Amarillo National Resource Center for Plutonium
A Higher Education Consortium of The Texas A&M University System, Texas Tech University, and The University of Texas System

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600 South Tyler • Suite 800 • Amarillo, TX  79101
(806) 376-5533 • Fax: (806) 376-5561
http://www.pu.org
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Electronic Resource Library

Dale Cluff, Ph.D., Texas Tech University
Karen Ruddy, Ph.D., and George Huffman, Amarillo College

The Plutonium Information Resource task is known as the Electronic Resource Library (ERL) and managed within Communication, Education, Training, and Community Involvement. The ERL provides international access to the centralized and easily searchable national archives of technical, policy, education, and historical information on plutonium. Reference http://plutonium-erl.actx.edu.

Amarillo College (AC)

During the reporting period, important collaborations and website enhancements continued. The collection, the plutonium catalog, and the number of times the website is accessed continue to grow.

1. **Electronic Digitization:** AC digitized 42,000 pages by April 1998, exceeding the FY99 deliverable of 40,000 pages.

2. **Website Activity:** The website has handled nearly 35,000 hits from launch date, January 6, 1997 through May 11, 1998. This number includes approximately 12,000 hits during the report period.

3. **Website Development:** Activities include completion of contractual arrangements and software development to enhance content and access for those who visit the website. Contracts were negotiated for the development of software programs by Data Research Associates (DRA) for the deployment and maintenance of the National Union Catalog on the topic of Plutonium (PuCAT). AC provided specifications to DRA programmers to develop software to map the comma-delimited data to the industry standard Machine-Readable Cataloging (MARC) bibliographic record in PuCat. This will allow linkage of the full text documents to the bibliographic records to be delivered by Texas Tech University. Staff developed a real time statistical program to provide current reports for any visitor to the website.

4. **Collaboration:**
   a) Renewing agreement between the Office of Scientific and Technical Information (OSTI) and AC Document Exchange Lab (DEL) to receive legacy documents for the PuCORE Collection,
   b) Negotiations are under way with J. James to link to the Electronic Barn Book (Neutron Cross-section Manual On-line),
   c) Working with New Mexico Junior College and Westinghouse Information Center to acquire Waste Isolation Pilot Plant (WIPP) documents pertaining to plutonium,
   d) Discussions under way with Lovelace Respiratory Research Institute to acquire documents related to plutonium/health physics,
   e) Negotiating with Mike Mulheim to acquire Nuclear Safety Journals,
   f) Working with the Department of Defense Technical Information Center office in Albuquerque to acquire documents pertaining to plutonium,
   g) Negotiating with American Nuclear Society (ANS), International Atomic Energy Agency (IAEA), American Chemical Society, American Physics Society and Health Physics Society are under way to obtain permission to digitize copyrighted materials.

5. **Copyright Document Delivery:** AC researchers continue to maneuver the software program that will allow the ERL to serve as an electronic document clearinghouse for copyrighted and other plutonium literature.

6. **Contract Renewals:** AC renewed contracts, written agreements, and letters of rights and permissions between the AC ERL and various vendors and agencies of bibliographic scientific and technical databases, including International Nuclear Information System (INIS), IAEA, ANS, and (OSTI).
7. **Project Management**: Produced systematic analysis of selection, acquisition, cataloging and processing of digital files. This is the first task for the DEL procedures manual. The Collection Verification Team (CVT) has been fully integrated into the selection process for all resources and services in the ERL.

**Texas Tech University (TTU)**

1. During the past quarter the TTU site of the ERL:

   a) Identified 98,489 records on plutonium in 53 separate databases
   b) Downloaded 96,113 bibliographic records on plutonium from 52 of the 53 databases.
   c) Delivered 9,765 bibliographic records from WorldCat and NTIS in ProCite, comma-delimited and WORD formats to the AC site.
   d) Updated configuration files for WorldCat, NTIS, DOE OpenNet, INIS, and Nuclear Science Abstracts.
   e) Downloaded all records from Nuclear Science Abstracts CD-ROM from the Amarillo ERL site.
   f)Parsed the very large retrieval files from Nuclear Science Abstracts into smaller, manageable files.
   g) Made presentation to Beth Perry on the value and procedures of the Plutonium Bibliography.
   h) Planned for random samples to check bibliographic comprehensiveness.

**Other Research Activities**

1. Collaborate with Dr. Abdurrahman with the MOX collection development.
   a) In process of digitizing MOXDAR copyrighted materials.
2. Plan and implement the MOXDAR website on the ERL server.
   a) MOX collection will be merged into PuCore.

3. Contract with vendors for ERL databases and services.
   a) DRA - PuCat database and software; NTIS database on CD-ROM; INIS database on CD-ROM; OCLC FirstSearch via Internet.

4. Renew contract with OSTI.
   a) Continuation as the source of legacy documents as well as a bibliography with over 92,000 bibliographic records for documents pertaining to plutonium contained in the Energy Database.

5. Initiate contract with DTIC.
   a) In progress.

6. ERL incorporates Collection Development (Verification) Team (CVT) guidelines.
   a) Completed.

7. TTU sends to DEL first 5,000 records for the PuCAT.
   a) Processed and delivered 9,765 bibliographic records from WorldCat and NTIS in ProCite, comma-delimited and WORD formats.

8. Publish scanning and training manual for DEL.
   a) Systematic analysis completed.

9. Perform first of two self-evaluations for ERL and DEL.
   a) Presented ERL instruction in late January to graduate students at Texas A&M University studying under Dr. Rube Williams. A study, information-seeking behaviors of users of scientific and technical information, will impact the design of the ERL through HTML pathways, search engines and links.
Environment, Safety, and Health
Environmental Restoration and Protection

Chemical Treatment of High Explosives: Granular Activated Carbon Applications

Mark Schlautman, Ph.D., and Elizabeth Carraway, Ph.D., Texas A&M University

The overall goal of this project is to identify and develop methodologies to enhance the removal of the high explosives (HEs) RDX and HMX from the perched aquifer at the Pantex Plant. Our approach is to investigate the efficacy of combining the existing granular activated carbon (GAC) adsorption system with various chemical treatment schemes including: (1) pretreatment of the GAC before its use in the adsorber column, (2) treatment of the HEs in the perched aquifer water before it enters the adsorber column and/or (3) treatment of the HEs after they have been extracted from the GAC. In all treatment scenarios investigated, consideration of GAC regeneration and reuse will be of primary importance.

Our major efforts this quarter were focused on the development of completely-mixed batch reactor (CMBR) systems for HE experiments (i.e., adsorption, extraction and treatment), GAC pretreatment, and the development of analytical procedures to quantify HE concentrations in these different systems. HE/byproduct adsorption from artificial groundwater (AGW) to GAC will be performed in 40-milliliter amber vials with Teflon-lined caps. The samples will be equilibrated for a suitable time period before analyzing the AGW for residual concentrations and calculating adsorption by mass balance. Following adsorption, the GAC will be contacted with acetonitrile and/or methanol in the vials to extract the HEs and by-products for analysis. Two different types of reactors will be used to chemically treat the HEs: vials similar to those used in the adsorption studies will be utilized for the reductive or hydrolytic degradation of HEs whereas a “merry-go-round” photochemical reactor with quartz tubes and a low-pressure mercury lamp will be used for HE photodegradation experiments. GAC pretreatment with strong soluble reductant (dithionite), strong acid (HCl), or strong base (N₂OH) will be performed in one-liter Erlenmeyer flasks wrapped with aluminum foil (to minimize photochemical reactions); to minimize the effects of oxidation by oxygen, reductive pretreatments will be conducted in an anaerobic chamber filled with 5% H₂ and 95% N₂.

Analytical methods to identify and quantify HEs in AGW and the extractant solutions have been developed using UV-visible spectroscopy (absorbency at multiple wavelengths) and gas chromatography/mass detection. Development of an analytical procedure using high pressure liquid chromatography (HPLC) has been hampered by the failure of our HPLC detector; we are now replacing the bad detector so that we can finish our development of all analytical procedures. Preliminary experiments for the reduction of RDX (14 ppm) by palladized iron (solid-to-water ratio of ~1%) showed an RDX half-life of approximately 70 to 80 minutes as determined by UV spectroscopy and HPLC. Preliminary photodegradation experiments showed an RDX half-life of about 5 minutes as determined by UV spectroscopy.

Feasibility of In-Situ Remediation of Residual High Explosives in the Vadose Zone Beneath the Pantex Plant: Laboratory and Field Studies

Kenneth Rainwater, Ph.D., Caryl Heintz, Ph.D., and Tony Mollhagen, Ph.D., Texas Tech University

The primary purpose of this project is to evaluate the potential for stimulation of in situ biodegradation to decrease the high explosive (HE) concentrations in shallow (< 30-ft depth) unsaturated soils at the Pantex Plant through appropriate laboratory and field experiments. The target areas for treatment are those contaminated by wastewater discharges from buildings in Zones 11 and 12.

Previous impedance microbiological studies of the metabolic potential of the soil from core samples taken from HE-contaminated Zones 11 and 12 showed soil from all depths contained cultivable bacteria. A visiting research associate from the Van Hall Instituut, Groningen, The Netherlands, conducted a study on bacteria isolated from these samples. Mr. Peppell isolated, described and identified (where possible) the heterotrophic bacteria isolated from these samples and from soil.
samples from a site known to be free of high explosives, IW-2. In addition, he developed methods and tested the ability of these isolates to grow in the presence of up to 200 ppm RDX and HMX.

Other projects undertaken include an intensive study carried out on one shallow (16-19 ft) sample of HE-contaminated soil from near Building 12-43. Previous tests provided a complex organic culture medium for the impedance studies. In this quarter, methods were developed to assess metabolic response of the organisms in the soil to simpler nutrient milieus, including single substrate broths. In addition, this study demonstrated the impedance response of the microbes in the samples to a nitrogen gas atmosphere, with distilled water replacing the nutrient medium. The positive metabolic responses obtained in these studies were encouraging with regard to the potential for soil.

A major development during this quarter was the involvement of the research team with the U.S. Department of Energy’s (DOE) Innovative Treatment Remediation Demonstration (ITRD) Program. Staff from the Sandia National Laboratory (SNL) manage the ITRD Program, and this specific effort is intended to support remediation of HE-contaminated soils and groundwater at Pantex and the Los Alamos National Laboratory (LANL). The Battelle Pantex Environmental Restoration team invited Dr. Kenneth Rainwater to participate as part of the technology review team. The review team includes scientists and engineers from Pantex, LANL, SNL, DOE, U.S. Department of Defense, U.S. Corps of Engineers, EPA, state regulatory agencies, and consulting firms. Two group meetings have been held, one at Pantex and one at Santa Fe, with intermediate conference calls. Through this interaction, the research team has formed alliances with the Idaho National Environmental Engineering Laboratory (INEEL) and the COE Waterways Experiment Station (WES). A proposal for ITRD funding will be submitted with INEEL to expand the soil column microcosm experiments, with the laboratory experiments to be performed at INEEL with soil provided by the Texas Tech University team. The INEEL staff has performed similar column tests for biofiltration testing, and will experiment with different nitrogen and organic vapor mixtures to stimulate HE degradation. WES staff are negotiating interaction with the TTU field demonstration experiment.

The layout of the field demonstration project for the Zone 12 source area was finalized, and a work plan was submitted to DOE. The eight 30-ft deep soil borings will be made with a geoprobe rig. Laboratory analyses of HE concentration and microbial activity will be performed on samples from the soil cores, with the bulk of the soil to be provided to INEEL for the soil column tests.

**Feasibility of In-Situ Remediation of Residual High Explosives in the Vadose Zone Beneath the Pantex Plant: Modeling Studies**

Daene McKinney, Ph.D., and Gerald Speitel Jr., Ph.D., The University of Texas

The research, conducted at The University of Texas at Austin, focuses on the biological and modeling aspects of the fate and transport of high explosives in Pantex soil. The objectives are to determine biological degradation rates through laboratory experiments and use these rates as an aid in obtaining a conceptual model to simulate the fate and transport of high explosives. Over the past quarter, progress has been made in both the laboratory and modeling portions.

Laboratory experiments on RDX degradation on soil sample are complete, and a thesis has been written. The results for the batch experiments using 14C-RDX showed that RDX degraders were indigenous to the contaminated soil located in the unsaturated zone and they degrade RDX to a significant extent under anoxic and microaerobic conditions. Little biotransformation was observed in the experiments conducted in an aerobic environment. The addition of phosphorus had little effect on the removal rate of RDX, except in the microaerobic experiment and anoxic experiment with organic carbon addition. However, the addition of a biodegradable organic carbon source significantly increased the rate at which RDX was degraded. Mineralization of RDX by the indigenous microorganisms also occurred in the vials. The extent of mineralization varied as a function of the type of nutrient(s) added.
and the environmental condition. Loss of original RDX from the soil was measured using HPLC analysis, and in all cases, the removal of unlabeled RDX was greater than the removal of the $^{14}$C-RDX. Therefore, the degradation rates were estimated in terms of a total mass loading and were largest when organic carbon was added. The half-lives for the degradation of RDX under anoxic and microaerobic conditions were roughly 70 days and 40 days, respectively. For comparison, the half-lives for aerobic degradation with and without phosphorus were 690 and 1390 days, respectively. However if the 95% confidence intervals were taken into account, the half-lives for aerobic degradation may be considerably larger.

In the past quarter, modeling efforts focused on developing a reasonable model for microbial activity in the vadose zone at Pantex and on simulating adsorption in UTCHEM-6.1. A biological model was developed to include the RDX degradation rates identified in the laboratory experiments into the computer simulations. The metabolic reactions are currently being incorporated into a one-dimensional input file. As stated above, the lab results indicate that anoxic or microaerobic conditions are required in order for microorganisms to metabolize RDX. Based on these results, additional soil parameter values required to correctly model the conditions at Pantex were identified through a search of existing reports. The most recent version of the code, UTCHEM-6.1, includes enhanced modeling of organic sorption to soil particles. In order to ensure the accuracy of this modification, UTCHEM-6.1 capabilities in simulating chemical partitioning into the soil phase are currently being analyzed based on RDX adsorption properties in Pantex soil. During the summer, simulations in UTCHEM using the one-dimensional input file will be conducted to determine the fate of RDX in Pantex soil under natural conditions. Then, the one-dimensional will be converted to a two- and three-dimensional file to obtain representative results for the contaminated area.

