9-2003

AFCI Quarterly Input – UNLV July through September, 2003

Harry Reid Center for Environmental Studies. Nuclear Science and Technology Division

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1.0 University of Nevada, Las Vegas (UNLV)

UNLV Transmutation Research Program. The University of Nevada, Las Vegas supports the AFCI through research and development of technologies for economic and environmentally sound refinement of spent nuclear fuel. The UNLV program has four components: infrastructure, international collaboration, student-based research, and management and program support.

1.1 Infrastructure Augmentation

1.1.1 Infrastructure Augmentation Scope

The infrastructure augmentation component of the UNLV Transmutation Research Program enhances UNLV's research staff, facilities, and academic programs to increase the ability of the university to perform AFCI research.

1.1.2 Infrastructure Augmentation Highlights

- **Ph.D. Program in Radiochemistry**. UNLV approved a proposal for a new Radiochemistry graduate program. The proposal was submitted to the Board of Regents of the University and Community College System of Nevada and the Board should address the proposal at their December 2003 meeting. If approved, the program could start as early as fall term 2004. The program will be a joint program between the Department of Chemistry and the Department of Health Physics and will be governed by the Graduate College.
- **M.S. Programs in Materials and Nuclear Engineering**. The proposal for new masters programs in Materials and Nuclear Engineering will be discussed at a Graduate College meeting next quarter. There appears to be support for this program by the UNLV administration, but the proposal has progressed slowly through the various committees.
- **Chemistry Professorships**. UNLV made offers on two tenure-track associate professorships in the Department of Chemistry. Kenneth Czerwinski, an actinide chemist, has accepted one of the positions and will start next quarter. The second position for a materials chemist is expected to be filled next quarter and commence Spring term 2004. These positions will be supported 49% by the UNLV Transmutation Research Program.
- **Facilities Progress Update**. Two facilities have completed their laboratory remodeling stage: the Transmission Electron Microscope user facility and the Interim Lead-Bismuth Eutectic Loop facility. The installation phases for the TEM and Pb-Bi Loop have started and should be complete within the next two quarters. Two other facilities, the Inductively Coupled Plasma Atomic Emission Spectrometer user facility and an interim Actinide Chemistry laboratory are progressing slower than expected and are still in the design phase for the ventilation system. The remodeling should go out to bid next quarter. The ICP AES and actinide chemistry equipment have arrived at UNLV and are awaiting installation, but additional ventilation is required in the rooms.

1.2 International Collaboration

1.2.1 International Collaboration Scope

The international collaboration component of the UNLV Transmutation Research Program enhances UNLV's breadth of scientific and scholastic experience. University collaboration is also an efficient conduit for international collaboration that benefits the national AFCI program. UNLV has ongoing relationships with the Khlopin Radium Institute (KRI) in St. Petersburg, Russia; the Institute for Physics and Power Engineering (IPPE) in Obninsk, Russia; and members of the International Molten Metal Advisory Committee (from Sweden, Germany, Belgium, and Italy).

1.2.2 International Collaboration Highlights

- **International Science and Technology Center (ISTC)**. The agreements and contracts to extend the collaboration with the Institute of Physics and Power Engineering, LANL, and UNLV over the ISTC Target Complex 1 located at UNLV have been signed and the contract to ISTC has been invoiced and paid. The Russian scientists who designed and built the TC-1 are planning to visit UNLV for the final installation within the next two quarters.
- **Khlopin Radium Institute**. The UNLV TRP Deputy Director and International Programs Adviser visited the Khlopin Radium Institute in St. Petersburg, Russia, to review progress on active collaborations (Task 15 (Iodine Sequestration) and Task 16 (Fluorapatite Waste Forms)) and discuss potential future collaborations. Samples for these tasks arrived this quarter and are part of their research activities. The KRI-built He-3 neutron detector for Task 6 arrived at UNLV and was tested this quarter. It is working perfectly and students are being trained on its modeling and use.

1.3 Student Research

1.3.1 Student Research Scope

The Student Research component is the core of the UNLV Transmutation Research Program with steadily increasing funds as the program evolves and capability expands. The milestones, schedules, and deliverables of the student research projects are detailed in the individual research proposals. UNLV currently has 16 student research tasks that include 37 graduate students and involve 34 faculty members. The tasks are divided below in terms of their research area: fuels, separations, and transmutation sciences.

1.3.2 Student Research Highlights

FUELS TECHNOLOGY

Metallic Fuel Pins (Task 1) Highlights.

- The mold filling process and solidification modeling have been combined and simulated together using the VOF-solidification algorithm.
- Since the casting process is very difficult and complicated, the software FIDAP alone is not enough for this kind of numerical simulation. Thus, two FORTRAN subroutines have been developed to link with FIDAP in the calculation.
- In the casting process, the velocity profiles are found increasing rapidly and then dropping off as solidification occurs.

- A new system design using a plug at the end of the mold which can control the backward pressure inside the mold has been suggested by ANL-West. Hence, a two-fluid VOF method will be used to include air and melt during the casting process.
- New methodologies and subroutines were developed to model the electrical conductivity in oxides, to study their potential use as materials (coils, etc.) in the system. The importance of different electrical conductivities is studied and simulated in the indirect induction heating (IH) process.
- A study of the indirect IH system was initiated to compare the indirect (IH) process with the direct (IH) process.
- The indirect (IH) system is used to heat insulating materials through the crucible made from electric conducting material (Outside indirect IH) or conducting material in the feedstock, in which most of the power deposits (Inside indirect IH).
- A comparison of the maximum temperature in the indirect induction heating system for different current densities, current frequencies, and coil numbers have been used for the indirect IH processes. All the dimensions of the system and the electrical parameters are kept the same as before.
- Efforts are beginning on the development of a numerical model that assesses the impact of americium transport from a heated melt. The heating rates with temperature profiles with the different power deposition to the crucible have been studied

Remote Fuel Fabrication (Task 9) Highlights.

- Graduate student Richard Silva continued the development of a simulation model with a Waelischmiller hot cell robot. He will continue to develop detailed 3-D process simulation models as his M.Sc. thesis project.
- Ph.D. student Jae-Kyu Lee continued his research on Concepts and Methods for Vision-Based Hot Cell Supervision and Control, focusing on rule-based object recognition.
- Undergraduate student Jamil Renno created simulations of fuel pin assembly (robotic insertion of pellets into cladding tubes) for the hot cell manipulator. Besides the correct insertion process, several accident scenarios were simulated.
- Two papers were accepted for presentation: G.F. Mauer and J. Renno, "Design and Virtual Testing of Robotic Assembly Processes for Hot Cells," ANS winter annual meeting, New Orleans, LA, November 2003; and, G.F. Mauer and J. Renno, "Design and Virtual Testing of Robotic Assembly Processes for Hot Cells," 10th International Conference on Robotics and Remote Systems for Hazardous Environments, Gainesville, FL, March 2004.

SEPARATIONS TECHNOLOGY

Systems Engineering Model (Task 8) Highlights.

- Implemented the Object Oriented Programming approach which remains three sections: First, Intermediate, and Last. Move command is also implemented to all three sections.
- The database has been created and tested using ACCESS of Microsoft. SQL server has been used to implement the database design.

