismuth Eutectic (LBE) systems, such as those under development for nuclear transmutation systems, as well as other applications. However, very little data regarding the mechanical properties of this alloy exists in the open literature, particularly in the temperature regime of interest for transmutation systems. To address this need, the UNLV research team, in collaboration with researchers from Los Alamos National Laboratory, has developed a research program to evaluate tensile properties of Alloy EP-823 stainless steel at elevated temperatures, which is not being performed at any other facility to date. Overall, results will lead to the development of a mechanistic understanding of the elevated-temperature deformation processes in this alloy as a function of thermal treatment.

RESEARCH OBJECTIVES AND METHODS

The focus of this work is to evaluate the effect of elevated temperatures (300-540 C) on the tensile properties of the candidate target material, Alloy EP-823. The impact of heat treatment on the tensile properties will also be evaluated. Test materials will be heat treated and machined prior to the measurement of their tensile properties at temperatures relevant to the transmutation applications.

Graduate student Martin Lewis will be trained on the mechanical testing equipment and surface analysis techniques. Deformation characteristics of tensile specimens will be evaluated by surface analytical techniques using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Metallurgical microstructures of the broken tensile specimens will be evaluated using standard methods such as polishing and etching. The morphology and extent of failure in each specimen tested will be studied using the SEM. TEM will be used to study high-temperature deformation characteristics including the distribution and nature of dislocations and other imperfections that will establish deformation mechanisms for the tested material.

Effect of temperature on mechanical properties will be determined and correlated with changes in microstructure for the different heat treatments. This work will serve as part of the work scope for the M.S. Thesis of Martin Lewis. The proposed research program will also generate the following data:

- Uniform elongation vs. temperature;
- Reduction in area vs. temperature;
- Yield strength vs. temperature;
- Ultimate tensile strength vs. temperature;
- Metallurgical microstructure vs. thermal treatment;
- Failure mode (ductile vs. brittle) vs. thermal treatment; and,
- Deformation modes (TEM).



Tensile testing machine with elevated temperature jacket.

RESEARCH ACCOMPLISHMENTS

Three batches of EP-823 alloy have been melted. Ingots processed by hot working converted them into round bars at an off-site facility. One batch of this material has been heat treated (quenched and tempered) at UNLV to produce a fully tempered martensitic microstructure. The hardness of the material has been measured, and experiments are well underway to machine tensile specimens from these heat treated bars.

Ambient-temperature tensile data will be generated as the test specimens become available. To allow tensile testing in the inert gas chamber, round wedges for specimen grips in the MTS were ordered. Currently, these round bars are being evaluated using MTS equipment to generate ambient temperature mechanical properties. The high-temperature, inert gas chamber for the high-temperature mechanical testing has arrived and has been installed. Service connections (water, 220V power, and gas lines) are currently being installed in the laboratory and connected to this experimental system.



Testing specimens.

Martin Lewis, a M.S. graduate student in the Mechanical Engineering Department presented a paper at the ANS student mini-conference in Reno, NV. "High Temperature Deformation Characteristics of Alloy EP-823" highlighted work completed on this martensitic stainless-steel from initiation of this project until November 2001.



Heavy duty torsion and tensile testing machine.

FUTURE WORK AND GOALS

The high temperature experiments on EP-823 will be initiated once the service connections for the laboratory are installed. The experimental campaign will then continue with the remaining alloy batches and the impact of heat treatments will be examined.

Research Staff

Ajit Roy, Co-Principal Investigator, Associate Research Professor, Mechanical Engineering Department
Brendan O'Toole, Co-Principal Investigator, Assistant Professor, Mechanical Engineering Department

Students

Martin Lewis, Graduate Student
John Motaka, Undergraduate Student

Collaborators

Stuart A. Maloy, Los Alamos National Laboratory

Task 11

Nuclear Criticality Analyses of Separations Processes for the Transmutation Fuel Cycle

W. Culbreth, T. Pang, and D. Beller

GOALS AND BACKGROUND

The separation and partitioning of used commercial reactor fuel is a vital component of any reprocessing or transmutation strategy. To process the high actinide fuels required for a transmutation effort, the Chemical Technology Division (CMT) at Argonne National Laboratory (ANL) is developing a pyrochemical separations process. Currently, this work is being done via small experiments. While this is more than sufficient to develop the technologies required to process actinide-bearing fuels, it does not allow for the direct investigation of criticality concerns that would be present in larger systems. As the volume of waste to be treated increases, a higher probability exists that fissionable isotopes of plutonium, americium, and curium can accumulate, forming a critical mass. These criticality events can be avoided by ensuring the effective neutron multiplication factor, k_{eff} , remains below a safe level. Monte Carlo simulations to evaluate k_{eff} are the best way to examine the criticality safety of the proposed separation processes, and will allow engineers to develop proper safety measures for the reprocessing and fabrication of high actinide fuels.

A related problem for handling high actinide fuels is the heat generated by the decay of the higher actinides. In particular, the presence of curium in transuranic wastes poses a significant problem. To minimize the impact of curium on the fabrication of actinide-bearing fuels, the process engineers and chemists would like to remove the curium from the fuel. Curium, however, not only poses a criticality concern, but also includes isotopes that generate a great deal of decay heat. This heat generation creates safety problems with regards to handling and storing curium. The decay heat can cause samples to melt very quickly if excessive quantities of curium are present. SCALE, a Monte Carlo code, simulates the scattering and absorption of neutrons. This technique permits assessment of what quantities of curium will result in a critical mass. This information is then combined with thermal transfer models to examine the decay heat issue, and evaluate thermally and critically safe storage configurations for curium-rich waste streams.