High-Rate Biological Treatment of Wastewater at the Pantex Facility as Alternative to the Existing Aerated Lagoon-Pond

Joseph Malina, Ph.D., and C. Cook, The University of Texas

The start of the project was delayed. The cause of the delay was difficulty in obtaining approval from the Department of Defense to collect samples of wastewater from the Pantex treatment facility in Amarillo, Texas. This hurdle has been overcome and samples will be collected on May 20, 1998.

Three activated sludge bioreactors and one rotating biological contractor have been fabricated by project personnel and are ready for operations. These bench-scale reactors will be used to acclimate the microbial consortium using wastewater that will be collected from the Amarillo treatment system. It is anticipated that preliminary results of the treatability studies will be available by the end of the next quarter.

Investigation of Lead and Heavy Metals Contaminated Surface Soils at Pantex Firing Ranges

Sheldon Landsberger, Ph.D., and Felfl Iskander, Ph.D., The University of Texas

During the past months we have focused our attention in two main areas. We completed a thorough library search on publications that involved lead-contaminated soil from firing ranges. Although there are numerous studies which involved soil contaminated from lead smelters and other sources, very few studies have involved firing ranges. As well, little or no data is available on the environmental impact or leaching behavior of the lead in the soil resulting from firing ranges. Work in the past three months has been hindered by the long wait to get permission to collect samples at Pantex and subsequent wait in arrival of the shipment. After an initial visit in January for a planning session, a follow up visit was undertaken in March to collect some 150 samples, including samples for Desmond Lawler in the Civil Engineering Department to conduct other experiments. Dr. David Barnes of the Center organized the sampling expedition and provided a random number output to collect the samples in a statistically
significant manner. About 225 kilograms of soil arrived at the University of Texas in April. Laboratory space to process the samples was arranged at the Center for Energy Studies. Process of the samples has begun. A second trip is planned to obtain additional samples including those from background areas.

The original plan was to analyze some 50-100 samples by x-ray fluorescence for lead, and neutron activation analysis for the other heavy metals. Since many more samples are anticipated to be analyzed there may be a short-fall in funds for analytical services. We have therefore begun exploring the possibility of using the facilities and resources at Pantex to do the determination of lead.

Treatment of Lead-Contaminated Surface Soils at Pantex Firing Ranges

Desmond Lawler, Ph.D., and Howard Lijestrand, Ph.D., The University of Texas

The development of a preliminary procedure for removing lead from contaminated soil and testing this procedure on soil samples spiked with lead have been the primary research activities for the period of February 1 to April 31, 1998. Soil samples from Pantex were obtained on May 1, 1998, and the initial separation of large lead fragments will begin in the following weeks. It is expected that this process will be the most time-consuming step of the treatment plan. However, it is not necessary to complete this preliminary separation step to achieve the starting point for the oxidation and precipitation studies.

Although the soil samples from Pantex were obtained only recently, preliminary tests have been conducted on uncontaminated soil spiked with lead to determine the effectiveness of various removal methods. For these initial tests, a solution of hydrochloric acid, adjusted to pH=1, was added to the spiked soil samples at a solid to liquid ratio of 1:10. The mixtures were stirred at 80 rpm for 24 hours. The liquid portion was decanted after settling for an additional 24 hours, and the remaining solids were air-dried. Future solid-liquid separations will be performed in a centrifuge to minimize the settling time and the adherence of soil particles to the evaporation basin. The remaining solids were measured for pH and digested in nitric acid on a hot plate.

Finally, the digested solution was filtered and the concentration of lead was measured using flame atomic absorption spectroscopy. The results of these tests and similar studies from a literature review have shown that adsorption due to ion exchange is the most predominant mechanism for lead binding to soil particles. Knowledge of the specific binding mechanism is the major factor in determining the proper removal technique.

In the next research period, the focus will be on washing the contaminated soil with an acidic solution to enhance desorption. The effectiveness of hydrochloric acid, acetic acid, and citric acid will likely be examined since these acids have the ability to form complexes with lead and thereby increase removal. The pH will be adjusted to the range 1<pH<3 to achieve acceptable lead removal while attempting to minimize the negative impact on the soil. The washing solution will be added to the contaminated soil, and the sample will then be placed on a mechanical stirrer for 24 hours. The washed soil will be rinsed with acidified water to remove residual contaminants. In the last of the soil washes, a dilute buffer solution will be used to neutralize the soil back to its original pH.

The emphasis of this research is the reduction of lead below the Toxicity Characteristic Leaching Procedure guidelines. In addition, the literature review has indicated several federal and state guidelines which will be used in determining the success of the removal method employed. However, lead shot used at firing ranges also contains from two to three percent antimony. Due to the high mobility and potential human health risks of antimony, consideration is being given to monitoring the removal of this metal as well as lead. The analysis for antimony would not necessitate any additional steps as each sample would still be tested using flame atomic absorption spectroscopy. It is anticipated that the preliminary separation of lead fragments and sieve analysis will be completed in the next quarterly period. The graduate student working on this project is Mr. David Kobe.
Environment, Safety and Health

Treatment of High Explosives by Adsorption and Biodegradation on Granular Activated Carbon

Gerald Speitel, Jr., Ph.D., The University of Texas

During the first quarter of 1998, biodegradation experiments continued and an initial desorption experiment was completed. Additionally, we visited the Pantex Plant and took samples from the groundwater treatment system.

Biodegradation experiments progressed very well during the quarter. In initial experiments, pH levels dropped below acceptable limits. The nutrient mix was altered to compensate for this problem. Additionally, experimental techniques and new equipment were utilized to further increase the accuracy of degradation data. For the first time, experiments exposed the bacterial cultures to a mixture of HMX and RDX. An initial biodegradation experiment achieved degradation of RDX from near 5 mg/L to below detectable limits. HMX was degraded from 1 mg/L to less than 0.45 mg/L. These results were obtained during batch experiments over an 18-day period. In subsequent batch tests, the two bacterial cultures were mixed and achieved even better degradation results. RDX levels, initially at 5 mg/L, reached undetectable levels within 12 days and HMX concentrations were reduced from 1 mg/L to below 0.3 mg/L over an 18-day period. The data suggest that degradation rates are increasing with every experiment, probably due to acclimation and/or natural selection processes.

An initial desorption experiment was completed. Desorption of RDX and HMX off granular activated carbon (GAC) will determine the effectiveness of bioregeneration of GAC. GAC was placed in a column, and RDX-contaminated water was passed through the GAC until the influent and effluent concentrations were equal (36 mg/L RDX). At this point, the adsorption capacity of the GAC was exhausted, although the equilibrium loading was not reached. The average concentration on the GAC was 325 mg RDX/g GAC, whereas equilibrium solid phase concentration should have been 398 mg/g (calculated from isotherm parameters). Clean water was then pumped through the spent GAC, and RDX was desorbed into the effluent. Effluent concentrations were measured over time to determine the rate and extent of RDX desorption. Under the conditions of the test, approximately 353 mg of RDX adsorbed in 18 hours, and about 270 mg RDX (76%) desorbed over 44 hours. A computer model based on the homogeneous surface diffusion model accurately predicted the desorption of RDX. This initial work is very promising from the viewpoint of bioregenerating GAC loaded with RDX.

In February, water and GAC samples were taken from the groundwater treatment system. Water samples were taken from the influent and effluent of the GAC adsorbers, and a sample of GAC was taken from the effluent end of the first adsorber. Influent concentrations were 1.29 mg/L RDX and 0.084 mg/L HMX, and effluent concentrations were 0.012 mg/L RDX and <0.010 mg/L HMX. The effluent RDX concentration was starting to approach the treatment limit because the GAC was nearly exhausted. Populations of heterotrophic bacteria in the treatment system were estimated with plate counts. Influent water had 6.1 x 10^4 cfu/mL; effluent concentrations were somewhat higher, with about 9.7 x 10^5 cfu/mL. Bacterial populations on the GAC were very low, with about 200 cfu/g dry GAC. Bacterial samples from the influent and GAC effluent were tested for the presence of RDX degraders. These were present in both samples; the organisms in the influent sample had a relatively high RDX degradation rate in preliminary experiments. We are now conducting additional tests with these organisms to determine if they are better than the organisms previously isolated from the Pantex soil.

Optimization of the Groundwater Pumping System at Pantex

David Barnes, Ph.D., and Richard Hartley, Ph.D., Amarillo National Resource Center for Plutonium

David Parker, Ph.D., West Texas A&M University

Perched groundwater beneath the Pantex Plant in Carson County, Texas is contaminated with the high explosives (HE) hexahydro-1,3,5-trinitro-1,3,5-triazine and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazozine commonly referred to as RDX and HMX, respectively. In addition to these HE contaminants, the perched groundwater also
exhibits evidence of solvent and chromium contamination. No contamination of the underlying Ogallala aquifer by Pantex Plant operations has been documented. In response to findings of contaminated groundwater, Pantex implemented a groundwater recovery and treatability study in 1995. At present there are fourteen groundwater extraction wells, two injection wells (which inject treated groundwater back into the perched aquifer upgradient of extraction wells), four passive vent wells, and several monitoring wells. The purpose of this study is to evaluate the effectiveness of the groundwater recovery effort.

There are several objectives paramount to this investigation. First and foremost is to determine if hydraulic containment of contaminated groundwater exists. Secondly, if containment is believed to be void or deficient in certain areas then recommendations will be made as to the number and location of supplemental extraction and/or injection wells to ensure that migration of groundwater off-site is terminated. Furthermore, once containment is established the study will then focus on the optimized pumping levels and rates to achieve the most cost efficient operation of the overall pumping system.

According to the January 1998 O&M Report (the most recent report that is in our possession) on the treatability study prepared by Mason & Hanger's engineering-environmental contractor, e²M, some 27,500,000 gallons of perched groundwater has been extracted, treated and re-injected into the perched aquifer. The recovery system was averaging approximately 41,000 gallons pumped per day which correlates to 1,230,000 gallons per month. Extraction wells PTX06-EW-10 and PTX06-EW-4 are currently the largest producers as of January 1998, reporting 311,210 and 295,710 gallons recovered to date, respectively. Other notables concerning the extraction wells PTX06-EW-8 and PTX06-EW-13, which are both reported as “Dry”, meaning they do not yield enough water for sustained pumping, and, wells PTX06-EW-5, PTX06-EW-11, and PTX06-EW-12, which have not yet indicated any flow. At the time of this report it is not known why these wells have not pumped.

Several groundwater reports, studies, publications, and flow models produced by various entities have been gathered from Pantex personnel. Data from these sources are currently being evaluated to determine the status of the hydraulic control at the site. Interpretation of these data is ongoing and an expected determination of hydraulic containment is anticipated in the coming months. The Zone 12 3-D groundwater model was received from Battelle/Pantex in early April and evaluation of this model has not yet been fully undertaken.

Concurrently, work is progressing on the literature review portion of the study. Several groundwater containment and pumping optimization publications are already in hand and being reviewed for their relevance to this project. The literature review is expected to last into the fall of 1998.

Computer hardware and software is being evaluated for the modeling requirements of this project. Comparisons of various manufacturers of Pentium II, 333 megahertz computers are being made and a final decision is expected by late April as to which system will be purchased. Software purchases will be Microsoft's Office Professional 97 which includes a word processor, spreadsheet, database, and presentation package. Technical software for groundwater modeling that is being considered is Visual MODFLOW with the graphic package Visual Groundwater, and FEFLOW which are all produced by Waterloo Hydrogeologic, Inc. Decisions for the possible choosing of Visual MODFLOW are: software is well-documented and accepted by various consultants and agencies, ease of data entry (since it is Windows™ based), compatibility with existing Pantex models, and price. Different optimizing programs such as MODMAN are being evaluated at well.

The graduate student on this project is Rick Gibson. Mr. Gibson is a Masters Degree Candidate in the Department of Life, Earth, & Environmental Sciences at West Texas A&M University.
Optimization of the Biodegradation of RDX and HMX

Robin Autenrieth, Ph.D., and James Bonner, Ph.D., Texas A&M University

The effects of anoxic and oxic conditions on the kinetics of the RDX and HMX degrading microbes were examined. This was the first step toward sequential anoxic/oxic slurry systems. Preliminary respirometric studies were initiated for future RDX and HMX experiments. Experiments were carried out to determine if lower carbon loading would still produce high degradation rates in support of work being done at UT-Austin (Dr. G. Speitel). Two new sets of microbes were isolated from samples taken (Feb. 1998) on-site from Pantex's two-stage, granular activated carbon (GAC) groundwater treatment system. They were tested for their abilities to degrade RDX and HMX.

Initial Rate Studies: The effects of anoxic and oxic conditions on the growth of the RDX and HMX degrading cultures were examined in initial rate experiments. Typically, the addition of biomass to our reactors rapidly produces anoxic conditions due to oxygen depletion. In these experiments, some reactors were allowed to produce these "passively anoxic" conditions. Other reactors were fed air to keep the dissolved oxygen levels (D.O.) and redox potentials in the oxic range, and still other reactors were purged with helium to encourage even more anoxic conditions ("actively anoxic"). The RDX-degrading microbes were exposed to 35 mg/L of RDX under these various conditions. The initial growth rates were then compared to those produced in reactors with no RDX added. The oxic conditions brought about, via influx of air produced, the best overall growth, with the growth in the RDX-exposed reactors nearly matching the growth in reactors without RDX. In this scenario, the D.O. ranged from 6.0 to 9.0 mg/L, and the redox ranged from 198-400 mV. The growth of the microbes under both passive and active anoxic conditions (D.O. < 1.0 mg/L, redox <198mV) was minimal when exposed to RDX. These results indicate that the presence of oxygen seemed to mediate some RDX toxicity. Parallel experiments were performed with the HMX-degrading culture with exposure to 4.0 mg/L HMX. In this case, there was no observed mediation in HMX toxicity in the presence of oxygen. However, the growth of these microbes and their corresponding oxygen depletion rates were high, and the addition of air could not raise the D.O levels above 4.5 mg/L. Therefore, the conditions generated were not as oxic as those created for the RDX-degrading culture. Future experiments will use pure oxygen as opposed to air in order to increase D.O. levels. The next step will be to examine the effects of oxic/anoxic conditions on RDX and HMX transformation and begin sequencing between oxic/anoxic conditions for optimization.