- Tables were modified completely so that redundancy is reduced. Four tables can take all the data from the VB interface. Tables have been designed for output so that reports can be generated from the developed interface by NCACM instead of AMUSE. Each table has filename as primary key so that foreign key relationship can be established.
- Several runs were made and charts for different inputs versus outputs were created. Based on these charts, there are some relationships between input and output which can be used for the optimization process in the system engineering modeling.
- The FLOWSHEET SIMULATOR code has been developed and is in use for the systems evaluations.
- User interface of Flowsheet-Simulator has been revised and improved.
- The TASK_INTEGRATION module has been successfully developed. User can build the task hierarchy from scratch or import it from the file which was saved before. The functions of this module are listed as follows:
    - Create a new TASK from scratch
    - User can dynamically add calculation module, simulation code, and chemical separation module such as AMUSE code to the main task
    - User can dynamically define the dataflow among all the tasks
    - Save result to database
    - Save result to XML file
- The above TASK_INTEGRATION module can be used to build the whole flowsheet to simulate the chemical separation process. User can then apply the different system study tools to study the system engineering modeling and analysis from the Task-Manager module.
- The TASK-MANAGER module has been successfully developed. From TASK-MANAGER module, user can access all the two other modules: TASK-INTEGRATION module and SOLUTION-MONITOR.
- User can also customize the desired system study plan such as the DOE study plan and Optimization plan. Parameter definitions are: Choose Design Variable, Objective Variable, and Define Constraint Condition.
- The SOLUTION-MONITOR module has also been successfully developed. User can view the system analysis result by way of graphic and table.

Criticality and Heat Transfer Analyses of Separations Processes (Task 11) Highlights.

- Graduate student Elizabeth Bakker completed a summer internship at Argonne National Laboratory.
- A heat transfer program was formed in MathCAD which determines maximum temperature inside storage form.
- Heat transfer tendencies of mixtures of americium oxide, curium oxide, cesium oxide, and strontium oxide were investigated.
- Storage solutions for separated cesium and strontium were investigated and a final report is in preparation.

Immobilization of Fission Iodine (Task 15) Highlights.

- Breakthrough experiments with the Fullerene-containing Carbon Compounds (FCC) material were carried out. The FCC pellets that were received from the V.G. Khlopin Radium Institute (KRI) were crushed with a mortar and pestle and packed into the glass column. The particle size distribution was not determined, however, the pressure required to achieve 20.0 mL/min flow rates for the FCC column was significantly higher than with the Natural Occurring Material (NOM) columns. The concentration of iodine in the vapor phase was 1.36×10^{-5} mol/L. The gas phase was approximately 50% saturated with nitric acid vapor as well. Experiments were conducted at a flow rate of 0.020 L/min
- Breakthrough experiments with the NOM activated carbon combinations were performed. We begun experiments with FCC and NOM scavenging of iodine during simulated fuel dissolution. We are performing additional elemental analysis (CSN) on KRI FCC material and NOM. We are continuing to investigate the formation of volatile iodides in aqueous suspensions of NOM with iodine. We have started examining the speciation of iodine remaining in water soluble forms after reaction of active iodine with NOM.
- We have tested various bases with NOM for their effect on iodine sequestration.
- We have started investigating the utility of hydroxide charged anion exchange resin for methyl iodide trapping. We are investigating the efficacy of removal of iodide from various strongly basic anion exchange resins. We are also investigating the potential of a mercaptan group (-SH) containing resin for methyl iodide trapping.
- We have measured surface areas of FCC materials using the BET method. Surface areas are lower than conventional activated carbon. We also examined reversibility and the effects of outgassing temperature and conditions on measured surface area. Comparing the material to a commercially available activated carbon shows very similar behavior.
- We have leached FCC material previously exposed to iodine at the KRI. Leaching of freshly exposed FCC with 0.1 M KI removed all of the “sorbed” iodine. We have demonstrated that iodine loaded at KRI can be thermally released as molecular iodine. Iodine can be released at relatively low temperatures. Iodine sorption has a large effect on the surface area of the FCC.
- We are continuing to investigate SPME analysis of methyl iodide. We are investing the formation of volatile iodides in aqueous suspensions of NOM with iodine.
- We have developed a calibration procedure for methyl iodide that is released by pyrolysis. We have measured the fraction of bound iodide released as methyl iodide from a NOM sample. We have investigated the influence of pyrolysis temperature on release.

Fluorapatite Waste Forms (Task 16) Highlights.

- NEXAFS spectra for the apatite samples have been measured. The obtained spectra are as follows:
  - Calcium L-edge NEXAFS for the hydroxylapatite, fluorapatite (clear crystal) and hydroxylapatite mixed with Zn powder,
  - Oxygen K-edge NEXAFS for hydroxylapatite and fluorapatite (clear crystal),
  - Phosphorous K-edge NEXAFS for hydroxylapatite and fluorapatite (clear crystal), and

- Fluorine K-edge NEXAFS for fluorapatite (clear crystal).

- Samples of synthetic fluorapatite and the model natural fluorapatite were obtained from the V.G. Khlopin Radium Institute (KRI) collaborators.
- We obtained Photoacoustic IR and IR imaging for two apatite samples from KRI. High resolution IR spectra for new apatite samples (from KRI) were obtained. Identification of each signal of those IR spectra is in progress.
- SEM data for the following samples were obtained: Hydroxyapatite, Zn metal + Hydroxyapatite, Mg metal + Hydroxyapatite, and Fluorapatite.
- Obtained following spectroscopic data for the new sample (from KRI), which was compared to data obtained from the synthetic hydroxyapatite standard using XPS, FTIR, and SEM.

TRANSMUTATION SCIENCES

Niobium Cavity Fabrication Optimization (Task 2) Highlights.

- Completed assessment of particle position detector and began procurement of electron grids and InGa system. Manipulator is designed to move piece under test and to measure electron beam current underway. In situ Ar cleaning and water removal system at 10^{-8} Torr being developed.
- Re-examining the multipacting code for mulipacting from muffin tin geometry.
- Revised the optimization routines for determining cavity geometry from resonant frequency and mode calculations.
- Flow studies were conducted and a modified baffle built and tested.
- Re-examining the multipacting code for mulipacting from muffin tin geometry.
- Revised the optimization routines for determining cavity geometry from resonant frequency and mode calculations with good results obtained.

LBE Corrosion of Steel (Task 3) Highlights.

- Continuing development of bench-scale lead bismuth eutectic (LBE) experiments.
- We measured the grain size in the annealed exposed LBE sample to be 40 microns, in agreement with previous measurements by other workers.
- Progress in Raman spectroscopy: The fluorescent background observed in the samples has been tentatively identified as a volatile/temperature sensitive surface contamination. When samples are baked, the background went away, indicating that it is volatile/thermally sensitive conface contamination.
- A manuscript describing our work was submitted to the *Journal of Nuclear Materials*. "Spectroscopic and Microscopic Investigation of the Corrosion of 316/316L Stainless Steel by Lead-Bismuth Eutectic (LBE) at Elevated Temperatures: Importance of Surface Preparation," by A.L. Johnson, D. Parsons, J. Manzerova, D.L. Perry, D. Koury, B. Hosterman, and J.W. Farley.
- We hosted a successful visit by Peter Hoseman, graduate student from Switzerland, visiting UNLV at the request of LANL scientist Ning Li. Hoseman made measurements of corroded steel samples using the SEM/EDAX on campus. He examined about 45 samples by SEM/EDAX and 6 samples by XPS.