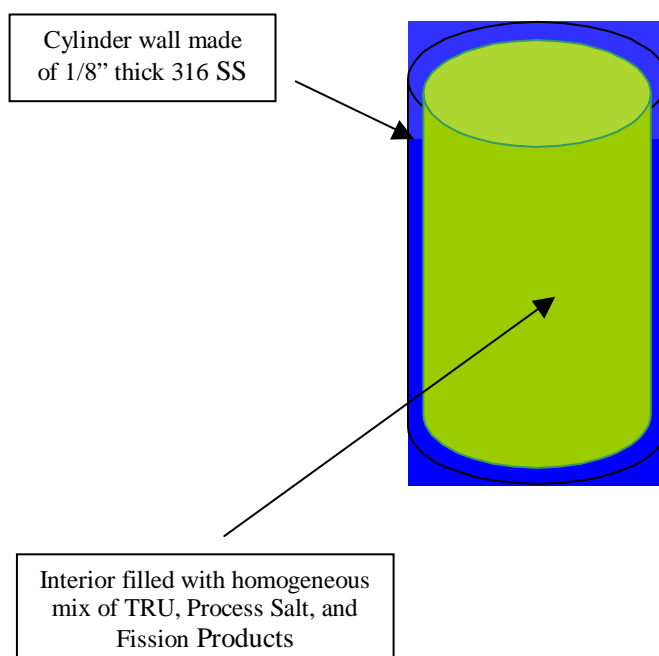
RESEARCH OBJECTIVES AND METHODS

The primary objective set out by the UNLV research team was to build expertise in criticality safety at UNLV, and then to use that expertise to analyze problems and develop tools for the CMT group at ANL in order to support the development of these new separations and partitioning technologies. For the first year, the UNLV research team set forth the following goals: (1) train the UNLV students to use the specialized codes necessary to examine criticality safety; (2) develop models, using these codes, to assess

neutron multiplication factors for geometries and material concentrations of interest to the chemists and chemical engineers developing the technologies; (3) develop software to incorporate criticality estimates into the existing ANL models for the pyrochemical treatment processes; and, (4) to bring the students to meet the chemists and engineers at ANL to identify, understand, and verify research objectives and goals established through collaboration with ANL. Additionally, the UNLV research team was requested to examine not only the criticality concerns, but also the thermal concerns associated with the storage of separated curium.

RESEARCH ACCOMPLISHMENTS

Through the meetings between the UNLV research team and the CMT at ANL, the modelers were able to gain significant insights with respect to the geometry of the equipment used in fuel separation along with scenarios that can lead to potential criticality events. Being able to actually see the equipment used allowed the modelers to better understand the complexity of working with radioactive and fissionable substances through glove boxes, which in turn



Cylindrical problem with TRU, process salt, and fission products.

allowed them to develop more useful alternative approaches that would minimize criticality risk while still being useable by the researchers and engineers at the CMT in these difficult conditions. Results from the criticality simulations were submitted as a report to ANL entitled, "Assessment of Criticality Safety for Cylindrical Containers to be used in the Processing of Spent Fuel". These results were subsequently integrated into the excel model developed by the CMT researchers to support the development of their experiments and flowsheets. The UNLV code package assesses the maximum mass of transuranic material that can be safely accumulated in a pyrochemical cell. This code was based on models developed by the students using the SCALE code to assess the safety of the pyrochemical cell as transuranics are accumulated.

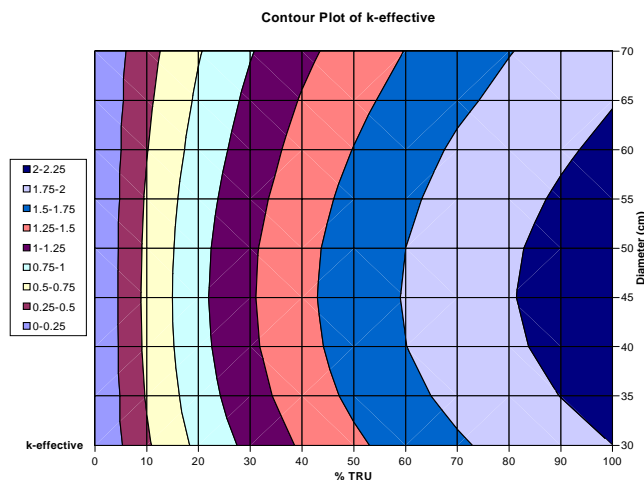
During this effort, the group's collaborators at ANL came to focus on the particular problems associated with separating and handling curium. As a result, ANL requested that the UNLV team re-direct their research to examine the potential for curium samples to "go" critical. Ms. Elizabeth Bakker (UNLV undergraduate Mechanical Engineering student) analyzed the problem using SCALE. This work was documented extensively in the "Fission and Thermal effects in Curium Separated from Spent Nuclear Fuel" report that was submitted to ANL. This report documents the thermal hazard involved with separating curium from spent nuclear fuel, the fissionable isotopes produced, and the maximum mass of curium that can be safely stored. This work also included parametric studies to determine k_{eff} values for specific geometries, component concentrations, radionuclide content, and fuel configurations.