Respirometry Studies: Work has been preliminary and focused on method development and instrument familiarity. Reactors are also being built for future RDX and HMX studies.

Carbon Loading: The RDX-degrading culture was exposed to lower levels of carbon to find the relationship between carbon and RDX degradation. It was hoped that lower carbon would need to be added in order to achieve our observed RDX degradation rates. This would be more economically feasible and would allow for more flexibility in generating various D.O. conditions by lowering culture growth rates. Carbon levels ranged from 0 to 5,000 mg/L (we normally use 2558 mg/L), and tests were carried out at 11 different carbon concentrations. The relationship between RDX degradation rates and increasing carbon levels was linear ($r^2=0.975$). Problems appeared at carbon levels higher than 2558 mg/L. Therefore, it was determined that the carbon level we normally use is optimal for this culture and that any alterations would reduce the amount of RDX transformation.

New Microbes: Two cultures were developed from water and activated carbon samples taken at Pantex. Water samples taken from influent and effluent water at the treatment facility, along with water taken in between GAC columns, was used to develop one culture. Another culture was grown from the GAC granules themselves. Both cultures were acclimated to 5 mg/L RDX and 1 mg/L HMX over 10 days. The resulting cultures were enriched and exposed to 40 mg/L RDX. The culture derived from water samples achieved 75% RDX transformation in 10 days compared
to 58% transformation by our current RDX-degrading culture. The addition of ammonium nitrate to the culture slowed the RDX transformation rate, yet nearly 50% was transformed after 10 days. The GAC culture was only able to transform 26% of the RDX after 10 days when no ammonium nitrate was added. However, the addition of ammonium nitrate enhanced RDX transformation for this culture, increasing RDX transformation to 51% after 10 days. The new cultures were subsequently exposed to 3.0 mg/L HMX, but less than 10% of the HMX was transformed after 10 days by each culture compared to 45% transformation by our HMX-degrading culture.

Plutonium Fate and Transport

Randall Charbeneau, Ph.D., The University of Texas

During the first quarter of this project, the approach for development of a resource text on plutonium in the environment has been reassessed. An advisory committee has been formed that includes representatives from the Center, Los Alamos National Laboratory, non-Center universities, and the private sector. A draft outline for the manuscript is being prepared and will be circulated within the advisory committee for comment. Once the outline is accepted, then a list of potential authors will be developed and authors contacted. The intent is to finish these steps during the next quarter.

Health and Safety

Aircraft Overflight: Accident Probability and Consequence Analyses

James Rock, Ph.D., Texas A&M University

Michael McNerney, The University of Texas

The Texas A&M team is ready to submit its manuscript on Bayes Rule for forecasting aircraft accident rates. We are turning our attention to a sensitivity analysis of the terms in the six-term model. Our goal is to rank each term on its marginal cost for unit improvement in the forecast accident rate. That would benefit public decision-makers who must act on the basis of environmental impact assessment information.

The University of Texas team obtained a customized version of the FAA Integrated Noise Model (INM) software, and is ready to select a replacement for Tracy Turen from two finalists. We expect a rapid acceleration of effort on adapting the INM software for flight track modeling of aircraft accident probabilities associated with arrival, departure and training operations conducted at Amarillo International Airport.

A teleconference was held on April 21, 1998. Participants were J.C. Rock, R. Hedtke, D. Kelly, T. Zimmerman, and J. Petraglia. We discussed priorities in light of the recent internal DOE review of the preliminary draft DOE EIS 0283, "Surplus Plutonium Disposition Environmental Impact Statement." Priorities include: (1) Bayes Rule Extension to Damage and Release Screening; (2) Accident Probabilities revised to eliminate portions of DOE Std 3014-96 associated with level flight into rising terrain, severe weather, heavy traffic and intersections; (3) flight track or flight trajectory model that predicts the expected reduction in accident frequency following efforts to move navigation aids.

Monitoring for Estimating Temporal Variability of Interplaya Recharge

Bridget Scanlon, Ph.D., The University of Texas

Don Reddell, Ph.D., Texas A&M University

Psychrometer data collection was initiated following completion of the boreholes and the instrument trench. The initial design plan required a total of 44 psychrometers to be installed in duplicate at a total of 22 locations in both the trench and in the boreholes. This was to include 7 monitored depths at two locations within the trench (total of 28 psychrometers) and 4 monitored depths in each of the two boreholes (total of 16 psychrometers). It was determined during installation of the boreholes that sufficient room was available to allow two additional depths to be monitored. Accordingly, psychrometer access tubes were installed in the boreholes to 5 and 15 feet below ground surface. As all of the required supplies for these additional depths were not available at the time of the January installation, BEG personnel returned to the site in early April and installed four additional psychrometers, thus bringing the total to 48.
Continuous soil samples were collected during auguring of the psychrometer boreholes. These samples have since been analyzed by BEG for gravimetric water content, chloride concentrations, and pore water electrical conductivities. We are currently awaiting the results for soil samples that were delivered to the Desert Research Institute in Las Vegas, Nevada, for analysis of stable isotopes (2H and 18O) in the pore water. Soil samples were sent to the University of Wisconsin for texture analysis and we are also awaiting those results. We will also be analyzing the samples for soil water potentials in the near future. The time domain reflectometry (TDR) system cable tester, multiplexers, and data logger have been ordered. The scheduled delivery of the system to Bureau of Economic Geology is May 15, 1998. Upon receipt of the components, Bureau personnel will perform laboratory tests to confirm the functionality of the system and a trip to the site will be scheduled for installation. Assuming there are no problems with the system components as received, installation will most likely occur in early- to mid June.

Human Reliability and Safety for Safe Handling and Long-Term Storage of Nuclear Components

William Kolarik, Ph.D., and Jeffrey Woldstad, Ph.D., Texas Tech University
Ian Hamilton, Ph.D., Texas A&M University

In order to jump-start this research project, the Co-PIs visited with the AT-400 team at Pantex in December. From this visit, as a result of a very productive meeting with the AT-400 team, we have become familiar with the unclassified parts of the project.

During the first quarter, progress has been made with the real-time reliability model. The prototype was successfully defended in Mr. H. Lu's doctoral defense in January. From that point, Ms. S. Lu has been involved in extending the model to the human factors/Pantex AT-400 focus. Pantex contact, Mr. Blair Rhodes, provided a limited amount of data from the welding operations. It consisted of physical data streams—current, rotation, and so on. The data was characterized graphically by transferring several cycles to a spreadsheet format and assessing its cyclical, on-off nature.

The prototype is now in the process of modification to deal with cyclical/choppy input data. Presently, it is being transformed to deal with the welding data characteristics. This is a significant part of the project in that the original prototype was developed to deal with a steady-state physical data stream. The on-off or choppy nature of a data stream poses several problems in modeling strategy and adaptation. These problems have been recognized and modeling counteraction strategies have been identified. The result sought in this endeavor is to develop a real-time reliability technology capability for the welding process. We expect a rather crude performance initially, but expect to be able to demonstrate the prototypes capability to link into this process or other processes characterized by cyclical data.

A literature review has been initiated in the areas of mistake-proofing and human error with application to materials handling and process control. Human performance data collected in real-time during previous Center supported tele-robotic work (Dr. Sung-Ha Park's Dissertation) is being compiled for testing in the reliability model.

During the next quarter, we will test our strategies for effectiveness. We will use simulated data that mimics the AT-400 welding data. Also during the next quarter, we will begin working on adapting the model to even more dynamic data, such as we see in human task monitoring and control. These modeling efforts are expected to constitute a significant portion of Ms. Lu's doctoral research project.

In addition, we are planning visits to several U.S. Department of Energy (DOE) facilities to speak with Human Factors Engineers regarding mistake-proofing issues at their sites. Input from these individuals will help us to construct realistic laboratory simulations to evaluate relevant human performance issues in DOE operations.

James Rock, Ph.D., Ian Hamilton, Ph.D., Brent Auverman, Ph.D., and Calvin Pamell, Ph.D., Texas A&M University

Ralph Ramsey, Ph.D., Texas Tech University

We spent the first quarter of this project organizing our team. We have four faculty members from three campuses of two university systems, and by the first of June we will have three full time graduate students committed to this project with prospects for hiring a fourth at TTU during the month of June. We are very pleased to report that because Prof. Parnell is helping without charging the project and Capt. Jim Lohaus, USAF, has chosen to pursue his thesis research work with us, we have leveraged the Center's resources beyond the proposed partial support for three faculty and three graduate students. Prof. Ramsey, of TTU-CE has agreed to join the team to replace Prof. Bethea, who resigned from this project. Prof. Auverman is gearing up to conduct plume transport research in the Amarillo region of the Texas Panhandle.

We have obtained copies of several plume transport software packages and are in the process of installing them to function on available machines.

We are seeking published reports of depleted uranium and weapons grade fissile material contaminated sites. We have obtained some data on the Bomarc Site in New Jersey, and are seeking data on other similar sites. Our goal is to discover the long term fate of metal oxide particles in the environment.

Mobilization and Uptake of Actinides and Heavy Metal Analogs by Plants

Lloyd Hossner, Ph.D., Texas A&M University

High biomass producing cultivars of sunflower (Helianthus annuus) and mustard (Brassica juncea) are potential candidates for phytoremediation of sites contaminated by Cr and U. Growth studies were conducted with these species to evaluate the effect of chelating agents on Cr and U uptake from diverse soils. Seeds of sunflower (cultivar hybrid 571) and mustard (cultivar 4260308; obtained from USDA, Ames, Iowa) were planted in four surface soils having different chemical and physical characteristics. Soils ranged from a calcareous Weswood (pH 7.6) to a very acid Crowley (pH 4.4) soil. Soils were treated with Cr at rates of 200, 300, and 600 mg Cr kg\(^{-1}\) as CrCl\(_3\) *6H\(_2\)O* or with 100 or 300 mg U kg\(^{-1}\) as UO\(_2\)(NO\(_3\))\(_2\) *6H\(_2\)O*. Chelates were applied at different rates, as chelated or non-chelated forms of Cr and U, and at different times of application. Uranium, at a rate of 300 mg U kg\(^{-1}\), was toxic to plants growing in calcareous Weswood soil but not in the acid soils. Chromium toxicity was observed in all soils when applied at 600 mg Cr kg\(^{-1}\) and particularly in those soils with a sandy texture. EDTA-chelated Cr and U affected plant growth more than oxalate or citrate chelates. Chromium and U complexed metal chelates did not affect plant growth as much as when chelates were added separately to the contaminated soils.

The absorption of free Cr\(^{3+}\) is highly pH dependent, but even at pH values as low as 4, this form is readily precipitated on the root surface and possibly in the apoplast, as Cr(OH)\(_2\). Hence, the translocation to the shoots is reduced. Once absorbed, the CrO\(_4^{2-}\) and organic forms of Cr are readily transported to the shoot. The relative toxicity of Cr follows the same general trend with CrO\(_4^{2-} ->\text{Cr}^{3+} ->\text{Cr-citrate}, \text{Cr-oxalate} -> \text{Cr-EDTA}. The absorption of the Cr\(^{2+}\)-organic complex was significantly greater (1.5- to 20-fold) for unhealthy plants, e.g., those that were exposed to Mn\(^{2+}\)-toxicity conditions for some time. This is attributable to a disruption of the membrane integrity and the resulting non-specific uptake of the Cr\(^{2+}\)-organic complex. The more tolerant plants are able to recover following an initial exposure to moderate levels of CrO\(_4^{2-}\), whereas, the more susceptible plants cannot. EPR spectroscopy indicates that in tolerant species the Cr\(^{3+}\) has been reduced to Cr\(^{2+}\). These results indicate that some plants may exhibit a specific or non-specific reductive stress-response to CrO\(_4^{2-}\) toxicity.

Mechanisms of heavy metal accumulation are related to phytochelatin (PC) synthesis and induction of a truncated version of glutathione-S-transferase (GST) whereby the latter is thought to shuttle the PC-heavy metal complex into the vacuole. Heavy metals also
induce the accumulation of anthocyanins, and in this case the nontruncated version of GST tags an anthocyanin precursor with glutathione, which allows for recognition and targeting into the vacuole. The \textit{gst} gene is induced by several environmental stresses and heavy metals. Amplification of a segment of the target gene was successful with PCR, and a radioactive probe was prepared. RNA extraction from Cr-treated and control seedlings has been accomplished, and transfer to a nitrocellulose membrane was successful. Northern hybridization of the probe with the induced mRNA was successful. RNA extraction from Cd-treated, Cr-treated, and control seedlings has been accomplished, and transfer to nitrocellulose membranes has been successful. Northern hybridization of the probe with the mRNAs induced by the heavy metal was successful. The results show that there was no induction of transcript message in the control plants, and a minor induction was observed in the Cd-treated seedlings. A moderate amount of transcript message was observed with the Cr$^{3+}$ treatment, and a very large amount of message was observed with the Cr$^{6+}$-treated seedlings. The molecular size of the Cr$^{6+}$ transcript was smaller than those from both the Cd and Cr$^{3+}$ treatments. It can be concluded that \textit{gmgs}26 gene expression was not only induced by Cd as shown by other workers, but was also induced by both Cr$^{2+}$ and Cr$^{6+}$. This is the first report of this gene being induced by Cr. The shift in the transcript size suggests that the one gene is transcribing two messages, thus two different proteins are being produced. This shift may have been regulated at the stage of transcription or later during post-transcriptional processing.