Environment-induced Degradation of Materials (Task 4) Highlights:

- Stress Corrosion Cracking (SCC) tests using self-loaded C-ring and U-bend specimens were conducted in aerated acidic solution at ambient temperature, 50°C, and 100°C. These test specimens are being periodically withdrawn from the cells for verification of crack initiation by optical microscopy. Results indicate that a C-ring specimen of Alloy HT-9 showed cracking in the acidic solution at 50°C. SCC testing in molten LBE using similar types of specimens is in progress at LANL.
- SCC testing using smooth and notched tensile specimens of Alloys EP-823, HT-9 and 422 were conducted under constant load in the Materials Performance Laboratory.
- SCC testing under controlled cathodic potentials (with respect to the corrosion potential) has been initiated. However, the single potentiostats (Model 273A) are currently malfunctioning. Therefore, all electrochemical testing including cyclic potentiodynamic polarization using these potentiostats are on hold. The eight-channel multi-potentiostat is currently being used for slow strain rate testing under controlled electrochemical potential.
- Fractographic evaluations by scanning electron microscopy are being continued. Microstructural analyses by optical microscopy are also in progress.

LBE Corrosion Modeling (Task 5) Highlights:

- Chao Wu successfully defended his thesis and received his M.S. degree from the Mechanical Engineering Department in July. His thesis title is "Study of Geometry Effects on Local Corrosion Rates for LBE Loop."
- Examinations of sudden expansion geometries were carried out in 2-D and 3-D models. Uniform Temperature along the length of the plate is assumed. A uniformly generated mesh is used. Different mesh sizes were tested to check the mesh independence.
- Preliminary results: initially, flow does not contain any species at inlet, while two plates have a fixed concentration of species. In this way the species on the plates will diffuse into the bulk region, and the expected corrosion rate along the length may vary due to the difference of local flow condition and concentration profiles normal to the wall. Hopf bifurcation occurs in this kind of symmetric sudden expansion domain, when Reynolds number reaches a certain critical value. Oscillation or vibration appears in the flow and the resultant flow becomes unsteady and periodic in time.
- Results verified by addition of monitoring cell to models. Mesh independence also examined.

Neutron Multiplicity (Task 6) Highlights:

- The ^{3}He Neutron Multiplicity detector prototype (60-element) and 304 Stainless Steel stand were delivered to the Harry Reid Center, set-up, configured, and operated continuously for hundreds of hours prior to shut down due to laboratory construction and maintenance. The ^{3}He system electronics and software all respond well within specifications for the system. Eight nuclear grade lead bricks were modified to fit into the target area of the ^{3}He detector system stand.
- Neutronics models for the 60-element ^{3}He system have been completed in both MCNPX and CONTROL nuclear transport code suites. Calculations of neutron capture efficiencies of the ^{3}He and ^{6}Li detectors were continued. These models are needed to calculate the intrinsic efficiencies of both detector systems; especially that of the ^{6}Li detector system in the cyclotron beam at UC Davis.

- The glass fiber neutron multiplicity detector prototype (^{6}Li glass fiber detector) is ~98% complete for all hardware and electronic card production (signal train, firmware). However, a stand-off configuration of the optoelectronic interfaces was determined to be required for the system due to charged particle beams passing in close proximity to the surface-mount electronics for the photomultiplier high voltage divider boards and pre-amplification circuits.
- MCNPX models of the ^{6}Li glass detector energy deposition using monolayer, bilayer, and double bilayer of 120 micron diameter core of active glass fiber have been completed. Relative energy depositions in the NucSafe ^{6}Li glass 6-element detector systems detector also were graphically depicted.
- Undergraduate student Dean Curtis, who is modeling the neutron detector systems, traveled to Russia in August and worked at the V.G. Khlopin Radium Institute for 10 days. He developed a model of the ^{3}He system and was trained in the KRI-developed CONTROL nuclear transport code.

Dose Conversion Coefficients (Task 7) Highlights:

- John Shanahan successfully defended his thesis and received his M.S. degree from the Health Physics Department in August. His thesis title is "Dose Coefficients for Radionuclides Produced in a Spallation Neutron Source."
- The quality check of the Dose Coefficient methodology/procedures has been completed in collaboration with Keith Eckerman (ORNL) and other university partners.
- The consortium cross checked the radionuclides in Category 1. DC's were calculated for some Category 2 radionuclides. Lack of available nuclear data for some radionuclides has delayed completion of some dose coefficient calculations. New databases are being investigated to try to resolve these issues.
- A fall meeting with the consortium has been scheduled for Nov 13-14.

Properties of Alloy EP-823 (Task 10) Highlights:

- Testing of two different heats of Alloy EP-823 was conducted at ambient and elevated temperatures. Tensile specimens of Alloy HT-9 have also been machined for mechanical properties evaluation at different temperatures. Type 422 stainless steel was heat treated for preparing test samples. Optical microscopy and SEM were used to evaluate the metallurgical microstructures and fractography, respectively.
- High-temperature tensile testing using specimen grips made of maraging steel in the presence of nitrogen were conducted. Testing was performed at ambient temperature, 100^{o}C, 300^{o}C and 400^{o}C. Data analyses are ongoing.

Radiation Transport Modeling of Beam-Target Experiments (Task 12) Highlights:

- Beowulf cluster was expanded. A total of 38 slave machine, 2 dual CPU masters are up and running.
- Benchmarked on shared memory systems and Beowulf cluster. In testing between MPI versions and PVM, MPI seems to be outperforming PVM by a factor of 3 on the Beowulf cluster.
- The new machines are AMD 2400's while the older slave machine were AMD 2000's. PVM now has the ability to load share. Testing is being done on this. MPI does not

currently support load sharing and will need another device to incorporate clave machines with different CPU speeds.

Oxygen Sensing in LBE (Task 13) Highlights:

- The software FLUENT was installed into the SUN server. Some preliminary simulation results on 3-D have been obtained for a simplified model.
- A study regarding the noise feature of the sensor was started.
- The experimental apparatus was shipped to LANL.
- Both sets of the experimental apparatuses were assembled at LANL and experiments were begun.
- Preliminary results have been obtained for transport simulation in the new oxygen control/measurement apparatus.

Positron Annihilation Spectroscopy (Task 14) Highlights:

- Measurements of residual stresses in welded specimens consisting of similar and dissimilar materials of heat-treated Alloy EP-823 and Type 304L stainless steel by positron annihilation spectroscopy (PAS) were performed at the Idaho State University. PAS data on three-point-bent specimens and cold-worked specimens were also generated.
- Metallographic evaluations of welded specimens by optical microscopy were completed.
- A new heat of Alloy HT-9, vacuum-melted at the Timken Research facilities, was processed for specimen preparation.
- Welded, cold-worked and bent specimens of Alloys EP-823 and HT-9, and Type 304L stainless steel have been sent to Atomic Energy of Canada Limited (AECL) for residual stress measurements by neutron diffraction technique.
- Three technical papers were presented at the International Surface Engineering Congress, 46th Annual Nondestructive Testing Forum and the 35th International SAMPE Technical Conference.