FUTURE WORK AND GOALS

The UNLV research team is working with their collaborators in the CMT at Argonne to develop and scope out additional criticality problems for analysis. One issue already identified relates to the criticality safety of the pyrochemical cells. The UNLV research team will also begin the evaluation of various candidate separations processes for efficiency, safety, reliability, and cost. These evaluations, along with the criticality safety analyses, are a vital component of the safety case for these processes, and are a necessary step in designing activities for process equipment and facilities that must begin in the not too distant future.

HIGHLIGHTS

- Ms. Bakker, Mr. Lowe, (Students, UNLV-ME) presented papers on this work at the American Nuclear Society Student Conference, as well as posters at the ANS Conference, both held in Reno, NV, in November 2001.
- Mr. Jason Viggato, a graduate student employed on this project, completed his graduate studies and went to work for Bechtel-SAIC as part of the Yucca Mountain Project, analyzing thermal and criticality problems for the proposed national nuclear waste repository (putting his training from the UNLV project to work).
- Two reports, "Fission and Thermal Effects in Curium Separated from Spent Nuclear Fuel" and "Assessment of Criticality Safety for Cylindrical Containers to be used in the Processing of Spent Nuclear Fuel," were prepared and delivered to the team's collaborators at Argonne National Laboratory.



Contour Plot of the Effective Neutron Multiplication Factor as a function of cylinder diameter and % TRU in the mixture.

Research Staff

William Culbreth, Principal Investigator, Associate Dean for Research, College of Engineering
 Tao Pang, Professor, Department of Physics
 Denis Beller, Los Alamos National Laboratory, TRP Intercollegiate Programs Coordinator, Harry Reid Center, UNLV

Students

Jason Viggato and Maurice Moore, Graduate Students
 Elizabeth Bakker and Daniel Lowe, Undergraduate Students

Collaborators

James J. Laidler, Senior Scientist, Chemical Technology Division, Argonne National Laboratory
 George F. Vandergrift, III, Senior Scientist, Chemical Technology Division, Argonne National Laboratory

Task 12

Radiation Transport Modeling of Beam-Target Experiments

W. Culbreth and D. Beller

BACKGROUND

The ability to accurately model the performance of an accelerator-target system and assess its performance is vital to the development of accelerator-driven transmutation systems. Los Alamos National Laboratories developed the MCNPX code suite, a Monte Carlo radiation transport code, for this purpose. This code is widely used by national programs and most international programs developing accelerator-driven systems to model the behavior of the accelerator-target system. These models are then used to assist in designing experiments, evaluating system designs, and other applications necessary to support the development of this technology.

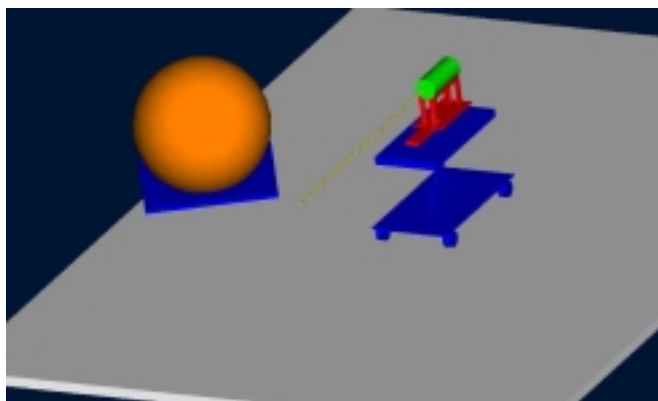
Through these modeling efforts, however, researchers have found that the uncertainties in the nuclear data within the reference libraries, and those introduced by assumptions within the computational methods used by MCNPX, lead to significant uncertainties in the predicted performance. These propagated uncertainties are even more significant at high energies. To address these uncertainties in the nuclear database, researchers are currently conducting experiments at national laboratory facilities (such as the LANSCE facility at LANL) to generate the data needed to benchmark the MCNPX models that predict neutron production and leakage rates from targets. Student researchers at UNLV are a part of this research effort, serving the effort by developing the models of the experimental systems and analyzing the data from the experiments.

RESEARCH OBJECTIVES AND METHODS

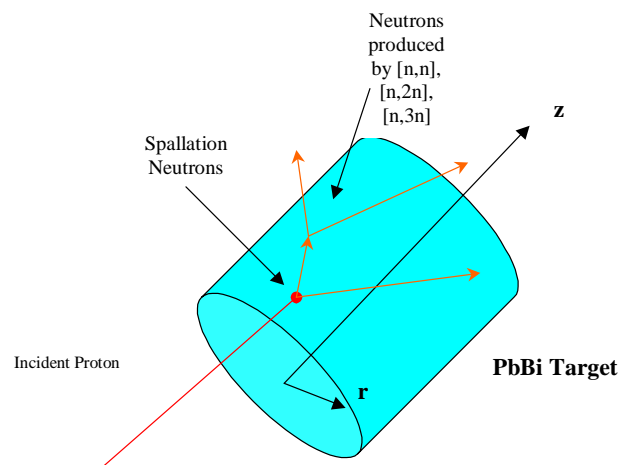
In the first year of the UNLV effort, researchers planned to develop the models of the experimental systems to predict the neutron flux and leakage from the experimental targets using the MCNPX code suite in order to help determine these missing parameters. To support these models, the researchers project, or estimate, values for the unknown parameters describing various events and phenomena occurring within the beam-target experiment. The results of these simulations will then be compared against the observed neutron leakage rates and energies. The estimates for the unknown parameters are then revised to correlate with the observed values (these parameters cannot be measured directly, and must be determined by inference). The resulting models will then be validated and benchmarked against data from future experiments. These models, even before being validated, have also been instrumental in designing the experiments themselves.