Dr. Jin Lee has joined the project and will conduct research at the Los Alamos National Laboratory on soil reactions and uptake of Pu by selected plants. This research will be conducted in collaboration with Dr. Moses Attrep and other staff at the Laboratory.

\textbf{Risk Characterization for a Mixed-Oxide Fuel Facility}

\textit{Randall Charbeneau, Ph.D., Sheldon Landsberger, Ph.D., and David Maidment, Ph.D., The University of Texas}

\textit{Ian Hamilton, Ph.D., Texas A&M University}

\textit{John Sweeten, Ph.D., Agricultural Research \& Extension Center}

\textit{David Barnes, Ph.D., and Carl Beard, Ph.D., Amarillo National Resource Center for Plutonium}

The risk assessment continues to move forward, on time, in a multi-faceted manner. First, a 100-page draft interim report, comprised of the preliminary work of the entire research team, has been completed. The document is under review currently, and editing is on-going. Further work is being done to: (1) revise agricultural impact numbers using different dose conversion factors, (2) calculate dose impacts during the early phase of a postulated incident (intermediate phase numbers were presented already), (3) perform a literature search of available studies regarding the failure of HEPA filters following overpressurization (many of the accidents postulated for the conversion and fuel fabrication facilities), and (4) literature search on additional information pertaining to both the conversion process and the mixed-oxide fuel fabrication process. An in-depth literature search has also been undertaken to determine the availability of plutonium release management practices, both nationally and internationally. In addition, data to be used in the GIS database efficacy-in-risk-communication section of the project has been obtained and is being decompiled. The environmental and health-and-safety team leaders have also gotten a "head start" on the transportation risk section of the assessment. The process team leaders are continuing research into determining an optimum throughput for each proposed facility that would minimize required resources (i.e., building space and workers).
Control of Electroslag Remelt Decontamination of Radioactive Contaminated Metal Scrap

Joseph Beaman, Ph.D., The University of Texas

This is a new project funded in April 1998. An update will be submitted next quarter.

A Decision Making Model for Materials Management of End-of-Life Products in the Pantex Plant

Hong-Chao Zhang, Ph.D., Texas Tech University
Frederick Ling, Ph.D., The University of Texas

Initial efforts were made on establishment of a feasible and acceptable architecture by the Pantex system. The system encompasses three major functions of waste management defined by U.S. Department of Energy (DOE), i.e., storage, treatment, and disposal. The emphasis of this research was on decision-making in management of non-nuclear materials dismantling and recycling from warheads.

The established initial system architecture consists of two modules, a disassembly module and a recycling module (see Figure 1). The disassembly module supports decision-making in identifying components in terms of reuse, re-manufacturing, disassembly, recycling, and classifying components under the requirements on environment, safety, and health issues. It can provide a summary report regarding disassembly route, disassembly cost and time, recyclable components, hazardous materials, amount and characters. The recycling module supports decision-making in material disposal methods in terms of recycling, landfill, and incineration. It can summarize these decisions in terms of optimization of recycling, statement of environmental impact, cost of disposal, and recoverable resources.

Since a large amount of environmental data such as materials properties, standards and policies are required in the decision-making, the system is designed with a capability of accessing public databases, i.e., EPA (Environmental Protection Agency) and DOE databases, via Internet by using common gateway interface (CGI) technologies.

The established initial system architecture was presented to Pantex Plant on March 18th. Dr. David Barnes conducted the meeting. Dr. James Luginbyhl and Mr. Bill Reamger from the Pantex Plant attended the meeting. The Pantex partners provided substantial recommendations on the system architecture. Also beginning the second quarter, project emphasis will be given to recycling and optimization.

Other Research Activities:

A presentation was given on March 18, 1998, at the Pantex Plant. Participants were: David L. Barnes, Ph.D., P.E., Programs Manager of Environment, Safety, and Health; James W. Luginbyhl, Ph.D., P.E., Section Manager, Pollution Prevention, Waste Management Department, Battelle Pantex; William Reams, P.E. Manager, Explosive Operation Department, Mason & Hanger Corporation.
Enzymatic Degradation of Pu/U “Suspect Contaminated” Waste

Caryl Heintz, Ph.D. and Kenneth Rainwater, Ph.D., Texas Tech University

The primary purpose of this project is to evaluate the potential for volume reduction and radionuclide separation of cellulose-based laboratory wastes with transuranic or low-level radioactivity. At the Los Alamos National Laboratory (LANL), work is regularly performed in glove boxes, such as in TA-55, with plutonium and other radionuclides that may leave residuals on the items within the box or the box’s internal surfaces. Normal maintenance of the glove boxes is done by cleaning with laboratory wipes and cheesecloth. When classified as “suspect waste”, these materials must be handled as transuranic or low-level radioactive wastes and disposed in special landfills or other repositories. Dr. Heintz has previously patented (U.S. Patent No. 5,597,728, issued January 28, 1997) an enzyme-based technology that could be used to treat cellulose, or cellulose-containing, waste items such as laboratory wipes, paper trash and laboratory garments which were known to be contaminated with Pu or U. This project is intended to demonstrate the technical feasibility of this process for treatment of the cheesecloth, wipes, and paper in LANL’s laboratory waste stream. This technology has been proven both with uranium-contaminated cotton in the patent held by Dr. Heintz, and with Pu-contaminated cotton by Dr. Jim Brainard of LANL who used a microbial source of the enzymes rather than the enzymes alone. The experiments with radioactive materials will be performed by a Texas Tech University (TTU) graduate student, Mr. Luke Swift, at the LANL facility under cooperation from Dr. Brainard and Dr. Larry Avens.

In the first quarter of FY98, the TTU research team, with Dr. Barnes, made two visits to New Mexico to discuss the project with the LANL scientists. The designs of cold experiments to be performed at TTU and hot experiments to be done at later at LANL were finalized. The first set of tests was begun at the TTU campus in the Department of Biological Sciences to evaluate possible inhibition of the enzymes by non-radioactive materials. The potential inhibitors will included lead, nitrate (both as soluble nitrate and as nitrate + cellulose), and slurries made from clean cheesecloth and lab wipes as provided by LANL. These tests will follow similar procedures to those employed in the original development of the patent.

New Polymers and Extractants for Plutonium Separation

Richard Bartsch, Ph.D., Texas Tech University
Keith Pannell, The University of Texas at El Paso

During the reporting period, the development of new bi-functional anion-exchange resins for sorption of plutonium from nitric acid solutions has been continued. As before, this development effort involved the preparation of novel bi-functional anion-exchange resins by Dr. Bartsch and his co-workers at Texas Tech University and evaluation of their performance in sorption of plutonium from nitric acid solutions by personnel in the Nuclear Materials Technology Division at Los Alamos National Laboratory (LANL).

In these bi-functional anion-exchange resins, there are two anion-exchange sites per repeat unit of the polymer. The resins are prepared by reaction of commercial poly (4-vinylpyridine) with alkylation agents which contain a positively charged function (quaternary ammonium or phosphonium group or a pyridinium group) in addition to a displacable halogen atom. Such bi-funcational anion-exchange resins were shown to exhibit superior plutonium sorption kinetics and efficiency compared to Reillex™ HPQ, a monofunctional anion-exchange resin which is the current industry standard for plutonium sorption.

Previous evaluation of the bi-functional anion-exchange resins for plutonium sorption from nitric acid solutions have involved single-stage sorption experiments in which the insoluble resin is shaken with the nitric acid solution followed by filtration of the resin and counting of the residual plutonium in the nitric acid solution. Although this experimental method is appropriate for determining the effect of structural variations within the resins upon their plutonium sorption behavior, it is not the methodology which would be utilized in practical application. In practice, a column of the anion-exchange resin will be utilized to
allow for processing of plutonium-containing waste solutions in a flow-through configuration. During the reporting period, a larger-scale synthesis of the most promising bi-functional anion-exchange resin was performed to produce 150 grams of resin which should be sufficient for the preparation of two 6-inch chromatography columns at LANL. The alkylating agent, (5-bromopentyl) trimethylammonium bromide, was prepared on a large scale. Due to size limitations of our laboratory pressure reactor, it was necessary to prepare the requisite amount of the resin batch-wise by reaction of the (5-bromopentyl) trimethylammonium bromide with commercially available Reillex™ HP-21 poly (4-vinylpyridine) in methanol at 100 °C. The large-scale synthesis was completed and 150 grams of the most promising bi-functional anion-exchange resin was sent to LANL for evaluation in the column-configuration sorption of plutonium from nitric acid solutions.

Interactions of the plutonium (IV) species present in 7 M nitric acid with bi-functional anion-exchange resins are also being probed by computer modeling at LANL. The results suggest that incorporation of a carbon-carbon double bond into the "linker" which connects the two anion-exchange sites in each repeat unit of the resin may provide more efficient complexation of the plutonium species than does the five methylene group linker of the presently most promising resin. By a mono-substitution reaction of cis-1,4-dichloro-2-butene with trimethylamine, the new alkylating agent was prepared. Reaction of cis-1-bromo-4-trimethylammonio-2-butene bromide with Reillex™ HP-21 poly (4-vinylpyridine) produced a new bi-functional anion-exchange resin which was forwarded to LANL for evaluation in single-stage sorption studies.

In another aspect of this work, Dr. Pannell and his co-workers at the University of Texas at El Paso continued the development of the larger-scale synthesis of a new actinide-complexing agent. Preliminary studies of this ligand at LANL indicated high efficiency in the separation of americium from plutonium. Dr. Pannell and his co-workers have obtained a crystal structure of the complexing agent.
Communication, Education, Training, and Community Involvement
Communication, Education, Training, and Community Involvement

Program Implementation

Program Management

Elda Zounar, Ph.D., Beth Perry, M.S., Cathy Dixon, Shirley Floyd, and Effie Harle, Amarillo National Resource Center for Plutonium

Philip Nash, P.E., Texas Tech University

The Center relies on Communication, Education, Training, and Community Involvement staff to facilitate community involvement by providing information to the public and to the media through electronic libraries, the Center website, quarterly newsletters and other print materials, the speaker’s bureau and invited speakers, and the Center’s exhibit program.

Communication Program

During the first quarter of 1998, Center staff continued external communications efforts on DOE-related issues of importance to the Amarillo community and managed a related project.

Center External Communications

Media

The Center received mention in 15 print articles and photos. The Center received two opinion editorials, three magazine articles including articles in Nuclear Materials Monitor and Pollution Engineering, one radio interview, and one television interview. The Center facilitated an additional opinion editorial. These numbers compare to 28 print articles, two opinion editorials, and 13 known electronic media hits in the first quarter of 1997.

Center communication staff 1) distributed a Center for Strategic and International Studies (CSIS) Report to the Amarillo Globe News, to the editorial department of the Dallas Morning News, and to a feature writer with the Dallas Morning News, 2) created packets of materials on the Center and disposition efforts and delivered those packets to The Austin American Statesman, The Bryan-College Station Eagle, and The Daily Texan (The University of Texas newspaper), and 3) facilitated an interview with the Center’s Nuclear Program Manager, Carl Beard, for Source Book, a utility companies publication.

Other Research Activities

The Center made presentations to the Waste-Management Education and Research Consortium, Carlsbad Monitoring and Research Center, and to the Center’s External Advisory Committee. Additionally, the Center made five presentations to small groups of people including Los Alamos staff and David Chaney and Roger Dintaman of DOE.

Center communication staff developed a new tabletop exhibit, developed presentation materials for Center researchers, and provided the Center’s conversion and mixed-oxide fuel risk characterization posters for display in Panhandle, Texas.

The Center published the first quarter, 1998, newsletter and the “What is Mixed-Oxide Fuel?” and “What is Plutonium?” fact sheets. These fact sheets have been distributed to the Center’s newsletter mailing list and Pantex employees. The fact sheets have been made available at presentations, on the Center’s website, at the Center’s exhibit, and at special events.

The Center’s fact sheet series has received high praise from David Geary, Director of Public Affairs of the Albuquerque DOE office. The list of published fact sheets consists of:

1. New Missions for Pantex?
2. Q&A on the Center’s Study
3. The End of the Cold War
4. Nuclear Energy
5. The U.S. Nuclear Fuel Cycle
6. Weapons Plutonium Conversion
7. What is Mixed-Oxide Fuel?
8. What is Plutonium?

Two additional fact sheets, Wastes and Regulatory Issues and Policy Aspects of Disposition, will be distributed during the second quarter.
Communication, Education, Training, and Community Involvement

Miscellaneous

The Communications Department handled two additional tasks that furthered the outreach efforts of the Center: 1) created a photo file of the Center's research projects at Texas A&M University and the University of Texas, and 2) developed the "Seaborgium" card.

Exhibit Program

The Center's exhibit was displayed for technical and professional audiences: Waste-Management Education and Research Consortium (WERC), Waste Management Symposia (3,900 attendees), Center's local External Advisory Committee, and the American Nuclear Society's Western Regional Student Researcher's Conference (100 students). Educational audiences that viewed the Center's exhibit during this reporting period include: Sam Houston Middle School Career Days (200 students attended) and the National Science Teachers (NSTA) Conference (16,500 attendees).

Speaker's Bureau

Center staff spoke to the public at the National Energy Education Development (NEED) Teacher Workshop, Fannin Middle School, at a middle & high school teachers workshop, at Amarillo Toastmasters Club #211, and the North Amarillo Lion's Club.

Science Information And Resource Center

Zane Curry, Ph.D., and Marie Gentry, Ph.D., Texas Tech University

The exhibit contract was awarded to Sparks Exhibits of Philadelphia on December 9, 1997. Drawings of the structures (not text and graphics) were received from Sparks Exhibits on January 23, 1998. Shop drawings of the exhibit structures by the investigators and Center personnel were approved on January 26, 1998. Sparks Exhibits of Philadelphia began fabrication of the structures.

In February investigators received proposed graphic layouts from Sparks Exhibits for review and mailed edits to the Center personnel. In late March, Sparks Exhibits sent revised final exhibit text and layout to the investigators and Center personnel for review. Investigators faxed corrections and comments back to Sparks Exhibits and Center personnel the same day.