1.3.3 Student Research Technical Summary

FUELS TECHNOLOGY

Metallic Fuel Pins (Task 1). The analysis of mold filling and solidification continues with progress being made for the consideration of these two features within one model. Analysis of the induction heating process of an Induction Skull Melter (ISM) is under study. Efforts are underway to validate the modeling procedure and specific comparisons are being made to previously published work. Few detailed modeling results have been reported by other researchers, making the validations an important part of the overall modeling process. Skin heating depths, power deposition rates, and other process parameters are being evaluated for use in upcoming furnace design simulations. Efforts are beginning on the development of a numerical model that assesses the impact of americium transport from a heated melt.

The mold filling process and the solidification modeling have been combined and simulated together using the VOF-solidification algorithm. The solidification could take place during the filling process. Since the casting process is very difficult and complicated, the software FIDAP alone is not enough for this kind of numerical simulation. Thus, two FORTRAN subroutines have been developed to link with FIDAP in the calculation.

In the casting process, the velocity profiles are found increasing rapidly and then dropping off as solidification occurs.

A new system design using a plug at the end of the mold which can control the backward pressure inside the mold has been suggested by ANL-West. Hence, two fluids VOF method will be used to include air and melt during the casting process.

Skin heating depths, power deposition rates, and other process parameters have been continuously evaluated for use in upcoming furnace design simulations.

Efforts are beginning on the development of a numerical model that assesses the impact of americium transport from a heated melt. The heating rates with temperature profiles with the different power deposition to the crucible have been studied.

We continue to work on the induction heating system of crucible modeling. The differences of the required heating time to reach the melting temperature by increasing the coil numbers have been studied.

A modified design of an induction heating system is about 3 times faster than the original design for the temperature to reach the melting point 1,400^{o}C. Figure 1.3.1 shows the time requirement for reaching the melting point using different coil numbers.

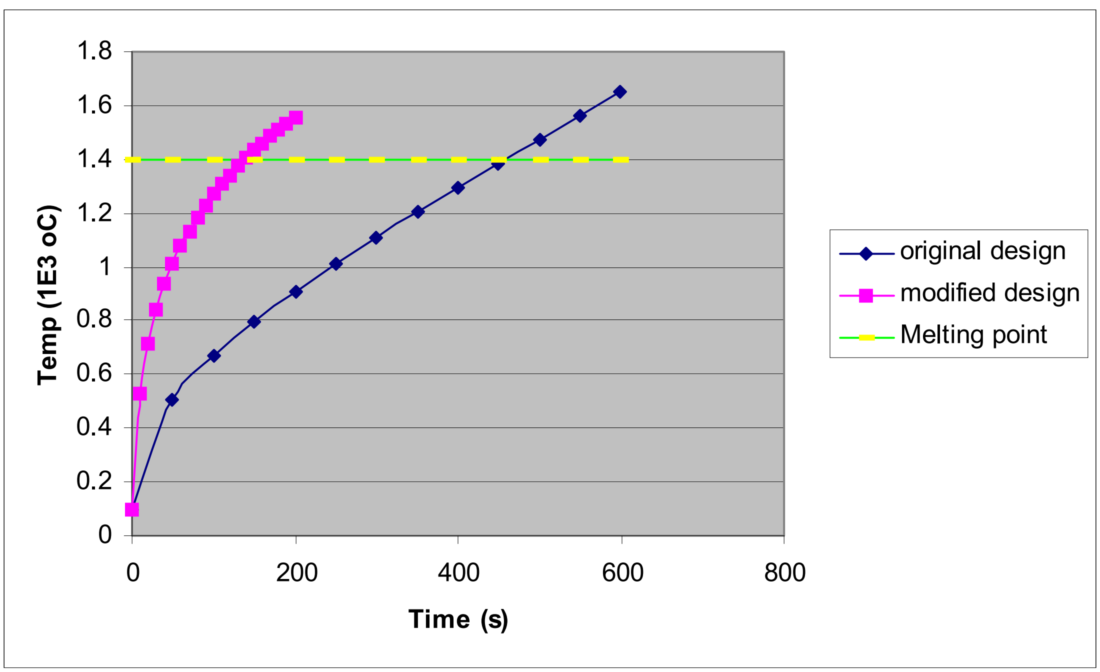

Figure 1.3.1. The time requirements for reaching the melting point using different coil numbers.

As in most materials, especially in the oxides, the electrical conductivity is strongly dependent on temperature. From former work we know electrical conductivity has great impact on the calculation of the two complex components of power deposition Q, i.e. C and S. A subroutine has been developed in the simulation of induction heating problem when the electrical conductivity is a variable value.

It will be difficult to use low electrical conductivity materials in the induction heating system. It will be necessary to add a pure material such Zr which has a high electrical conductivity compared to ZrO_2 powder. Zr acts as a “conductor” during the induction heating process. The location of the “conductor” material, shape, and volume are important factors during the numerical modeling.

Remote Fuel Fabrication (Task 9). The objective of this project is the design and evaluation of manufacturing processes for AFCI fuel fabrication. The large-scale deployment of remote fabrication and refabrication processes will be required for all transmutation scenarios. The evaluation of the fabrication processes will create a decision support data base to document design, operations, and costs. Fabrication processes required for different fuel types differ in terms of equipment types, throughput, and cost. Differential cost implications of various fuel choices will be assessed. Another aspect is the assessment of robotic technology and robot supervision and control, and the simulation of material handling operations using 3-D simulation tools with view towards the development of a fully automated and reliable, autonomous manufacturing process. Such development has the potential to decrease the cost of remote fuel fabrication and to make transmutation a more economically viable process. An added benefit would be the potential for large reductions in dose to workers. This project is being conducted in close cooperation with the fabrication development group at Argonne National Lab.

During the present reporting period, the robot simulation model for robot control under Matlab Control software was improved farther by graduate student Jamil Renno. Matlab controls the spatial robot model, comprising a geometric model as well as the robot dynamics. Thus a realistic simulation of the forces and torques present during robot motion is being generated. Mr. Renno developed a simulation for pellet placement from a bin, and for inserting a row of pellets into a fuel rod.

Several accident scenarios associated with pellet placement and insertion were explored and analyzed. Efforts were initiated to expand the simulations to other processes, such as pellet unloading, pellet tray loading and unloading from sintering oven, grinding, and dimensional inspection.

Graduate student Jae-Kyu Lee continued his work on Object Recognition using a knowledge-based system. The schematic diagram for an Algorithm for Recognition is as follows:

Preprocessing stage (off-line):

- Step 1: Extract interesting points from model image
- Step 2: Calculate edges and loops data
- Step 3: Evaluate surface invariance using transformation invariance of mid-point of loops
- Step 4: In case of 3D, evaluate loop connectivity of super perimeter

Recognition stage (on-line):

- Step 1: Extract interesting points and build test vector sets

- Step 2: Pick one model image dataset and compare with test scene data to find co-edges and loops
- Step 3: Evaluate DOU values and verify hypothesis
  Step 4: Regenerate matching results
- Step 5: Go to the step two and pick next model image dataset and repeat the remaining steps until the last model

The following describes a series of task experiments.