RESEARCH ACCOMPLISHMENTS

In the first year, the UNLV research team completed the modeling and analysis of experiments conducted to assess neutron leakage, sodium activation, actinide fission, and neutron multiplicity. Through participation in the MCNPX workshop at UNLV, the research team received the training in using the code that allowed the students to participate directly in the modeling and analysis of the experimental campaigns conducted at LANSCE. The first collaborative experimental campaign was the neutron leakage test experiments on LANSCE. Preliminary results from the experiment are in good agreement with the model projections for the neutron energy spectra. Refinements of the model to improve the agreement are currently underway.



Schematic of the Experiment at LANSCE, December 2002.



Leakage of High Energy Neutrons from a Spallation Target.

FUTURE WORK AND GOALS

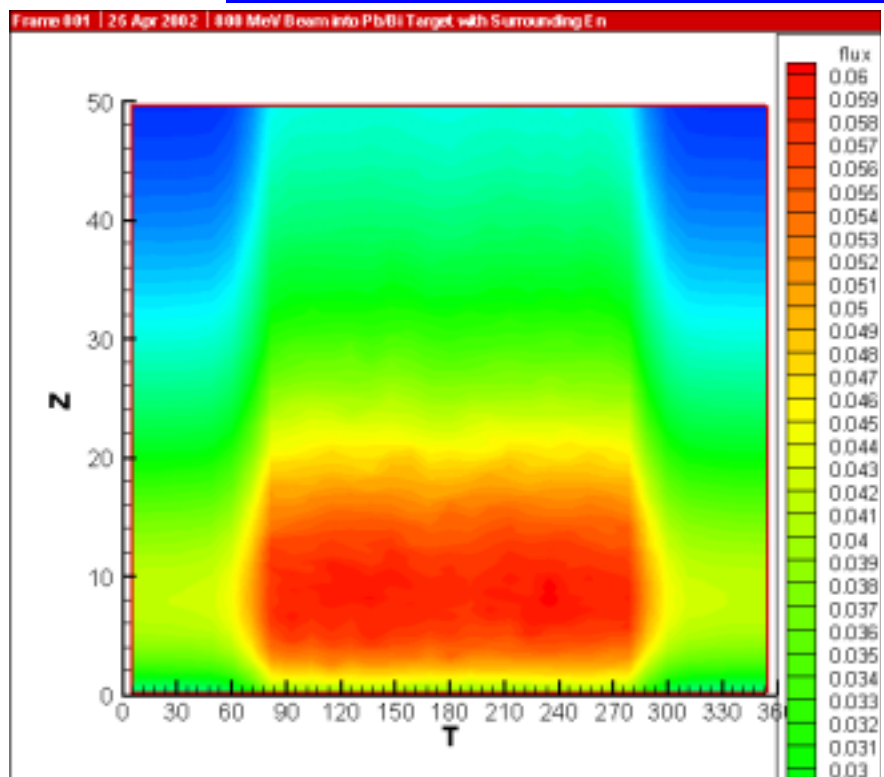
The simulation of experiments at LANSCE will continue, modeling both already completed experiments (to benchmark the codes) and to assist the planning and analysis of future experiments. For example, the research team has been added to the experiments led by Dr. Pitcher (LANL) to analyze the activation induced by neutrons passing throughout the sets of foils attached to the spallation target. Work will also continue in support of the neutron spallation experiments.

The UNLV team also plans to develop a benchmark program for the neutron leakage tests and other tests related to transmuter development. This program will parallel the international benchmark experiments and modeling conducted by the OECD nuclear energy agency and cooperating laboratories. As part of this effort, a comprehensive, three dimensional CAD image of the LANSCE experimental set-up will be developed to ensure accurate geometric data for MCNPX modeling.

HIGHLIGHTS

- Based on the success to date in supporting the LANL/LANSCE experiments, UNLV has been asked to collaborate on experiments at the Idaho Accelerator Center (IAC). Suresh Sadenini, a graduate student in the UNLV Mechanical Engineering department accompanied Prof. William Culbreth (UNLV-ME) to visit the IAC to plan for an experimental campaign for the summer 2002. IAC staff invited Mr. Sadenini to assist with the experiment, provide simulations, and analyze data.
- Students presented their research at the American Nuclear Society Conference in Reno, November 2001.
- Mr. Daniel Lowe, student in the UNLV Mechanical Engineering Department, has been invited to spend six weeks at LANSCE to conduct MCNPX simulations and assist with the planned neutron spallation tests. His work contributed to the preparation of a benchmark program for these tests.