Informing the Agricultural Community about Plutonium

Paul Vaughn, Ph.D., Texas Tech University

John Sweeten, Ph.D., Texas A&M Experiment Station

Project staff met with District I Extension personnel in Amarillo to develop procedures and dates for focus group meetings. Following that initial meeting, focus group sessions were held with county extension personnel and their agricultural committees in eight counties near Pantex. The purpose of the focus groups was to identify specific questions and concerns the agricultural community had regarding the current and proposed activities related to plutonium storage, plutonium conversion, and mixed-oxide fuel. Several follow-up meetings with local county extension personnel and other agriculturists in the area were held to identify other specific concerns.

Utilizing data collected from the focus group sessions and other meetings, project staff identified approximately 100 questions to be answered. Answers to the questions were written by project staff and submitted to Center staff for review.

At a subsequent meeting with Center communications personnel and TTU project staff agreed to develop pamphlets and a guide for county extension personnel for distribution to the agricultural community. Project staff also agreed to develop a set of visuals for the guides, which will be distributed to each of the nine counties in the immediate Pantex area. This is in accordance with the project objective to develop a flexible plan for communicating information to the agricultural community.

Education Program

During February, March, and April, information about the Center's Education Program was presented in 107 schools with an audience of approximately 8,304 students and teachers. The following projects and activities are some...
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of the ways the Center participates in the community through the Education Program.

**K-12 Education Projects**

**West Texas Environmental Project for Integrative Studies in Science and Mathematics (WTEP)**

*Richard Powell, Ph.D., Texas Tech University*
*Christine Purkiss, Ph.D., West Texas A&M University*

**Recruit teachers for 1998 WTEP**

Twenty-four individuals have been recruited for the summer phase of this project which includes three days of classroom work and an extended field trip to sites in the western portions of Texas, Oklahoma, Kansas, and Nebraska. The teachers will focus on sustainability with an emphasis on water and the Ogallalla Aquifer. This study will furnish background knowledge and context in which to develop integrative curriculum.

**Hold teacher advisory panel meeting**

The 24 1998 participants met in Lubbock on March 30 to develop a conceptual framework for the summer study and curriculum to be developed this summer. Participants were assigned several books to read and review. Preliminary plans were made for the field trip during this quarter.

**Secondary School Physics Curriculum**

*Jan Spears, Ph.D., West Texas A&M University*
*Terence Ahern, Ph.D., Texas Tech University*

**Simulations for the Interactive Physics Teachers Manual**

were translated from Macintosh to PC format during the last reporting period. This project has ended. The final version of the manual was delivered in February, and the final report was completed in April 1998.

**Middle School Science Resource Manual**

*Gerald Skoog, Ph.D., Texas Tech University*
*Treasure Brasher, West Texas A & M University*

On May 1, 1998, Treasure Brasher presented a workshop on a unit from the Middle School Resource Manual at the National Science Teachers Association (NSTA) convention in Las Vegas, Nevada. During April and May, participants were recruited for the Summer 1998 training session on the use of the Middle School Resource Manual, the selected participants were notified, and the training sessions were planned.

**Building Foundations For Mathematics And Science Success**

*George Mann, Ph.D., West Texas A&M University*
*Richard Powell, Ph.D., Texas Tech University*

Project activities for this reporting period include completion of Cool School and Intercession classes and preparation of evaluations. Current emphasis is on planning for the Fall 1998 project activities and analyzing data gathered from the Spring 1998 project activities.

More West Texas A&M University (WTAMU) teacher education students than were originally planned were able to receive training and access to mathematics and science curricular materials developed by prior Center-funded projects. WTAMU redesigned the department's elementary methods classes this year, and taught the methods in a block. These students received training from four WTAMU professors and developed master lesson plans over the four areas. The interns had access to effective lesson plans through project training and curricular materials.

Follow-up interviews with the interns indicated that they performed well, and they were able to make modifications and adjustments as needed. Evaluations by the professors indicated that students later taught with poise and confidence and motivated the elementary students to learn.

Class offerings included 15 different topics presented by 24 interns. Interns team-taught classes at a number of different schools for a maximum teaching experience. Thirteen master teachers oversaw interns' and students' progress. Six site managers completed the personnel teams. The Panhandle Independent School District and five schools in the Amarillo Independent School District hosted 244 students for the Cool School and Intercession classes.
On the last day of the AISD Cool School, AISD provided transportation for participating students to the WTAMU campus. Interns served as tour guides and assisted master teachers and WTAMU professors in teaching about engineering technology, environmental science, and mathematics using ropes. The children participated fully in the experience. This gave students first-hand experience with university professors who talked about careers and used hands-on application of principles.

The principal investigator has reviewed the evaluation instruments designed to measure the effectiveness of the project.

**Texas Prefreshman Engineering Program (TexPREP)**

*Charles Kellogg, Ph.D., Texas Tech University*

*Therese Jones, Amarillo College*

During this reporting period, the primary activities consisted of recruiting students and planning for the summer TexPREP program, as follows:

**Recruitment and Publicity Activities**

Amarillo middle schools broadcast information about the program. In April 1998 all 8th grade classes in Hereford Junior High School had the opportunity to hear a presentation about the Amarillo TexPREP program. Tascosa High School classes heard presentations on April 21.

Approximately 1,500 TexPREP application packets were sent to 115 area middle and high schools; 140 packets were sent to prospective 2nd and 3rd year participants during February. Completed applications were organized by mid-April. Interaction with groups such as Texas Alliance for Minorities in Engineering (TAME), Los Barrios, Lubbock Coalition for Math, Science & Engineering, National Association for the Advancement of Colored People (NAACP), and others continues. Instructors and staff for summer 1998 TexPREP were hired by May 1.

Panhandle Regional Planning Commission has been awarded funding again this year by Amarillo TexPREP. A contractual arrangement for a $95-per-week stipend and transportation costs, as needed, was made for students qualifying for the programs. The AmarilloPREP stipend award process examines academic interests and grades, and the award is determined by financial need. Arrangements were made for free lunches to be provided to all participants through the City of Amarillo Parks Department Summer Lunch Program.

**Planning Activities**

Requests for area engineers and scientists to speak to TexPREP students have been made.

Plans for field trips are underway, particularly for the two combined Amarillo PREP/TexPREP-Lubbock trips funded by the Center. The second year students' overnight trip to New Mexico to tour the Waste Isolation Pilot Project (WIPP) site, space museum, endangered species fish hatchery, and Carlsbad Caverns is planned for July 8-10. The third year students' five-day trip to Nevada to tour the Yucca Mountain Site and Palo Verde Nuclear Power Plant is planned for July 12-17.

**Regional and National Science Bowl**

The Regional and National Science Bowl is an academic competition developed for teams of high school mathematics and science students and their coaches. The competition is designed to encourage students and teachers to achieve excellence in the sciences.

The Pantex Plant Regional Science Bowl, February 1998, involved 175 students and sponsors who formed 29 teams representing 18 schools from the Texas Panhandle and central and southern Texas. The Texas A&M University (TAMU) Regional Science Bowl held February 1998 involved 90 students and sponsors who formed 13 teams that represented 11 schools from the central and southern areas of Texas. Support from the Center allowed the winners from the Pantex Science Bowl and from the TAMU Regional Science Bowl to compete in the U.S. DOE's National Science Bowl finals May 1-4 in Chevy Chase, MD, moderated by Secretary of Energy, Federico Peña, and Bill Nye, "the Science Guy."
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PACES-On-Tour

The Promotion and Awareness of Careers in Engineering and Science (PACES), under the umbrella of the Society of Mexican American Engineers and Scientists (MAES) toured Texas Panhandle schools in March. Teams of students from Texas A&M University (TAMU) visited 17 schools and appeared before approximately 3,000 students. Their messages to middle and high school students are: (1) Stay in school. (2) Get a strong foundation in science and mathematics. (3) I was where you are just a few years ago; if I can get a technical education, you can too. Reports from teachers indicate the TAMU students are up-beat, have great energy, and deliver a strong, positive message.

JASON Project

The JASON Foundation's, JASON IX, Oceans of Earth and Beyond, is a program designed to study the structure of shallow, mid-water, and deep ocean environments and the life they support. After a period of research, students learn by way of an electronic field trip with actual on-site scientists. In preparation for the broadcast, Amarillo students conducted their own explorations in area lakes and streams.

The Center supported the local broadcast for Amarillo Independent School District (AISD) in March. Over 2,000 AISD middle school students, two marine biology high school classes, and 78 teachers participated in pre-broadcast research, news and discussion groups, interactive exercises on current and past projects, and viewed video and sound clips. Participants continue interaction with the JASON Project via the Internet On-line Systems.

Fannin Middle School Discovery Laboratory

The Discovery Lab is in constant demand with 150 students working in the laboratory daily. In the lab, Science and Math students can connect to the JASON Project through the JASON On-line System.

Traveling Chemistry Road Show

The Traveling Chemistry Road Show is a portable, interactive chemistry demonstration that travels to schools throughout the Texas Panhandle demonstrating the wonders of science to elementary, middle and high school students. During March and April the show traveled to 14 schools with nearly 1,800 students in attendance.

High Plains Regional Science Fair

The High Plains Regional Science Fair held in February was host to 463 students with 325 science projects. The “Ion Propulsion,” project of Eric Davis of Amarillo High School and the “Harmful Pathogens in the Air We Breath,” project of Amanda Landis of Happy High School, will represent the High Plains Region at the INTEL International Engineering and Science Fair in Ft. Worth, Texas in May.

Tri-State Fair Discovery Expo

The Tri-State Fair Discovery Expo will be a science experience for children of all ages. The Expo promotes excellence in mathematics and science and will provide hands on activities designed to stimulate students’ excitement with the wonders of science. It will be held at the annual Tri-State Fair, a regional event that was attended by 120,000 people in September 1997. The Center, the Pantex Plant, and The Don Harrington Discovery Center are collaborating to provide a unique science experience that will draw fair attendees to the Expo and serve as a motivator for area teachers to plan science field trips. The Discovery Center will host numerous interactive activities, the Pantex Plant will have exhibits about their activities, and the Center will provide the Plutonium Disposition exhibit.

Graduate Education

Technical Graduate Education for the Texas Panhandle Via Distance Learning

Edward Anderson, Ph.D., Texas Tech University
Sheldon Landsberger, Ph.D., The University of Texas

The objective of this program is to "establish a means by which Texas Panhandle technical employees can have access to high quality graduate education courses." Texas Tech University (TTU) offers a distance learning Master of Engineering graduate degree with considerable latitude for allowing up to one-
half of the credits to be transferred from other institutions and disciplines. The Texas Higher Education Coordinating Board is now modifying its distance learning regulations so that other state universities may offer programs outside their “designated areas.” The TTU program provides a vehicle for the consortium to participate in degree granting programs.

The Nuclear and Radiation Engineering Program at UT Austin has developed a Health Physics Masters Program in collaboration with UT San Antonio. Several students have been recruited for this program and several courses have been developed. These courses can be offered in the Texas Panhandle region. Considerable effort has been dedicated to reformatting the UT Austin Radioactive Waste Management courses for distance delivery.

The feasibility of distance learning is being determined through a combination of (a) historical information analysis, (b) analysis of current information associated with telecommunications capabilities in the Texas Panhandle, (c) analysis of survey research results, and (d) evaluation of investigative results on the best technology to meet the objective.

Information regarding items (a) and (b) has been gathered over a two-year period. Regarding item (c), the audience has been defined, a survey process has been designed, and two survey instruments are nearly complete. The first instrument is for regional employers and the second is for their respective employees. Each group will be asked the same or similar questions. Results will be compared. Survey results will provide information about interests, education objectives, curriculum and logistics preferences, and availability of on-location facilities.

To establish a broad potential audience, the PIs have contacted other facilities including the University of Texas at El Paso, Commanche Peak Nuclear Power Station, and Los Alamos Scientific Laboratory.

The PIs have investigated the best technology to meet the project objective. They have visited the Waste-Management Environment Research Consortium (WERC) of New Mexico State University, and the Western Heights School District of Oklahoma City, both of which offer distance learning courses. The WERC program operates a two-way, interactive audio/video program using fiber optics, satellite links, and specialized studio-classrooms at both ends of the communication. The Western Heights District program uses two-way compressed audio/video with other personal computer (PC) based tools such as shared electronic whiteboards and chat rooms. Although they operate some studios, most of the Western Heights facilities are simply an appropriately equipped PC in an existing classroom. Teaching appeared to be similar in both programs. After evaluating these two approaches, the PIs have elected to pursue the Western Heights model using Internet communication channels. The necessary software, hardware, and communication channels have been identified and satisfactorily demonstrated in the Lubbock area. A demonstration is planned for May in the Amarillo area. All the computer networks in the Texas Panhandle have been identified and their capabilities have been determined. A cost comparison of the various commercial and educational communication channels is underway and should be completed in May.

Long Distance Graduate Education
Sheldon Landsberger, Ph.D., and Julie Mercer, Ph.D., The University of Texas

During the reporting period long distance graduate education for the Nuclear and Radiation Engineering Program at the University of Texas has been developed. Promotional efforts for the Health Physics Option Master's Program had favorable results. Employees of Texas Department of Health have shown an interest in the program and have begun to apply. Two to three new courses will be developed to accommodate this new area, while two courses in Radiological Medical Physics will be offered by the University of Texas San Antonio Health Science Center. Researchers visited to the University of Texas at El Paso and WERC at New Mexico State University where students expressed an interest in applying for the Health Physics masters program. The Director of WERC asked for a detailed syllabus of the Radioactive Waste Management course given
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at UT Austin with the possibility of including it in their long distance program. Exchanges with Dr. Mitty Plummer from the University of North Texas resulted in his willingness to advertise UT Health Physics courses as part of their curriculum for Commanche Peak Power Plant.