Experiment 1: Verify Probabilistic Viewing Effect in 3D
Before we start 3D object, first, we verify the probabilistic viewing effect. To do so we try to find a match between the same objects only their image is taken in different viewing angle at 0°, 15°, 30°, respectively. For the first match, recognition between the same images shows extra loops inside. Such an unwanted loop match is common in 3D real object recognition due to problems in real image. This is due not only to round off and environment error but also the errors from viewing itself. Each matching algorithm in 3D has been applied to each surface as well as to the super perimeter. After finding the right match of loops we evaluate the degree of uncertainty (DOU). By following the DOU values, we make a decision which strategy is the best for the processing the recognition. During the evaluation of DOU value we also employ the rank system. The rank system is also known as weighted k^{th} nearest neighbor or WkNN. In our research such weighted value (or so called extra credit) is given when the loop belong to surface also belongs to the super perimeter as well. Such a case of matching results will be stored into different datasets by best bin first (or BBF) algorithm.

Experiment 2: Find Model Object from Test Scene C
Here 3D object recognition from a real image is tested. As always, there is no prior knowledge from the test scene except points set coordinates. The procedure is the same as 2D until the loop search. However, after evaluating DOU values, we implement both a super perimeter search as well as a surface search. We compare the highest scores from each step.

- Step 1: Generating Test Vector
- Step 2: Find Edge Match and collect Co-edges from Test Vector Sets
- Step 3: Search for the Loop and evaluate DOU Value
- Step 4: Parallel Process to search for Super Perimeter and Surface

SEPARATIONS TECHNOLOGY

Systems Engineering Model (Task 8). The objectives of this task are the development of a systems engineering model and the refinement of the Argonne code AMUSE (Argonne Model for Universal Solvent Extraction). The detailed systems engineering model is the start of an integrated approach to the analysis of the materials separations associated with the AFCI Program. A second portion of the project is to streamline and improve an integral part of the overall systems model, which is the software package AMUSE.

AMUSE analyzes the UREX process and other related solvent extraction processes and defines many of the process streams that are integral to the systems engineering model. Combining these two tasks is important in ensuring that calculations made in AMUSE are accurately transferred to the overall systems model. Additional modules will be developed to model pyrochemical process operations not treated by AMUSE. These modules will be refined as experiments are conducted and as more knowledge is gained in process steps.

Efforts have started on the storage of all results in a MS-Access database to speedup and streamline the analysis of multiple runs (parametric studies for design purposes). An Object Oriented Programming (OOP) approach has been developed and implemented for the final three sections of the new modeling approach (First, Intermediate, and Last sections). Discussions were held with ANL researchers to clarify data transfer and data update issues for the AMUSE code. This will clarify the data flow within AMUSE. A number of AMUSE analyses were conducted to demonstrate the ability of the code to store the data, plot the data, and to obtain feedback from ANL on how to improve the interface. The AMUSE code can now be called from within MATLAB as part of the Systems Engineering Modeling effort.

Input files and results files can be successfully generated for individual runs and for multiple runs through MATLAB calls. Refinements will be made to this approach to allow for more runs and to allow for optimization. We have successfully implemented the OOP which remains three sections. Move command is also implemented to all the above three sections. The database has been created and tested using ACCESS of Microsoft. SQL server has been used to implement the database design. Tables were modified completely so that redundancy is reduced. Four tables can take all the data from the VB interface. Tables have been designed for output so that reports can be generated from the developed interface by NCACM instead of AMUSE. Each table has filename as primary key so that foreign key relationship can be established. It enables user to easily handle the data for a particular flow sheet which the structure of database design.

Several runs were made and charts for different inputs versus outputs were created. Based on these charts we have got some relationship between input and output which can be used for optimization process in the system engineering modeling.

FLOWSHEET-SIMULATOR has been developed which has the following features:

- Create a new FLOWSHEET from scratch
- Open a FLOWSHEET from export file
- Open a FLOWSHEET from SQL server database
- Edit the FLOWSHEET by simply visually dragging and dropping
- Save result to database
- Save result to export file
- Call AMUSE code to run

The great advantages for the FLOWSHEET-SIMULATOR development are that it is developed using OOP technologies and can hide all the information about connection with AMUSE and data flow with database, export file and report file. FLOWSHEET-SIMULATOR provides the entire friendly interface for user to implement all the functions.

Task-Integration module is continuously developing to allow the following:

- Create a new task from scratch
- User can dynamically add simulation module, simulation code, and chemical separation module such as AMUSE code to the main task

- User can dynamically define the dataflow among all the tasks
- Save the simulation results to the developed database
- Save the simulation results as XML file

We can use the above Task-Integration module to build the whole flowsheet to simulate the chemical separation process. User can then apply the different system study tools to study the system engineering modeling and analysis from the Task-Manager module. The Task-Manager module has been designed. Currently, we are in the coding phase.

Criticality and Heat Transfer Analyses of Separations Processes (Task 11). The success of the AFCI program will rely upon the ability of radiochemists to separate spent nuclear fuel. The Chemical Technology Division at Argonne National Laboratory is actively involved in the development of pyrochemical separation technology that minimizes the usage of strong acids with the subsequent problems involved in disposing of the acidic residue.

Small scale experiments are being validated at ANL to separate spent nuclear fuel, but they must be scaled up to accommodate the large amount of commercial spent fuel that must be treated. As the volume of waste to be treated is increased, there is a higher probability that fissionable isotopes of plutonium, americium, and curium can accumulate and form a critical mass. Criticality events can be avoided by ensuring that the effective neutron multiplication factor, k_{eff}, remains below a safe level. NRC regulations normally allow an upper value of 0.95 for k_{eff}. This parameter can be computed for any combination of fuel and geometry using Monte Carlo neutron transport codes. Scale 4.4a from the Oak Ridge National Laboratory and MCNP4C2 from the Los Alamos National Laboratory are two codes that are regularly used to assess criticality.

Immobilization of Fission Iodine (Task 15). The recovery of iodine released during the processing of used nuclear fuel poses a significant challenge to the transmutation of radioactive iodine. This task will develop and examine the use of Fullerene Containing Carbon (FCC) compounds as potential sorbents for iodine release from the reprocessing of nuclear fuel. This work will also include the development of bench-scale testing capabilities at UNLV to allow the testing of the FCC material in a simulated process off-gas environment. This experimental capability will also be used to test other potential sorbtion materials and processes, such as natural organic matter (NOM) and other promising alternatives. This work also examines the development of a process to convert the sorbed iodine into a ceramic material with the potential for use as either a transmutation target or as a waste form in a partitioning and sequestration strategy.

Fluorapatite Waste Forms (Task 16). Fluorapatite, fluorinated calcium phosphate, has been identified as a potential matrix for the entombment of the zirconium fluoride fission product waste stream from the proposed FLEX process. If the efficacy of fluorapatite-based waste-storage can be demonstrated, then new and potentially more-efficient options for handling and separating high-level wastes, based on fluoride-salt extraction, will become feasible. This task is a dual-path research project to develop a process to fabricate a synthetic fluorapatite waste form for the ZrF_4, FP waste stream, characterize the waste form, examine its performance under environmental conditions, and correlate the behavior of the waste form with natural analogs.