Neutrons per Square Centimeter per Incident 800 MeV Proton on a Lead Bismuth Target



Research Staff

William Culbreth, Principal Investigator, Associate Dean for Research, College of Engineering
Denis Beller, Los Alamos National Laboratory, TRP Intercollegiate Programs Coordinator, Harry Reid Center, UNLV

Students

Ashraf Kaboud and Suresh Sadenini, Graduate Students
Daniel Lowe, Undergraduate Student

Collaborators

Raymond Klann, Argonne National Laboratory

Program Information

Transmutation Research Program Infrastructure Augmentation New Faculty and Staff

Ajit K. Roy received his Ph.D. in Metallurgical Engineering from Case Western Reserve University, Cleveland, OH in 1981. His specialty areas in metallurgical engineering include mechanical metallurgy, physical metallurgy, alloy development, failure analysis, and metallurgical characterization. Additional expertise in corrosion engineering includes environment-assisted cracking, localized corrosion, galvanic corrosion, and electrochemical principles. He brings his knowledge to UNLV as an Associate Research Professor. Currently, he serves as Principal Investigator for a number of research projects for the Transmutation Research Program and the Yucca Mountain Project. These include the following tasks: "Delayed Hydride Cracking of Spent Fuel Cladding under Repository Conditions," "Hydrogen-Induced Embrittlement of Candidate Target Materials for Applications in Spallation-Neutron-Target Systems," "Development of a Mechanistic Understanding of High-Temperature Deformation of Alloy EP-823 for Transmutation Applications," and, "Use of Positron Annihilation Spectroscopy for Stress-Strain Measurements."



Longzhou Ma received his Ph.D. in Mechanical Engineering from West Virginia University, Morgantown, WV in 2001. His experience in superalloy environmental-assisted crack propagation studies, fracture mechanics analysis, microstructure characterization using SEM, TEM, and optical microscopy, as well as materials failure analysis augment his role in the Transmutation Research Program. Other areas of expertise include heat treatment, physical metallurgy investigation, material deformation, and manufacturing process development. Dr. Ma interned at Special Metal Co. in Huntington, WV and with the Exposure Assessment Branch of NIOSH in Morgantown, WV. He authored and co-authored several publications. Prior to enrollment at West Virginia University, he worked as a Metallurgical Engineer in China. Dr. Ma's work as a graduate assistant in China and West Virginia and his dissertation work on environmental-assisted crack growth model and microstructure characterization in superalloy INCONEL 783 characterizes his suitability as a Research Scientist within UNLV's Harry Reid Center for Environmental Studies.

Robert J. Fairhurst joined UNLV's College of Sciences in June 2002 following completion of his Ph.D. degree at the University of Houston, Texas. He brings to UNLV extensive experience operating equipment and performing analytical techniques. These experiences include operating the JEOL JXA electron microprobe (EMP), JEOL JSM-6330F scanning electron (SEM), and x-ray diffractometer Gadds. Additionally, he is knowledgeable in ICP-AES, inductively-coupled plasma atomic emission spectrometry, various mass spectrometry techniques, atomic absorption spectroscopy, gas chromatography, and high performance liquid chromatography. He served as a research assistant when he was a Ph.D. student and taught introductory chemistry laboratories, including honors sections. His knowledge and background proves to be an asset while operating the Electron Microanalysis and Imaging Laboratory at UNLV.



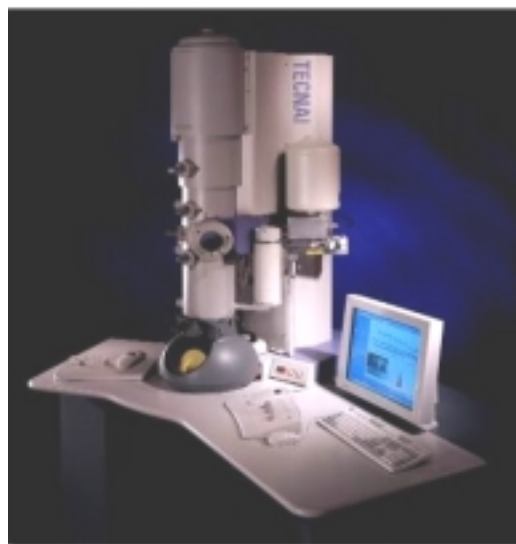
Transmutation Research Program Infrastructure Augmentation New Equipment and Facilities

Materials Performance Laboratory

The UNLV Materials Performance Laboratory (MPL) has numerous research and development capabilities in areas of metallurgical and corrosion engineering using state-of-the-art techniques. MPL is well equipped to study the effect of heat treatment on the resultant metallurgical microstructure and mechanical properties of engineering metals and alloys at ambient and elevated temperatures in the presence of an inert atmosphere. The susceptibility of many metallic materials and alloys to environment-induced degradation such as localized corrosion, stress corrosion cracking (SCC), and hydrogen embrittlement (HE) can be evaluated in MPL using both conventional and electrochemical test methods. Environment-assisted cracking behavior such as SCC and HE, which are of major concern in different energy-related applications such as nuclear power generation, oil and gas exploration, and geothermal energy development, can be precisely determined under constant load and slow-strain-rate (SSR) conditions in different aqueous environments of interest. The susceptibility of these alloys to localized corrosion such as pitting corrosion; crevice corrosion, and intergranular attack can be evaluated by electrochemical polarization techniques at ambient and elevated temperatures. In essence, this world class UNLV research laboratory is capable of materials characterization as functions of numerous metallurgical and environmental variables related to engineering applications. Pictures of equipment in the MPL can be found on pages 3, 13, 24, 25, and 35.