PIs followed up with the Instructional Media department at UT-Austin in preparation for delivering the first course in Health Physics this fall. Much effort has been given to formatting the Radioactive Waste Management lectures to be presented via remote distance learning. The next set of lectures is being developed. This project is off to an excellent start. PIs look forward to disseminating the "Needs Survey" to Pantex and to industries in the Panhandle.

Miscellaneous Education Activities

1. The Center was represented at the National Science Education Leadership Association workshop held at the National Science Teachers Conference in April 1998, attending sessions on PRIME Science, a program that coordinates all areas of science; International Science Olympiad, a competitive science, math, and technology event that requires knowledge and problem solving skills; and Science Assessment.

2. The Center’s Education Program Local Impact Report was shared with members of the External Advisory Board and U.S. Department of Energy official, Dave Chaney, in information packets. Approximately 300 reports were mailed to federal and state-elected officials, Department of Energy officials, local city and county officials, education administrators, and local civic leaders among others.

3. School administrators in the Carson County towns of Panhandle, Skelleytown, White Deer, Groom and Claude received a visit from the Center’s Education Program Manager in April. Each was given a packet of information about the Center and Education programs supported by the Center.

Training

Plutonium Reference Book
Darleane Hoffman, Ph.D., Seaborg Institute for Transactinium Science
Clinton Nash, Lawrence Livermore National Laboratory
Marye Anne Fox, Ph.D., The University of Texas

In consultation with the Center staff, we have reinterpreted the scope of the deliverable volume as defined in the relevant contracts. We have decided that this volume is to be a multi-authored volume, which the G.T. Seaborg Institute for Transactinium Science (GT-ITS) will edit and contribute to, reviewing the major advances in plutonium chemistry since 1967. That year corresponds to the completion of J.M. Cleveland’s The Chemistry of Plutonium which is thought to have been authoritative to that point. The GTS-ITS contribution will focus on advancements in the chemistry of plutonium since 1970. It is preferable to have individual authors contribute chapters in their own areas of expertise, with the detailed choice of material to be covered to be left according to the author’s own good judgment. An examination of the scant recent review literature in plutonium chemistry reveals that there is a great need for a volume such as this.

The GTS-ITS has begun the process of identifying and contacting potential authors for the various chapters. This process is continuing and no final determinations have been made as yet.

The GTS-ITS has begun to reconsider whether the Sci Finder task package is appropriate for our needs, particularly in light of our new focus on the generation of a review volume as opposed to a comprehensive annotated bibliography. Although no final decision has been made, it seems likely that the Sci Finder task package will be returned for a refund. It is possible, however, that other ‘per-use’ Chemical Abstracts information products such as STN Easy will be employed. It is felt that these may be more appropriate for our immediate needs.
Progress in Theoretical Studies of Aqueous Plutonium Chemistry

In order for the GTS-ITS to gauge the effectiveness of the use of relativistic effective core potentials in conjunction with ab initio quantum chemistry programs to study the theoretical chemistry of plutonium ions in solution, we have used this method to develop MCSCF wave functions for gaseous UO in its quintet, triplet, and singlet states. Although this species is perhaps only remotely related to the problem at hand, namely predicting the behavior of plutonium and plutonyl ions in solution, it is necessary as a first step to compare results of our method with available experimental data. Such data is available for uranium monoxide in the gaseous state. In addition, the study of this ion serves to elucidate many of the same issues that must be considered for the more complex plutonium species.

We have found excellent agreement between calculated and experimental bond lengths at both the multiconfigurational self-consistent field and quasidegenerate perturbation levels of theory. The calculated electronic structure of UO corresponds to that inferred by Kaledin and Heaven from their study of the electronic spectrum of the molecule. Our next step is to use these multiconfigurational wave functions in conjunction with relativistic configuration interaction methods in order to gauge the importance of spin-orbit coupling in these systems. In this way, we hope to determine the potential importance of spin-orbit coupling in plutonium-containing species.
Nuclear and Other Materials
Analytical Development


Purnendu Dasgupta, Ph.D., Texas Tech University

The current quarter is earmarked for design, engineering, drawing and purchasing the components for systems based on small furnace heaters and tubular graphite heaters. Components for the design based on small furnace heaters have been purchased. We have already assembled the parts and have also done trial measurements. From the initial results, it appears that the system based on the small furnace heater is sufficient for the purpose and is quite promising. As such, we have not purchased anything for a graphite heater system. We have also placed an order (Control device corporation) for a Photo Diode Array detector (PDAD) and it is expected to be in the laboratory very shortly.

Figure 1 shows the schematics of the complete system. Part numbers for each of the components are given in the figure. A thermocouple measures the furnace temperature and feeds the relay that controls the temperature by controlling the power. The furnace is rated for heating up to 1093°C and can reach 700°C with a rise time of 2 minutes. At this temperature, an equimolar mixture of NaCl and KCl, kept in silica tubing, melts completely. For optical measurements, a Xenon flash lamp is used as the light source. The light is carried through an extended UV optical fiber (silica) which is coupled to another piece of optical silica fiber (from which the outer coating is removed) which is encased in a ceramic tubing. A similar arrangement is used for taking light out of the heated sample. Though we do not have the PDAD, a charge coupled device (CCD) with a monochromator is used for initial evaluation. The CCD analyzes light from the output fiber. Initial testing reveals that the sample tube and optical fibers can handle the temperature conditions. Also, a wavelength range of 300-600 nm will be available, according to the trial measurements. One modification suggested by the initial trial is the sample tube geometry. A circular silica sample tube may not be ideal due to its lensing effect leading to light alignment difficulty. A rectangular sample tube will be more efficient and will be rugged with respect to alignment aspects. We are in the process of getting rectangular sample tubes.

Dr. Larry Avens from Los Alamos National Laboratory visited our laboratory and was satisfied with the progress of the project. Dr. Poruthoor, who is currently working on this project, is leaving Texas Tech to take up a position at Monsanto. This might cause some delay in progress of the project, until a substitute is found.

Figure 1: Schematic Of Spectrometer
Nuclear and Other Material Studies

Improving Spectroscopy Calibration and Limit of Detection

Clifford Spiegelman, Ph.D., and James Rock, Ph.D., Texas A&M University
Frits Ruymgaart, Ph.D., Texas Tech University
Robert O'Brien, Battelle PNL

During this first quarter of the project, we organized our team, presented our first seminar in Amarillo, and laid the foundation for future collaborative work. After the seminar concluded, we engaged in discussions of broad-based chemometric and statistical needs to support the Pantex mission.

As a result of this meeting, Frits Ruymgaart and Cliff Spiegelman are developing the necessary statistical theory to find the effects of sample contamination among several calibration methods. They seek a calibration method that is robust in the presence of unknown contaminants.

For most spectrographic measurements and most measured compounds, only a small part of the spectra corresponds to each measured compound. Typically the parts of the spectra that respond to the input compound are not well characterized by chemical theory. Thus, there is an urgent need for chemometric methods that can identify the important peaks in the calibration data. The seminar presented a variety of modern chemometric peak selection algorithms that were developed by Spiegelman and his co-authors. A copyrighted shareware MATLAB toolbox that automates these selection algorithms is available from TESS, Inc.

Other Research Activities

- We are currently planning for a quality control seminar to be given by Mr. Robert O'Brien of Battelle, PNL, at the Center's site in Amarillo, at West Texas A&M University (WTAMU), and at Texas A&M University (TAMU).
- A paper based, in part, upon the Center's presentation has been submitted to Technometrics for peer review and possible publication. Technometrics is an official journal of the American Statistical Association and the American Society for Quality Control.
- Prof. Cliff Spiegelman and Dr. Jim Rock from TAMU met Prof. Fritz Ruymgaart from Texas Tech at the Center in Amarillo on April 10, 1998 to conduct a one-day seminar. Colleagues from Pantex, the Center and WTAMU participated in this seminar, creating some lively dialogue about: "Selection of Peaks (Variables) for Calibration."

Rugged Miniaturized Mass Sensors for use in Plutonium Processing

Emile Schweakert, Ph.D., and William James, Ph.D., Texas A&M University

We have completed the design of a prototype mass analyzer for the on-line detection of volatile contaminants. The design is based on new technology (U.S. Patent 5,659,170) which combines an innovative means of ionization with Time-of-Flight Mass Spectrometry, ToF-MS, in a roughing pump vacuum (mtorr). The goal is to build a miniaturized device capable of detecting elemental and molecular species in the mass range of 1 to 500 amu. A key component is a miniaturized mass analysis chamber. We have already one available which is 12" in length, 6" in width, and 5" in height. This chamber together with a small pumping system and the electronics for ToF-MS should readily fit into an attache case. In a portable configuration, data acquisition, display and archiving can readily be handled by a laptop computer.

In addition to designing the prototype ToF-MS instrument and procuring a chamber for mass analysis, we have acquired most of the hardware and supplies needed for building an operational system. We have assembled a new Microsphere Plate Detector, MSP, including a voltage divider of our own design. The performance of the MSP device has been tested and was found to be equivalent to the conventional Microchannel Plate Detector. The MSP has a decided operational advantage. This is a rugged detector which can operate in mtorr vacuum and is thus uniquely suited for our mass analysis system. The timing electronics for the prototype will be configured with commercially available modules. The research scientist working on this project is Dr. Michael J. Van Stipdonk.
Materials Science

Alpha Effects on Encapsulating Materials of Plutonium

Ron Hart, Ph.D., Texas A&M University
Kenan Ünlü, Ph.D., The University of Texas
Gene Carlisle, West Texas A&M University

The radiation damage and associated surface and microstructural changes produced in stainless steel and beryllium by high fluence alpha particle irradiation from plutonium are being studied to understand materials degradation problems that may occur during the long-term storage of weapons grade plutonium (WGPu). The study progressed this quarter with emphasis on completion of a Monte Carlo code to determine the depth distributions of both He and lattice displacements produced in stainless steel due to alphas emitted from WGPu. As expected, the greatest concentrations occur at the surface with an approximately linear decrease to a depth of 11 μm. The alpha current density at the interface between WGPu and stainless steel was also determined as a function of time, energy, and angle. The code results give a fluence of 6.7E14/cm² after the first year with the fluence increasing to 7.2E16/cm² after 100 years. The non-linearity is due to the buildup and decay of Am-241. These results compare favorably with our initial estimate of 1E15/cm²-year for the alpha current density from Pu-239.

Two polished Be samples were received this quarter from Dr. Bill Modemann, Pantex. These will be implanted with He-3 next quarter and analyzed using neutron depth profiling. A polished single crystal sample of Be was also received this quarter and will be used for Rutherford backscattering and channeling analysis of He-4 implants.

Other Research Activities:

A paper entitled, “Radiation Degradation Due to Alpha Damage in Stainless Steel,” by Mehmet Saglam was presented at the American Nuclear Society, Western Student Conference, March 26-28, 1998, Austin, Texas and will be published in the proceedings of the conference.

A paper entitled, “Helium-3 and Boron-10 Concentration and Depth Measurements in Alloys and Semiconductors Using NDP,” by Kenan Ünlü and Mehmet Saglam was accepted for presentation at the 1998 Symposium on Radiation Measurements and Applications at the University of Michigan during the week of May 11.

A paper entitled, “The Effects of Alpha Irradiation on Stainless Steel,” by J. D. Shipp and R. R. Hart has been accepted for presentation at the international youth forum: "Youth and the Plutonium Challenge" at Obninsk, Russia, July 5-10, 1998.

Characterization and Formation of Corrosion Precursors on Beryllium and Stainless Steel for Weapons Applications

Landsberger, Ph.D., Felib Iskander, Ph.D., Juan Sanchez, Ph.D., Arumugam Manthiram, Ph.D., and Harovel Wheat, Ph.D., The University of Texas

Two graduate students were appointed to the project, Li Zhao and Thomas DeFee. Both students enrolled in a full-semester graduate level corrosion of materials course, taught by Dr. Harovel Wheat, to sharpen their knowledge of corrosion characteristics. In February, Bill Modemann, from Pantex, visited The University of Texas (UT) to brief the project team on the previous corrosion studies conducted on the AL-R8 containers and beryllium cladding at Pantex. From the meeting, the UT corrosion team learned that the beryllium cleaning and machining solvents contained dilute amounts of chlorine in the form of trichloroethane (TCA) and trichloroethene (TCE). It is believed that the chlorine may be responsible for pitting corrosion that has been observed on the surface of the beryllium cladding. The inside of the stainless steel vessel may be vulnerable to attack from chloride vapors generated by the residual TCA or TCE that may be present on the surface of the beryllium. Throughout the month of February, Li Zhao and Thomas DeFee conducted research in the library pertaining to the properties of beryllium and stainless steels. By the end of February, the corrosion team consisted of Dr. Landsberger, Dr. Juan Sanchez, Dr. Arumugam Manthiram, Dr. Harovel Wheat, Dr. Felib Iskander, Thomas DeFee, and Li Zhao.
Nuclear and Other Material Studies

In the second week of March, Drs. Landsberger, Manthiram, Sanchez, and Wheat traveled to the Center. From the meeting, a division of labor was established between UT and West Texas A&M University (WTAMU). The UT corrosion team was to be responsible for conducting experiments and data analysis of the corrosion study. It was also determined that the UT corrosion team was responsible for the modeling and characterization of the beryllium corrosion (actual beryllium corrosion experiments to be conducted by WTAMU). It was determined that Thomas DeFee would work with Dr. Wheat in setting up corrosion of stainless steel experiments and Li Zhao would work with Dr. Sanchez on characterizing and modeling of corrosion of beryllium.

Celotex samples were received near the end of March from the Pantex supplier, Associated Machine Technology. Two AL-R8 containers arrived at UT in the first week of April. One of the AL-R8 containers contained the stainless steel vessel and the Celotex packing; the other container contained Celotex only. In the following week, Celotex extraction procedures were received from Bill Moddeman. In the same time period, Dr. Manthiram located a commercial lab that can perform ion chromatography on Celotex samples to determine fluorine content. Upon receiving materials and test procedures, testing could now begin. Dry Celotex samples were prepared for Neutron Activation Analysis (NAA) by Thomas DeFee and Felib Iskander. The results of the NAA procedure conclude that there is chlorine present in Celotex and it is easily detected by this procedure. Identical samples were delivered to Dr. Manthiram for elemental analysis using different methods (EDS, SEM, etc.). The samples will be tested with different methods to establish a consistency in the data. Thomas DeFee and Felib Iskander prepared and tested equipment for reflux extraction of Celotex. The actual sample extraction and subsequent NAA tests are scheduled to occur in the first week of May.