Characterization of the material will be accomplished through probing the molecular-scale electronic and geometric structure of the materials in order to relate them to macroscopic properties, with the goal of developing techniques to evaluate and predict the performance of different waste-form materials. Time and funding permitting, other waste forms for the zirconium fluoride, fission product salt waste stream will be examined and benchmarked against the fluorapatite matrix baseline.

TRANSMUTATION SCIENCES

Niobium Cavity Fabrication Optimization (Task 2). Multipacting is one of the major loss mechanisms in rf superconductivity cavities for accelerators. This loss mechanism limits the maximum amount of energy/power supported by the cavities. Optimal designs have been identified in others' studies. In practice, these designs are not easily manufactured. Chemical etching processes used to polish the cavity walls result in a nonuniform surface etch. A nonuniform surface etch will leave some unclean areas with contaminants and micron size particles. These significantly affect mutipacting. Further, a nonuniform etch will leave areas with damaged grain structure, which is not good for superconducting properties. Typically, the depth of chemical polishing etch ranges between 10 to 150 microns.

It is the purpose of this study to experimentally model the fluid flow resulting in the chemical etching of niobium cavities with the aid of a baffle. The current etching process with baffles does not uniformly etch the cavity surface. Multiple cavity cell geometries are being investigated. Optimization techniques will be applied in search of the chemical etching processes that will lead to cavity walls with near ideal properties.

LBE Corrosion of Steel (Task 3). The goal of this task is to achieve a basic understanding of corrosion of steels by Lead Bismuth Eutectic (LBE). There have been previous studies of LBE, especially by the Russians, who have over 80 reactor-years experience with LBE coolant in their Alpha-class submarine reactors. The Russians found that the presence of small amounts (ppm) of oxygen in the LBE significantly reduced corrosion. However, a fundamental understanding and verification of its role in the corrosion of steels is still very incomplete.

We are carrying out a program of post-experiment testing and analysis on steel samples that have been in intimate contact with LBE. We have employed surface analysis techniques, including Scanning Electron Microscopy (SEM), Energy Dispersive X-Ray (EDAX) spectroscopy, and X-ray Photoelectron Spectrometry (XPS), and laser Raman. These techniques, applied to the steel surface, have probed the surface morphology, elemental analysis and oxidation states as a function of position. The measurements were made using the facilities at UNLV. Chemical alterations and resulting chemical species are studied at the steel surface. We plan to use powder X-ray diffraction in the near future. In addition to these well-established laboratory-based instrumentation approaches at UNLV, we have begun to use a state-of-the-art synchrotron-based spectroscopy and microscopy technique, the X-ray fluorescence microprobe at the Advanced Light Source, at Lawrence Berkeley National Laboratory. We are characterizing spectroscopically the stainless steel before and after interaction with LBE to determine their composition, including minor components such as chromium and nickel. The research moves toward establishing a rigorous experimental database of experimental measurements of LBE and its reactions with steels. Such a database can be used by DOE scientists and engineers in engineering efforts to control, avoid, and/or minimize the effect of corrosion of steels by LBE.

Environment-induced Degradation of Materials (Task 4). During the past two years of this project, the primary effort was focused on evaluating the effect of hydrogen on the cracking behavior of candidate target materials namely, Alloys EP-823, HT-9 and 422 in aqueous environments of different pH values at ambient and elevated temperatures. More recently, emphasis is being placed to evaluate the cracking behavior of these materials in molten lead-bismuth eutectic (LBE) environment at much higher testing temperatures so as to compare the cracking susceptibility in environments containing molten metals and aqueous solutions, respectively.

The most recent tests to evaluate the cracking susceptibility were primarily based on two state-of-the-art techniques known as constant-load and slow-strain-rate (SSR) methods. Simultaneously, efforts were made to determine the localized corrosion (pitting and crevice corrosion) behavior in similar aqueous environments at ambient and elevated temperatures using electrochemical polarization techniques. However, these techniques cannot be applied to LBE environment. Therefore, the work scope described in the original proposal has been modified to include additional testing methods to suit the high-temperature LBE environment. Although, testing still will be continued to complete the original matrix involving all three alloys in aqueous environments using constant-load, SSR, and polarization techniques, testing has also begun in both aqueous and LBE environments using self-loaded C-Ring and U-Bend stress-corrosion-cracking (SCC) test specimens.

All tested specimens are examined metallographically. Further, the scanning electron microscope (SEM) was used to determine the extent and nature of cracking in the tested specimens. The thrust of this overall testing program is to evaluate the environmental and radiation effects on the cracking behavior of candidate target materials.

LBE Corrosion Modeling (Task 5). This project combines chemical kinetics and hydrodynamics in target and test-loop lead-bismuth eutectic (LBE) systems to model system corrosion effects. The goal is to produce a predicative tool that can be validated with corrosion test data, used to systematically design tests and interpret the results, and provide guidance for optimization in LBE system designs. The task includes two subtasks. The first subtask is to try to develop the necessary predictive tools to be able to predict the levels of oxygen and corrosion products close to the boundary layer through the use of Computational Fluid Dynamics (CFD) modeling. The second subtask is to predict the kinetics in the corrosion process between the LBE and structural materials by incorporating pertinent information from the first subtask.

Neutron Multiplicity (Task 6). The goals of this task are to measure the neutron leakage from 15, 20 and 40-cm diameter Pb-Bi / Pb targets and to compare these empirical measurements with MCNPX results. These measurements are essential in validating and benchmarking MCNPX modeling results of target materials. The neutron leakage measurements should provide a systematic set of precision data that will enable direct comparison with code calculations.

Two detector systems, which employ independent technologies, are employed. Comparisons of results obtained from both should remove many uncertainties and permit the derivation of relative measurements in the few percent range at the 95% Confidence Level (CL). A 60 detector element ^{3}He tube based system and a prototype neutron sensitive glass fiber-based system was built in Russia and successfully operated at UNLV this quarter. A glass fiber detector prototype is very close to completion and should be finished by next quarter. MCNPX models of the ^{3}He system have been developed and will be integrated with target models. Models of the glass fiber detectors have also been developed.

Dose Conversion Coefficients (Task 7). A research consortium comprised of representatives from several universities and national laboratories has been established as part of this task to generate internal and external dose conversion coefficients (DCC) for radionuclides produced in spallation neutron sources. Information obtained from this study will be used to support the siting and licensing of future accelerator-driven nuclear initiatives within the U.S. Department of Energy complex, including the Spallation Neutron Source (SNS) project. Determination of these coefficients will also fill data gaps for several hundred radionuclides that exist in Federal Guide Report No. 11 and in Publications 68 and 72 of the International Commission on Radiological Protection (ICRP).

Properties of Alloy EP-823 (Task 10). The purpose of this project is to evaluate the elevated temperature tensile properties of Alloy EP-823, a leading target material for accelerator-driven waste transmutation applications. This alloy has been proven to be an excellent structural material to contain the lead-bismuth-eutectic (LBE) nuclear coolant needed for fast spectrum operations. Very little data exist in the open literature on the tensile properties of this alloy. The test material will be thermally treated prior to the evaluation of its tensile properties at temperatures relevant to the transmutation applications. The deformation characteristics of tensile specimens, upon completion of testing, will be evaluated by surface analytical techniques using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The 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. The resultant data may also provide guidance in developing future target materials possessing the improved metallurgical properties, and enhanced LBE corrosion resistance.