Transmission Electron Microscope (TEM)

A state-of-the-art transmission electron microscope (TEM), the TECNAI-F30-SUPER-TWIN series TEM, will be available for research needs at UNLV's Harry Reid Center for Environmental Studies. The Transmutation Research Program at UNLV (formerly the Advanced Accelerator Applications Program) purchased this equipment. This highly versatile tool used to explore in-depth structure within the microscopic world in disciplines spanning life sciences and materials sciences. This acquisition institutes tremendous scientific advancement for research at UNLV and within the research community.



Electron Microanalysis and Imaging Laboratory (EMIL)

The JEOL-5600 Scanning Electron Microscope (SEM) is optimized for imaging micron to millimeter scale topography. The SEM is equipped with a backscattered electron (BSE) detector and an Oxford ISIS EDS system, capable of qualitative analysis. Topographic and compositional images can be processed on the screen to show pseudo-color and critical point measurements of features. The images can also be combined, allowing for easy comparison of samples or different magnifications.

The JEOL-8900 Electron Probe Microanalyzer (EPMA) offers quantitative, non-destructive chemical analysis of solid materials on a micron scale. Four automated wavelength dispersive spectrometers and an energy dispersive spectrometer collect a full spectrum of X-rays at once. These spectrometers can examine up to eight elements at one time and obtain high-precision X-ray maps and line scans of spatial variation in chemical composition. Additional detectors permit the production of "real time" images or automated images in tandem with X-ray mapping to further characterize the area of interest.

Pictures of equipment in the EMIL can be found on pages 3, 35, and 36.

Program Highlights 2001-2002

January 18, 2001

UNLV hosted TRP Mini-Workshop for UNLV researchers and National Laboratory personnel

February 2, 2001

UNLV TRP website <aaa.nevada.edu> launched

March 29, 2001

Call for Proposals and supporting documents distributed

March 29-April 1, 2001

UNLV TRP Recruiting Booth at ANS/HPS Student Conference

April 4, 2001

UNLV TRP Intercollegiate and International Program Coordinators establish offices at UNLV

May 24, 2001

Summer term begins; 4 student research task proposals receive funding to start

June 29, 2001

UNLV TRP Special Workshop and Tour for DOE-NE visitors and MOU Signing Ceremony: UNLV Pres. Harter and DOE-NE Dir. Magwood

July 1, 2001

Dr. Ajit Roy joins UNLV's Mechanical Engineering Department

August 27, 2001

Fall academic term begins; 8 new student research tasks start

October 5-7, 2001

UNLV TRP students and staff sponsor booth and Transmutation Poster at the Harvest Festival in Pahrump, Nevada

October 9, 2001

AMUSE Code Training at UNLV, conducted by ANL staff

November 9-15, 2001

UNLV TRP Conference Committee organizes participation for 24 UNLV students and 11 faculty members at ANS and ADTTA conferences in Reno, NV

November 9-11, 2001

Accelerator Applications Embedded Sessions in ANS Student Mini-Conference, Reno, NV organized by UNLV — 14 papers presented by UNLV TRP students covering all 12 Tasks. One Best Session Paper award received.

November 11-15, 2001

ANS Accelerator Applications and ADTTA Conference in Reno, NV. 3 papers presented by UNLV TRP faculty.

November 12, 2001

International Molten Metal Target Advisory Group meeting, Reno, NV: UNLV proposal for use of ISTC Target agreed upon, establishment of International Advisory Committee recommended.

December 2, 2001

Dr. Longzhou Ma joins UNLV's Harry Reid Center

December 12-14, 2001

UNLV administrators visit the Institute for Physics and Power Engineering and the Institute For Nuclear Power Engineering, Obninsk, Russia

December 16-18, 2001

UNLV administrators visit the Khlopin Radium Institute and St. Petersburg State Institute of Technology, St. Petersburg, Russia

January 14-18, 2002

MCNPX Training at UNLV

January 16, 2002

TRP Student Poster Session

February 12-13, 2002

UNLV hosted national AAA University Workshop

May 28, 2002

ISTC Target arrives from LANL for new LBE loop facility

June 1, 2002

Dr. Robert Fairhurst joins the College of Science

June 20, 2002

TEM (valued at over \$2 million) purchased from FEI for \$1.3 million.

Transmutation Research Program Financial Statement

Program Administration	\$2,209,194
Program Support	
Labor	\$178,882
Other Costs (e.g. travel, conference support, supplies)	\$192,958
Infrastructure Augmentation: New Faculty and Staff	\$121,115
Infrastructure Augmentation: Facilities and Equipment	\$1,553,739
Los Alamos National Laboratory Subcontract (Intercollegiate Programs Coordinator)	\$162,500
Student Research Tasks	\$790,806
Labor	\$524,323
Other Costs	\$266,483
Total	\$3,000,000
Labor	\$824,320
Other Costs	\$2,175,680