In parallel to the Celotex analysis, Li Zhao has worked with Dr. Sanchez on the modeling and characterization of corrosion of beryllium. Li has been familiarizing herself with a Thermo Calc software package that will perform thermal calculations based on the phase diagrams of binary beryllium alloys. The goal of these calculations is to predict the corrosion behavior of beryllium in chloride and fluoride environments based on the temperature, relative humidity, and other environmental parameters.

**Gallium Interactions with Zircaloy Cladding**

*Ron Hart, Ph.D., Texas A&M University*

*Kenan Ünlü, Ph.D., The University of Texas*

Work continued on beam-driven studies of the interaction of Ga with fuel cladding. Three additional implants of 100 keV Ga to fluences of 1, 3, and 10E17/cm², respectively were performed into a Zircaloy-IV sample heated to 400°C. Rutherford backscattering analysis using 280 keV He-3 is in progress. In an attempt to confirm the formation of Ga-Zr compounds, additional electron microprobe analysis and initial x-ray diffraction measurements have been performed on a previously implanted sample. A low-energy (3 keV) Ga ion beam of good intensity has been obtained using the 10 kV accelerator at Texas A&M. The target heating unit of this system was successfully modified and tested to provide the required 400°C target temperature. A low-energy, high fluence implant of Ga into a heated target of Zircaloy-IV will be performed in the next few weeks. Computer modeling of fission-fragment-induced lattice displacements in Zircaloy is continuing.

**Other Research Activities:**

Ron R. Hart accompanied Rick Hartley, Carl Beard, and other Center investigators on a visit to LANL on April 1 and 2. Interaction was primarily with personnel of the Chemical Science and Technology Division at LANL.
Nuclear and Other Material Studies

High Explosives Program

Javad Hashemi, Ph.D., and Darryl James, Ph.D.,
Texas Tech University

Grant Willson, Ph.D., The University of Texas

Explosive Compression of Buckminsterfullerene

Three Dimensional Compression. Work has continued on the three-dimensional compression experiments. A new technique has been developed that allows loading of a highly densified sample into the workpiece prior to detonation. The sample mixture (C\textsubscript{60} + quenching material) was loaded into a die set where it was pressed into the exact dimensions of the sample chamber. It is possible to press pre-cursor materials that are not air sensitive to densities of approximately 4.5 g/cm\textsuperscript{3} at Pantex. The oxygen sensitive materials that require pressing under an inert atmosphere could be pressed to 2.6 g/cm\textsuperscript{3} at the University of Texas. Densifying the sample results in generation of higher pressures because of the reduction in compressible void volume.

A sample consisting of 20\% (by weight) C\textsubscript{60} and 80\% of 200 mesh nickel was pressed at Pantex to 4.56 g/cm\textsuperscript{3}. This sample was detonated for compression in early March. The design of the apparatus was the same as that described in previous reports. The product was extracted from the workpiece by cutting the steel sphere in half, drilling the sample material, and collecting the shavings. The shavings were dissolved in acid and the carbon material recovered by centrifugation. Analysis by X-ray diffraction revealed the only product to be graphite. Another compression experiment consisting of a pressed sample containing nanometer grade nickel as the quenching material is assembled and waiting pad clearance for detonation. The nanograde metal should provide more rapid quenching of the sample and reduce back transformation of carbon phases. Successful production of diamond requires more efficient quenching. It is necessary to reduce the temperature of the sample while the pressure is still high.

A workpiece consisting of a solid copper sphere rather than steel was tested as a means to more rapid quenching. The copper fractured into fourteen distinct pieces; the segments correspond to the convergence of the detonation fronts created from each detonator. Optical metallography was used to determine the nature of the failure of the copper sphere. Casual observation of the recovered copper pieces leads to the conclusion that the sphere failed because the inner portions entered a molten state, thereby radically reducing the spall strength of the entire sphere. Closer inspection revealed the copper did not actually melt. The duration of the elevated temperatures was sufficient to only induce recrystallization. Thus, the fracturing process was the result of the solid sphere being unable to endure the intense tension forces experienced during unloading. High shear stresses caused the surface to rupture where the shock fronts converged while the extreme deformation of the core was caused by the enormous tension forces. From this analysis, it is obvious that modifications to the design would be required to reduce the magnitude of the tension waves in order to recover the copper sphere intact. However, since the copper does not become molten, this becomes reasonable design goal. We will simulate copper spheres with steel cladding in the next quarter.

Diamond synthesis represents only one use of the compression tool we have developed. We are interested, for example, in the opportunity for the high-pressure synthesis of carbon nitride, \( \beta \)-C\textsubscript{3}N\textsubscript{4}, a compound predicted to have a hardness equivalent to diamond. To that end, we have loaded two workpieces with pre-cursor materials that are designed as precursors of carbon nitride. The organic pre-cursor materials being tested are 2-amino-1,3,5-triazine, C\textsubscript{3}N\textsubscript{4}H\textsubscript{6}, and tetracyanoethylene, C\textsubscript{6}N\textsubscript{8}. The first contains the proper ratio of carbon to nitrogen but also contains hydrogen, while the latter consists solely of carbon and nitrogen, but not in the stoichiometric ratio as found in carbon nitride. Both workpieces are in the assembly process at Pantex.

One Dimensional Compression: Unusual experimental data that do not match modeling predictions has been collected in the 1-D tests. The models predict flyer velocities that should result in compression forces of approximately 25 GPa, which is more than sufficient to destroy C\textsubscript{60}, because this structure
is stable to only 16 GPa in nonhydrostatic compressions. However, unchanged $C_{\text{iso}}$ was found to be the major product in all the Pantex experiments. Two experimental techniques have been used to determine flyer velocity to check modeling accuracy. These are Velocity Interferometer System for Any Reflector (VISAR) and a technique based on piezoelectric quartz pins. The flyer velocity measured by both techniques matched that predicted by the model.

Flash X-ray photography was used to determine the nature of the flyer after detonation. The shock wave produced from the explosion resulted in the generation of tension waves that exceeded the spall strength of the steel flyer, resulting in localized spalling of the material. Jets of molten metal were emitted from the center of the flyer and the remainder of the flyer deformed into a bowl shaped structure. The velocity of this lower mass jet of metal was what was being measured by VISAR and the quartz pins, not the velocity of the more massive flyer as a whole. The remainder of the flyer travels much more slowly than predicted due to the high degree of deformation. These experiments provide an explanation for the discrepancy between the models and the experimental results.

A redesign of the 1-D compression was required that does not include a flyer. The new design is shown in Figure 1. The design consists of two sets of high explosives placed on opposite sides of a sample chamber. Sandwiched between the explosives and the chamber are steel spall plates. The pressure waves generated at each surface after detonation are transmitted to the center of the sample chamber where constructive interference occurs. Hence, the pressure seen by the sample is approximately twice the pressure generated by each explosive. The waves, now in tension, continue to the opposite side of the sample chamber where they encounter the spall plates. The plates are designed to absorb the transmitted waves. They will fail but thereby maintain the integrity of the sample chamber. The bolts also aid in the recovery of the sample. Initial tests used a design with a bolt on just one side. The chamber cracked and failed on the unbolted side because the compression caused too much deformation for the steel to endure. However, the bolt provided a small degree of movement and kept the steel from cracking. A subsequent test using bolts on both sides proved the sample chamber could survive the detonation and the products are currently being analyzed at UT.

Figure 1: Redesign Of 1-D Compression Tool That Does Not Include An Explosively Driven Flyer. Note: “HE” Stands For High Explosive And “Det” Stands For Detonator.

Mechanisms of Formation of Trace Decomposition Products in Complex High Explosive Mixtures

James Woodyard, Ph.D., West Texas A&M University
Ken Rainwater, Ph.D., and Reed Richardson, Ph.D., Texas Tech University

The goals of this project are to identify and synthesize high explosive decomposition products that are produced during storage and aging of the current weapons stockpile. Laboratory experiments are being set up to cause the aging processes, and analytical devices at West Texas A&M University (WTAMU), Texas Tech University (TTU), and Pantex will be employed to characterize the aging effects. The project enjoys the cooperation of Mike Lightfoot of the Applied Technology group at Mason & Hanger, and Dr.
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Ben Richardson, now of Engineered Carbons, Inc., Borger, Texas, formerly of the Applied Technology group.

In the first quarter, meetings were held in Lubbock (once) and Canyon (twice) to design the aging studies and to finalize staffing requirements. Justin Brown, a Master's student, was selected from Texas Tech, and will be available to work at Pantex this summer as a research associate. Justin Brown is pursuing the proper security clearance for this assignment. Dr. Caroline Burgess, the post-doctoral researcher and John Heh, an undergraduate student who will become a graduate student in the WTAMU chemistry program on May 16, were both hired for the WTAMU team. Dr. Burgess will be moving to Canyon June 1. She is presently serving out a teaching responsibility at the University of Texas - Permian Basin (UTPB), teaching physical chemistry. She has been carrying out extensive literature searches from UTPB since March. Accumulation of pertinent literature has started with the assistance of John Heh. The literature searches are focused on estane, HMX, TATB, and Kel-F 800.

The high-speed NMR spin system is currently being installed at the Bruker headquarters in Massachusetts on the extra CP/MAS probe housed at WTAMU. The installation of this system on our existing probe saves the cost of an entire new probe. The modified probe will be tuned to the appropriate frequencies for carbon and hydrogen (protium), and should be capable of spinning samples at speeds of up to 16 kHz, beyond the current limit of only 6 kHz.

The design of the aging study has been finalized. The HE will be exposed to combinations of radiation (UV light, fluorescent light, and darkness), temperature (ambient and 50°C), and humidity (high, medium, and low). The appropriate chambers, ionization sources, and chemicals for the baths are being procured. Construction of the chambers and start of the aging study will commence upon receipt of supplies. It is hoped that access to a radioactive source will be made possible through Pantex or one of the universities. The first study will investigate the induced decomposition of TATB. Paperwork has been initiated to get the TATB moved to a staging area in Lubbock.

Materials for High Gradient Magnetic Separation of Radioactive Materials

Rodger Walser, Ph.D., The University of Texas

This is a new project funded in April 1998. An update will be submitted next quarter.

Plutonium Processing and Handling

Gallium Removal

C.V. Philip, Ph.D., Texas A&M University
Max Roundhill, Ph.D., Texas Tech University

During the first quarter we have been improving the analytical procedures both for estimating the effectiveness of the thermal removal of gallium as its suboxide from cerium oxide, and for determining the composition of the material that drops from the copper wire. This second target goal developed from a recent collaborative interaction with staff scientists at Los Alamos National Laboratory where we agreed that the concept of introducing a copper wire collector into an apparatus for removing gallium from plutonium was one of very high potential. We are proceeding on the basis that this feature will be designed into the equipment that is eventually used for the removal of gallium for plutonium. In each case the analytical data were obtained by inductively coupled plasma (ICP) measurements on aqueous solutions prepared from samples that had been obtained by the thermal treatment of gallium and cerium oxide mixtures at Texas A&M University at temperatures where it is expected that the volatile gallium suboxide will form.

The data that we have collected at Texas Tech University (TTU) to assess the effectiveness of the removal of gallium from cerium were obtained by dissolving the residual material after the thermal treatment in aqueous acid solution, and then measuring the gallium concentration in the solution by ICP at a wavelength where cerium does not interfere. These data for two sets of samples that were obtained using a set of slightly different experimental conditions show that, with the exception of one set of conditions, the
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residual percentage of gallium in the cerium oxide surrogate ranges from 0.9% to 6.9%. These data show that gallium can be effectively removed by sublimation as its suboxide.

The data that we have collected here at TTU to determine the composition of the material that is found to drop from the copper collector were obtained by dissolving this material in aqueous nitric acid solution (10%), and then measuring both the gallium and copper concentrations in the solution by ICP. Since gallium readily forms alloys with most metals, including copper, it is important to know the composition of this metallic bead. This information is important because a knowledge of the percentage of copper in the material that drops from the collector will allow for a good estimate to be made of the rate of loss of this copper collector alloy formation with gallium during the operation of the process for removing gallium from plutonium. In addition, since the gallium that is removed must subsequently be disposed of, these data are important in deciding the manner in which this procedure can be carried out in a safe manner. These analytical data for gallium and copper in the drop for four separate experiments show that the ratio of gallium to copper ranges from 24 parts gallium to 76 parts copper, to 32 parts gallium to 68 parts copper. For this limited number of measurements these values are consistently close to each other. If further work confirms these values, it is clear that the "gallium droplets" forming on the copper collector contain a large amount of copper. Additional measurements are needed to verify whether such a high copper content can always be expected to be found, and to also explain from the chemistry and metallurgy why such a large amount of copper is deposited.

Several experiments were conducted to identify the benefits of a copper-collector as well as the reactions of other materials in gas streams with vapors of gallium suboxide. Elemental analysis by atomic absorption (AA) spectrometry, FT-IR (both mid and far IR) spectrometric analysis, BET surface area and pore size distribution measurements, and powder X-ray diffraction scanning were used for the characterization of materials.

Distance between copper collector and the oxide bed does not have any effect on gallium removal or conversion. Hydrogen gives better conversion than H2/Ar. The rate of conversion increases with increase in temperature and gas flow rates. When gallium trioxide is heated in H2 or H2/Ar gallium suboxide vaporized and deposited of cooler parts of the quartz 'U' tube and a white powder is produced. Sometimes the powder is gray colored. The powder is not sublimed readily on heating. Heating at 950°C in a reducing gas (H2 or H2/Ar) both white and gray powders sublimed in about thirty minutes. Air oxidation of gallium suboxide vapors produces a nonvolatile white powder which deposits on the quartz 'U' tube right inside the furnace. The far IR spectrum of the oxidized product is very similar to that of the white deposit collected on the cooler parts of the quartz during the heating of Ga2O3 in H2 or H2/Ar.