Tensile tests were performed at ambient temperature, 100, 300 and 400^{o}C using cylindrical specimens fabricated from quenched and tempered Alloy EP-823 (heat number 2054). Three different tempering times (1.25, 1.75 and 2.25 hours) were used followed by an air-cooling. These test materials were identified as 2054S, 2054T and 2054U, respectively.

The results are shown in Figures 1.3.2-1.3.5 showing the effect of testing temperature on the resultant yield strength (YS), ultimate tensile strength (UTS), percent elongation (%El) and percent reduction in area (%RA) as a function of the tempering times. An examination of the Figures 1.3.2 and 1.3.3 clearly indicates that both the YS and UTS were gradually reduced with increasing testing temperature, as anticipated. On the other hand, the ductility parameters (%El and %RA) were not significantly affected due to the increased testing temperature. Additional tests are in progress at 500 and 600^{o}C involving similar materials. It is well known that for martensitic stainless steels, there may be a sudden drop in YS and UTS at temperatures exceeding 400^{o}C. Simultaneously, the ductility parameters may be enhanced due to the increased plastic flow of the test materials at temperatures above 400^{o}C.

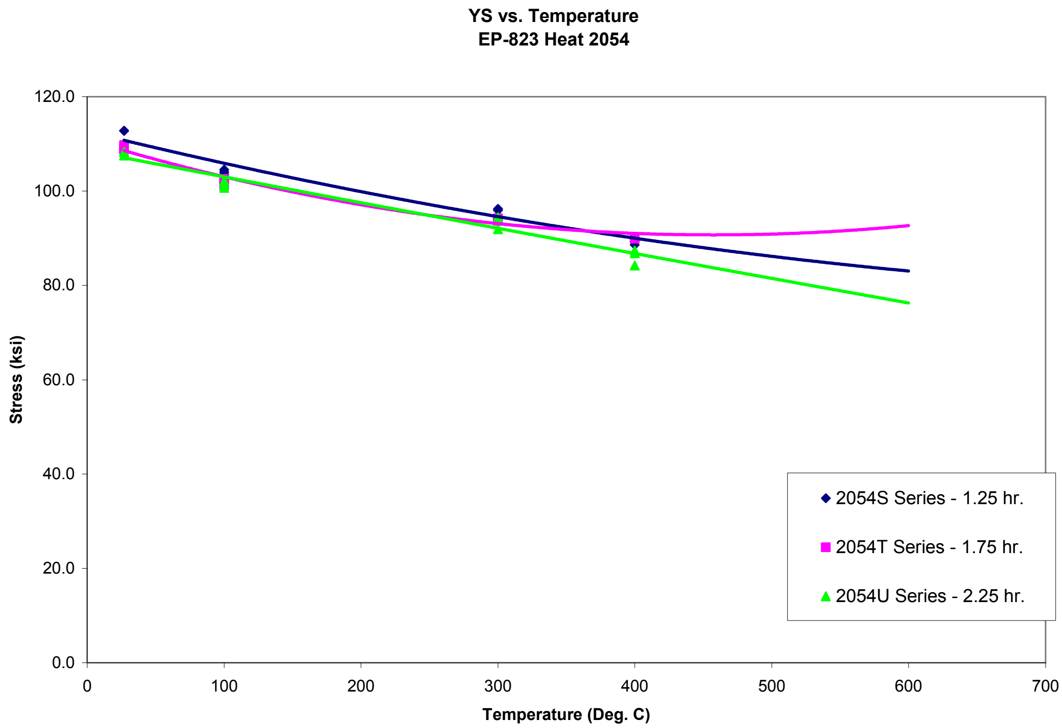

Figure 1.3.2. Yield Strength versus Test Temperature

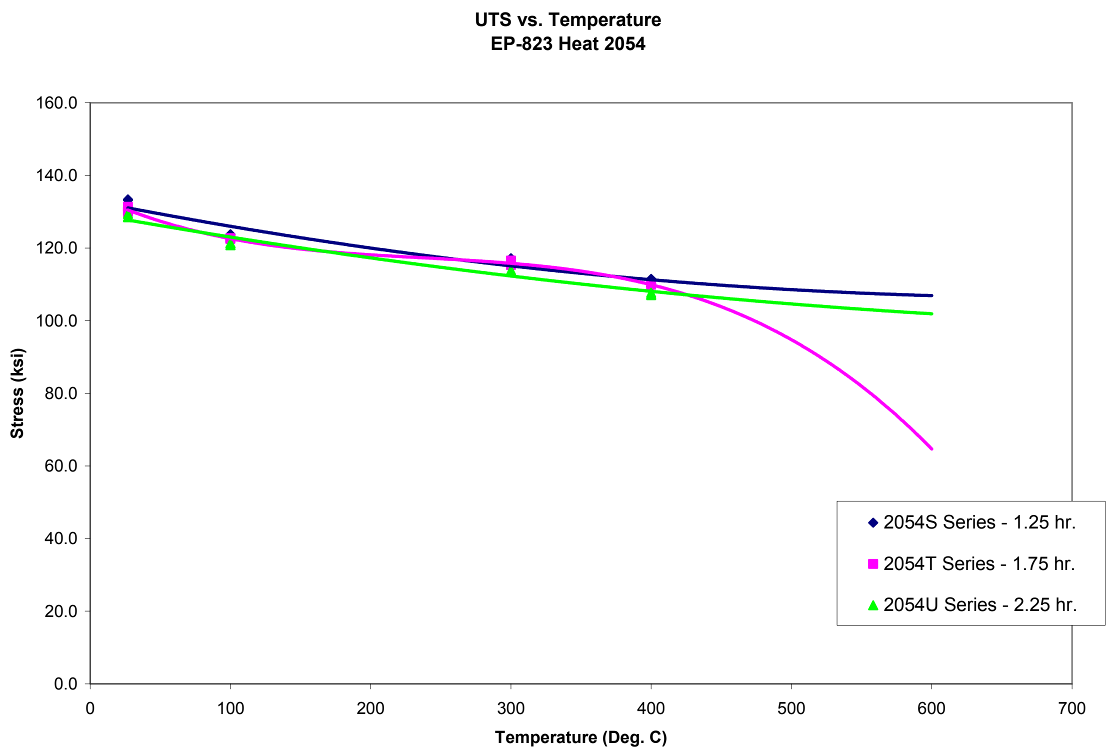

Figure 1.3.3. Ultimate Tensile Strength versus Test Temperature

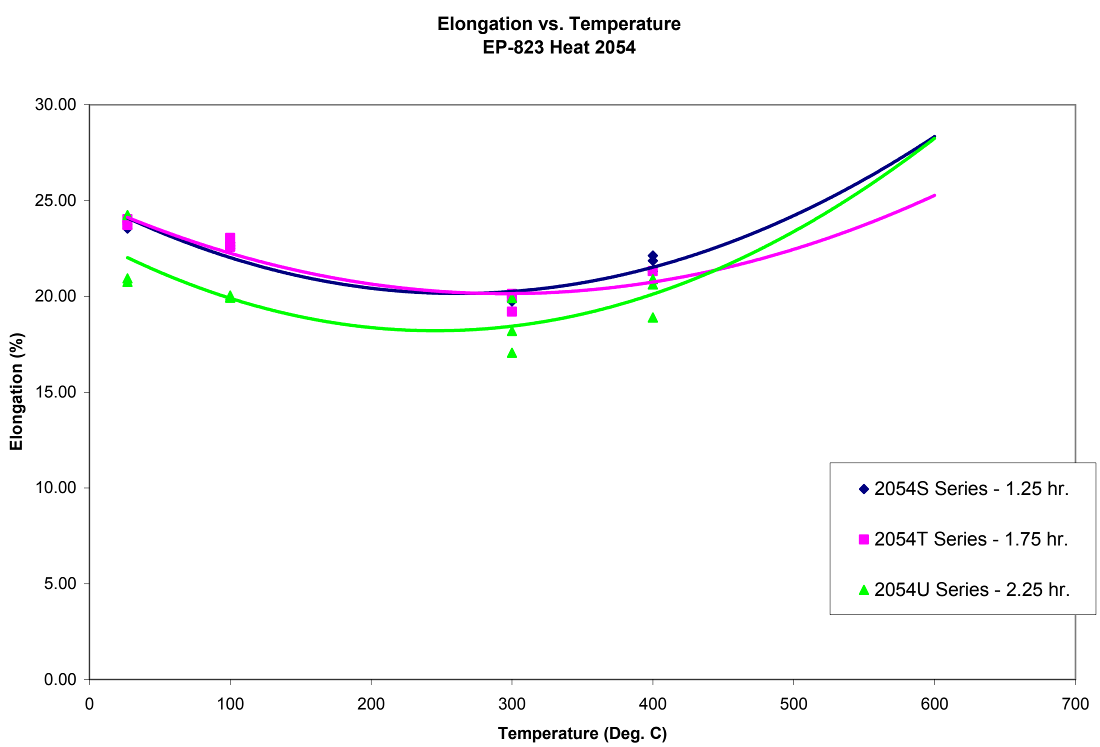

Figure 1.3.4. Percent Elongation versus Test Temperature

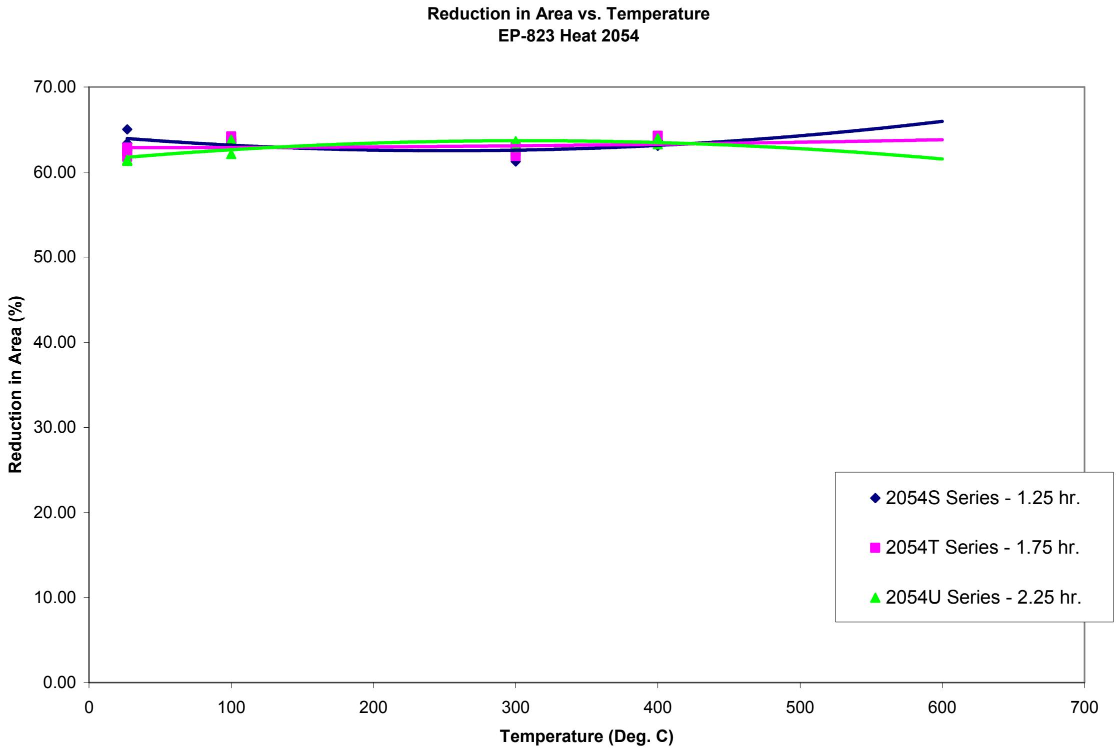

Figure 1.3.5. Percent Reduction in Area versus Test Temperature

Fractographic evaluations of the broken tensile specimens by SEM have just been initiated.

Radiation Transport Modeling of Beam-Target Experiments (Task 12). The AFCI program will rely on the use of accurate calculations and simulations of criticality and shielding for the separation process of the long-lived isotopes that present a significant safety hazard in commercial spent fuel. To help design and verify the safety of the separation process, the neutronics code MCNPX will be used to model the distribution of neutron flux within the fuel blanket and to determine the neutron multiplication, k_{eff}. However, the cross section libraries and computational methods used by MCNPX at these neutron energies still have some uncertainty and will require validation.