Student Research Task by Task			
	FY01	FY02	Total 12-month Budget
Task 1	\$97,379	\$44,058	\$141,437
Task 2	\$127,146	\$34,001	\$161,147
Task 3	\$98,896	\$95,605	\$194,501
Task 4	\$108,615	\$37,144	\$145,759
Task 5	\$40,655	\$68,355	\$109,010
Task 6	\$58,952	\$80,580	\$139,532
Task 7	\$55,565	\$104,435	\$160,000
Task 8	\$57,701	\$92,762	\$150,463
Task 9	\$21,609	\$64,924	\$86,533
Task 10	\$57,175	\$41,560	\$98,735
Task 11	\$41,308	\$68,815	\$110,123
Task 12	\$25,805	\$84,174	\$109,979
Totals	\$790,806	\$816,413	\$1,607,219

Infrastructure Facilities Augmentation	
Khlopin Radium Institute – Neutron Detectors	\$47,500
Electron Microscopy Imaging Laboratory Support	\$63,000
Materials Performance Laboratory Support	\$143,239
Transmission Electron Microscope Purchase	\$1,300,000
Total	\$1,553,739

Transmutation Research Program Organizational Chart

**Director, Anthony E. Hechanova
(Harry Reid Center)**



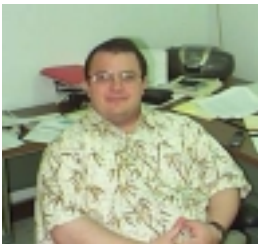
Harry Reid Center Executive Director Donald Baepler and TRP Director Anthony Hechanova at the Low Energy Demonstration Accelerator Facility in Los Alamos, NM.

Program Administration

**Finance Director, Patricia Baldwin
(Harry Reid Center)**



**Deputy Director, Harry Reid Center
Gary S. Cerefice**



**Deputy Director, College of Engineering
William G. Culbreth**



**Deputy Director, College of Sciences
Malcolm F. Nicol**



**International Programs Coordinator
Ning Li (LANL)**

Ning Li and IPPE Laboratory Head Evgeny Yefimov with Russian-built loop at UNLV.



Paul Newman and Denis Beller. The Academy Award-winning actor spent the day at UNLV to hear about transmutation and waste issues.



**Intercollegiate Programs Coordinator
Denis Beller (LANL)**



**Conference Coordinator
Kathleen D. Lauckner (HRC)**

**Science Adviser, National Program
Thomas Ward**



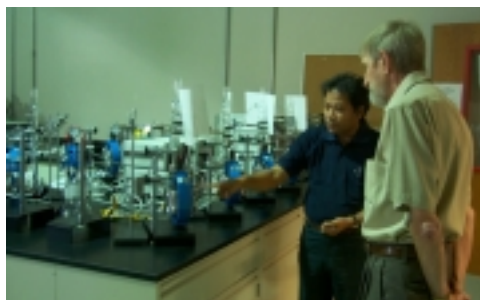
Thomas Ward and Khlopin Radium Institute General Director Alexander Rimski-Korsakov in St. Petersburg, Russia.

Transmutation Research Program Support Staff and Students

Materials Performance Laboratory College of Engineering



*Konstantin G. Zobotkin, MPL
Research Associate, College
of Engineering.*

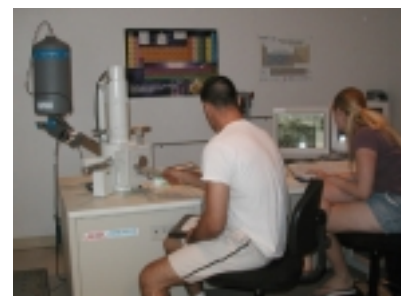


*Mechanical Engineering Associate
Research Professor Ajit Roy (left)
explains some MPL experiments.*

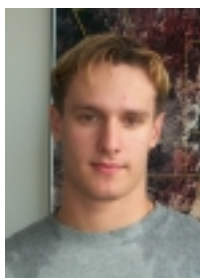


*Robert Fairhurst
EMIL Research Scientist
College of Sciences*

Electron Microanalysis and Imaging Laboratory, College of Sciences



EMIL Scanning Electron Microscope



Demian Gitnacht (U)



*Longzhou Ma, TEM Research
Scientist, Harry Reid Center.*

Transmission Electron Microscope Harry Reid Center



Cheryl Gustafson (U)

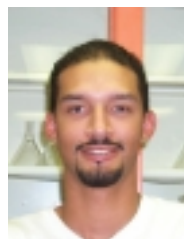
Harry Reid Center Student and Staff Support



Christina Crossan (U)



Ingrid James (U)



*John Knoten (U)
Webmaster*

*Stephanie Kamagai (G) and
Richard Turner (U), not pictured.*



*Elizabeth Johnson
Technical Writing*

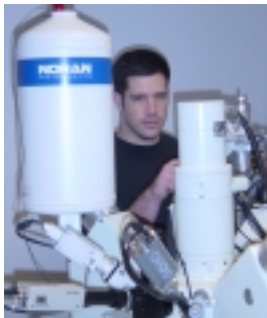
Photo Gallery

Transmutation Research Program Student and Faculty Researchers

College of Sciences, Department of Physics Task 3



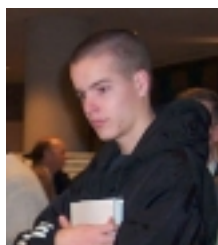
*Principal Investigator John Farley (top left),
Dr. Dale Perry, LBNL, (top center),
Professor Allen Johnson (top right),
Graduate Students Dan Koury (left) and
Brian Hosterman (center right), and
Undergraduate Denise Parsons
(bottom right).*