Oxygen Sensing in LBE (Task 13). Although liquid lead-bismuth eutectic (LBE) is a good candidate as a coolant in fast nuclear systems, it is known to be very corrosive to stainless steel, the material of the carrying tubes and containers. Such a corrosion problem can be prevented by producing and maintaining a protective oxide layer on the exposed surface of stainless steel. The proper formation of this oxide layer critically depends on the accurate measurement and control of the oxygen concentration in liquid LBE. YSZ (Yttria Stabilized Zirconia) oxygen sensors, using molten bismuth saturated with oxygen as the reference, have been utilized to accurately measure the concentration of oxygen dissolved in LBE.

Positron Annihilation Spectroscopy (Task 14). The purpose of this collaborative research project involving UNLV, ISU, and LANL is to evaluate the feasibility of determining residual stresses in cold-worked, plastically-deformed (bent), and welded materials using a nondestructive method based on positron annihilation spectroscopy (PAS). This technique uses γ-rays from a small MeV electron Linac to generate positrons inside the sample via pair production. This method is known to have capabilities of characterizing defects in thick specimens that could not be accomplished by conventional positron technique or other nondestructive methods. The generated data will be compared to those obtained by other methods such as neutron diffraction and X-ray diffraction (for thin specimens), and ring-core (destructive-for thick specimens) methods. During the initial phase, residual stresses induced in experimental heats of austenitic Type 304L stainless steel, and martensitic Alloy EP-823 have been determined by X-ray diffraction, PAS and ring-core techniques. More recently, efforts are ongoing to include Alloy HT-9, another martensitic stainless steel to perform similar measurements on this alloy using all four techniques. Later, irradiated materials may be evaluated. Low-level radiation will be induced in the test specimens at the ISU, followed by residual stress measurements using the PAS method.