Harry Reid Center Task 6



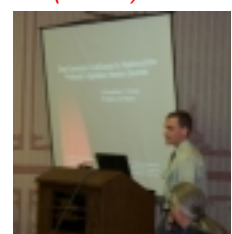
*Principal Investigator Carter D. Hull (top left),
Health Physics Professor William H. Johnson (top right),
Graduate Student Steven Curtis (bottom left),
Undergraduate Student Dean Curtis (bottom right)*



Health Physics Department Task 7



*Principal Investigator Phillip Patton (top left),
Professor Mark Rudin (top right),
Graduate Students John Shanahan (below)
and Yayun Song (not pictured)*



Transmutation Research Program Student and Faculty Researchers

College of Engineering Tasks 1, 2, 4, 5, 8, 9, 10, 11 & 12



Georg Mauer



Tao Pang (Physics)



William Culbreth



Darrell Pepper



Yitung Chen



Ajit Roy



Brendan O'Toole



Robert Schill, Jr.



Mohamed Trabia



Zhiyong Wang



Samir Moujaes

Not pictured: Randy Clarksean (Mechanical Engineering) and David Hatchet (Chemistry, Task 4)

Students

G = Graduate Student, U = Undergraduate Student



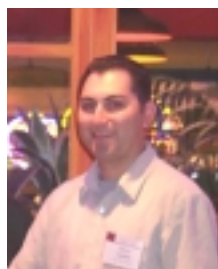
Xiaolong Wu (G)



Jianhong Li (G)



Satishkumar
Subramanian (G)



Jason Viggato (G)



Chao Wu (G)



Anoop
George (G)



Kanthi Dasika (G)



Lijian Sun (G)



Mohammad
Hossain (G)



Qin Xue (G)



Mark Jones (G) and Raymond Kozak (G)



Daniel Lowe (U) and
Ashraf Kaboud (G)

Not pictured: Tim Atobalele (U), Elizabeth Bakker (U), Yulien Chen (U), Myong Holl (U), Paul Lawson (U), Jae-Kyu Lee (G), Martin Lewis (G), Greg Loll (U), Maurice Moore (G), John Motaka (U), Sridhar Munaga (U), Suresh Sadenini (G), Richard Silva (G), and Aaron Tippetts (U).

Acronyms

AAA	Advanced Accelerator Applications
ADTTA	Accelerator-Driven Transmutation Technologies and Applications
ALI	Annual Limit on Intake
AMUSE	Argonne Model for Universal Solvent Extraction
ANL	Argonne National Laboratory
ANS	American Nuclear Society
AVS	American Vacuum Society
BNL	Brookhaven National Laboratory
CAD	Computer Aided Design
CFD	Computational Fluid Dynamics
CMT	Chemical Technology Division
DAC	Derived Air Concentration
DC	Dose Coefficient
DCAL	Dose Calculation code
DOE-NE	U.S. Department of Energy, Office of Nuclear Energy, Science and Technology
EMIL	Electron Microanalysis and Imaging Laboratory
FGR	Federal Guidance Report
HE	Hydrogen Embrittlement
HPS	Health Physics Society
HRC	UNLV Harry Reid Center for Environmental Studies
ICAPP	International Congress on Advanced Nuclear Power Plants
ICRP	International Commission on Radiological Protection
IPPE	Institute for Physics and Power Engineering, Obninsk, Russia
ISM	Induction Skull Melter
ISTC	International Science and Technology Center
ISU	Idaho State University
KRI	Khlopin Radium Institute, St. Petersburg, Russia
LANL	Los Alamos National Laboratory
LBE	Lead Bismuth Eutectic
LBNL	Lawrence Berkeley National Laboratory
LANSCE	Los Alamos Neutron Science Center
LCS	LAHET code system
Linac	Linear accelerator
MCNP	Monte Carlo n-particles code
MCNPX	Monte Carlo n-particles code extremely high-energy version
MOU	Memorandum of Understanding
MPL	UNLV Materials Performance Laboratory
MTS	Material Testing System
NACE	National Association of Corrosion Engineers
NERAC	DOE Nuclear Energy Research Advisory Committee
OECD	Organization for Economic Co-operation and Development
ORNL	Oak Ridge National Laboratory
RF	Radio Frequency
SCC	Stress corrosion cracking
SEM	Scanning Electron Microscope
SIMS	Secondary Ion Mass Spectrometer
SNS	Spallation-Neutron-Source
SSR	Slow Strain Rate
TEM	Transmission Electron Microscope
TRP	Transmutation Research Program
TRU	Transuranium Actinides
UNLV	University of Nevada, Las Vegas
UREX	Uranium Extraction process
XPS	X-ray photoelectron spectroscopy

The Last Page

References

UNLV Transmutation Research Program references, current activities and other miscellaneous information can be found on the TRP website at <http://aaa.nevada.edu>

Credits

The University of Nevada, Las Vegas Transmutation Research Program is administered by the Harry Reid Center for Environmental Studies under the auspices of the U.S. Department of Energy (Grant No. DE-FG04-2001AL67358).

This report was produced by Anthony Hechanova, Elizabeth Johnson, and Gary Cerefice.

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