MOX Fuel Performance Evaluation

Lee Peddicord, Ph.D., Texas A&M University
Gregory Gellene, Ph.D., Texas Tech University

This quarter the work focused on the completion of thermal models to be incorporated into the COMETHE code to predict MOX fuel behavior at high burnups. This work has been completed and a report was written summarizing the developments. This activity has been carried out by John Alvis, a graduate student from Texas A&M University who is working at Belgonucléaire in Brussels, Belgium. He is collaborating with Dr. Marc Lippens, Senior Scientist at Belgonucléaire who is in charge of fuel performance modeling. The modeling work was based on irradiation data owned by Belgonucléaire from tests the company has conducted in-house and in cooperation with international partners. Assessments of the models with data from irradiation experiments show good agreement between calculations and measurements. In addition, attention is being given to more detailed phenomena governing fission gas behavior. This work is being undertaken by John Alvis and Greg Gellene. The effort is divided into an examination at the engineering level as well as consideration of the role of more basic physical phenomena at the crystallographic level which might determine this behavior.

The purpose of this project is to conduct thermal and mechanical analyses of weapons
MOX fuel in light water reactors using state-of-the-art computer models. The goal is to verify the efficacy of fuel designs under power reactor conditions. The activity during this past quarter has been to complete the thermal modeling and produce a report summarizing this activity. Additional efforts included assessments of specific phenomena relating to the fuel performance of MOX fuel.

John Alvis, a graduate student from the Department of Nuclear Engineering at Texas A&M University, is in Brussels, Belgium, working directly with Belgonucléaire (BN). BN is the developer of the COMETHE fuel performance code which is the most extensive code for addressing MOX fuel under power reactor conditions. At Belgonucléaire, Mr. Alvis is interacting with Dr. Marc Lippens, Senior Scientist who directs the fuel performance modeling group at BN. The work deals with the assessment of models for the thermal behavior of oxide fuel at high burnups. In addition, Professor Greg Gellene of Texas Tech University is investigating more basic physical phenomena relating to fission gas behavior in MOX fuel.

The analysis of the COMETHE modeling of recent experiments was completed. The results of this analysis demonstrated that the current thermal models implemented in the code are capable of accurately predicting fuel temperatures up to high burnups. However, fission gas release at low temperatures and high burnup is still generally underestimated by COMETHE. Comparison to recent experiments confirmed the under-prediction in this regime. The under-prediction is partly attributable to burst release of fission gas and not problems with the thermal models. The current fission gas release models are not equipped to deal with a burst release and therefore cannot accurately predict incidents of burst release of fission gas. No further improvement in the thermal models is necessary based on the current analysis. The fission gas release models may need to be reviewed to incorporate burst release of fission gas from the grain boundaries.

Several issues associated with the effect of heterogeneity on the thermal performance of MIMAS fabrication method still remain. An effort was made to try and quantify any penalties or benefits of heterogeneous fuel compared to homogeneous fuel. Heterogeneous MOX fuel of the MIMAS form at 100% theoretical density can be considered as a mixture of UO₂ with spherical UO₂-PuO₂ agglomerates. The net thermal conductivity of the mixture can be estimated based on the theory of conduction of dispersed systems. The object of this study was to try to quantify the effects of the Pu rich agglomerates on the thermal conductivity of a heterogeneous system due to the distribution of the enriched plutonium, the resulting local burnup distribution, and local porosity development.

It was concluded that the presence of the Pu rich agglomerates have very little effect on the net thermal conductivity until a pellet average burnup of approximately 40 GWd/MtM is reached at which time porosity begins to develop in the homogeneous fuel. From 40 GWd/MtM until porosity saturation is reached at ultra-high burnups, heterogeneity has a large positive effect on the thermal conductivity due principally to the local burnup. The porosity develops quickly to saturation due to the high local burnup in the agglomerate leaving the matrix relatively free of either burnup effects or porosity development until the ultra-high burnups are reached.

The temperature distribution across the agglomerate can be estimated based on the theory of conduction. The object of the next study was to try to quantify the temperature increase due to the presence of the Pu rich agglomerate. The temperature increase due to the Pu rich agglomerate was approximately 5°C. It was concluded based on the results of this analysis that the presence of Pu rich agglomerates does not significantly affect the temperature distribution in the fuel.

Also, a study was conducted to determine if the presence of Pu rich agglomerates resulted in any latent stresses in the fuel matrix. An attempt was made to estimate the stress resulting from the presence and growth of fission gas bubbles and relate that to the stress resulting from the presence of the agglomerate. The principal factor contributing to the stress resulting from the presence of gas bubbles is the bubble size. Of the assumptions used in the analysis, the lack of resolution probably has the largest impact.
Resolution plays a large role in gas precipitation by controlling the amount of gas atoms dispersed in the matrix. At high temperatures, resolution is ineffective in maintaining gas in solution because the gas diffusion coefficient is large enough to return gas to the bubbles as soon as it is ejected by collision with an energetic fission fragment. However, at lower temperatures a much larger fraction of the gas is atomically dispersed in the matrix.

It was determined that bubble growth by resolution and coalescence also effects the assumption that all the bubble radii are the same. When bubbles are subject to processes that change the bubble size in a discontinuous manner, a bubble size distribution develops during the growth stage. The larger bubbles are also more difficult to maintain in mechanical equilibrium with the surrounding material. Mechanical equilibrium is usually maintained by a flow of vacancies to the bubble to provide the additional volume needed to accommodate the simultaneous influx of gas atoms. The vacancy supply problem becomes more of an issue as the bubbles continue to grow and the mechanical equilibrium is lost.

The conclusion of this phase of the work was that this analysis was at best an estimate of the pressure and stress associated with fission gas bubbles. A more detailed analysis where the limiting assumptions have been relaxed would provide a more detailed look at the life of a bubble.

Also as part of the project, during this quarter, Greg Gellene met with research staff of Belgonucléaire. The main topic of the discussion was the apparent “memory” effect for fission gas release following an initial burn-up. It seems that after some burn-up, fission gas appears to diffuse to the grain boundaries faster than predicted by any realistic diffusion model. This higher diffusion rate then seems to become a permanent new property of the fuel. It happens for UO$_2$ and MOX fuels. A mechanism was considered in which the oxygen potential produces locally in the grains of higher oxides of U which may create microchannels between UO$_2$ boundaries in the grain increases mobility of gases to the grain boundaries. The phenomena will be considered in more detail during the upcoming quarter. The initial work will be to consider crystal and thermodynamic properties of the UO$_2$’s to see what might be favored. An important (and maybe little considered) potential point is the locally high pressure within the grain from initial fission gas during burnup. An attractive feature of this mechanism may be that the microchannels, if produced, would be expected to be long lasting giving the memory effect.

Continuing reviews were also made of the literature focusing on other code systems which either have MOX capability or be used to assess MOX in LWR’s. References are being identified relating to: TRANSURANUS/METEOR, ENIGMA, FRAPCON-THermal-3, ENIGMA, START, and FALCON ESCORE/FREY.

Finally, discussions were held at the end of the quarter with Oak Ridge National Laboratory concerning the MOX Demonstration Tests in the ATR reactor in Idaho. ORNL has an interest in being able to calculate the performance of the ATR pins. Three pins are under irradiation and one is scheduled to be removed in the summer with a burnup of 8 GWd/MtM. COMETHE represents the capability in the US to calculate MOX fuel performance. Work was begun in collaboration with ORNL to assemble the input parameters for this analysis.

**Benchmarking of Neutronics Codes**

*Naeem Abdurrahman, Ph.D., The University of Texas*

*Theodore Parish, Ph.D., Texas A&M University*

**Generation of Cross Section Libraries.** In order to be able to perform MCNP benchmark calculations for temperatures other than 300K, special libraries were needed for various temperature conditions typical of LWRs. The task for this reporting period consisted of developing NJOY capability and developing a comprehensive library we called UTXS (University of Texas Cross Section Library). The library has been generated for typical temperatures of US PWR, BWR, and the Russian VVER.

The current version of the UTXS is UTXS6, which is based on ENDF-B/VI. The UTXS6 has
gone through a preliminary validation process. The preliminary validation consisted of checking the library structure, comparing cross section plots with those from LANL, and benchmarking against selected set of critical experiments from the "International Handbook of Evaluated Criticality Benchmark Experiments." The UTXS6 benchmark results were also compared with those obtained using LANL ENDF60 obtained for the same set of experiments.

The plot comparisons with LANL ENDF60 libraries were done only for 300K. From these comparisons, we noticed small differences between the two libraries in the resonance regions. This is due to using smaller tolerances in UTXS in reconstructing those resonances from the resonance parameters.

The libraries are currently available on the web at http://radon.me.utexas.edu. A username and password security has been implemented to monitor downloading the libraries. Interested users can browse the directory that lists all the files for the various materials and temperatures, and if interested, can request the username and password on-line to get authorization to download the libraries. A report has been prepared on the UTXS libraries and will be sent to the Center under a separate cover.

Evaluations and Calculations of Esada Experiments. The evaluation of single region PuO$_2$-UO$_2$ fueled critical experiments performed at the WERC facility within ESADA Plutonium program (1967) has been revised and the revised report delivered to ORNL. About 55 different single region critical core configurations were present in ESADA experimental program. Evaluations of both single region core configurations were presented in that report.

Evaluations of ESADA multi-region critical experiments including 35 different critical core configurations were revised and the revised report delivered to ORNL. Multi-region core configurations were constructed in three ways; salt and pepper, concentric region, and core configuration with different lattice pitches.

Evaluations of power distribution measurements for ESADA experiments were performed and the evaluation report delivered to ORNL. Evaluations for power distribution with both single and multi-region core configurations are included in that report. Twenty eight different cases were selected for power distribution evaluation report.

Power distribution calculations for single region core configurations were performed for 8 different core configurations. Power distribution calculations for concentric region and salt and pepper core configurations have been started.

Evaluations and Calculations of Saxton Experiments. The evaluation of Saxton Critical Experiments continued with MCNP calculations for flux. Reaction rates and flux estimates showed an important bias in epithermal and fast flux measurements by 238U foil method due to 235U impurity, especially for the locations placed in water reflector. Good agreement between calculations and measurements was obtained for the thermal flux.

The sensitivity calculations for the Saxton Critical Experiments began with a study for the self-shielding effect of PuO$_2$ particles in UO$_2$ matrix. Although the study does not predict the bias produced by the self-shielding effect because of lack of information regarding the average particle size, it indicates the importance of this phenomenon for large H/Pu ratios. Thus, this study showed that the effective multiplication factor for cores with 0.56-in lattice pitch is quite insensitive to particle size, while that for cores with larger lattice pitch is more sensitive. In MCNP criticality calculations PuO$_2$ particles were modeled as lattices of spheres of 20, 30, and 40 microns in diameter.

As part of the evaluation of the codes being benchmarked, a statistical analysis of the calculated k-effectives from the Saxton critical experiments was performed. The k-effectives were calculated using WIMS-D4m and DIF3D. This material is an addendum to the final report for last year's TAMU activities in benchmarking which was also submitted in this period.

A paper entitled, "Criticality Analysis of the Saxton Plutonium Program Using the WIMS-D4M and DIF3D Codes," was presented at the
A sensitivity analysis on Saxton type fuel pins was begun to evaluate the effects of various modeling options in various lattice codes. More specifically, a comparison was performed for the results from the following deterministic codes:

- WIMS-D4M (ENDF/B-V nuclear data library)
- CASMO-3 (CASLIB evolved from ENDF/B-IV)
- WIMS7a (JEF 2.2 nuclear data library).

The k-effective values from pincell calculations with each of these codes have been analyzed as a function of fuel rod pitch.

In order to be able to compare the results from WIMS7a with those already obtained using other code systems, a 19x19 MOX fuel rod assembly has been formulated and is being tested. This model employs the 2D calculation module in WIMS7a.

For the next period, an evaluation of the Saxton single-region cores will be performed using the code WIMS7a.

Water Reactor Options for Disposition of Weapons Plutonium

Marvin Adams, Ph.D., and Dmitri Anistratov, Ph.D., Texas A&M University

This project is mostly a collection of unfinished tasks from the former project, "Water-Reactor Options for Disposition of Weapons Plutonium." Funding for the current project is from carryover of FY97 funds that were originally allocated to the former "Water-Reactor Options" project.

The project has four tasks: 1) Continued participation in the US/Russia Joint Technical Working Group, 2) Continued study of the MOX fuel experiment underway at the ATR in Idaho, 3) Continued study of transients in MOX-fueled reactors, and 4) Continued study of MOX fuel with burnable absorbers. A related task, funded directly by ORNL instead of the Center, is to study "flexible" fuel cycles that can gracefully handle interruptions in the supply of MOX fuel.

Dr. Adams continued to participate in the US/RF Technical Working Group on water-reactor options for disposition of weapons Pu. The main activity this quarter was to begin preparations for the upcoming meeting in St. Petersburg, Russia, scheduled for June 17-19. At this meeting Dr. Adams will present work from the benchmarking effort, performed mostly by Dr. Naeem Abdurrahman and his associates at UT and by Dr. Igor Carron of TAMU, with some work done by Dr. Adams's student Helen Nasr.

There was progress on the task of calculating power distributions in the MOX fuel experiment that is underway at the ATR in Idaho. During this quarter we obtained drawings of the MOX test capsule and the surrounding Be reflector. We also requested and received an MCNP input file so that we could deduce certain dimensions and coordinates that were not shown on the drawings. From this geometric data, which is fairly complicated, we are building the geometry portion of an input file for the code SNAC, which will ultimately be used to calculate power distributions in the test capsule. After our geometry input is complete (which is a large job) and ORNL has sent us all necessary sources and cross sections, we will calculate power distributions, beginning with relatively crude spatial and angular and energy grids. We expect to complete these initial crude calculations in the next quarter, with more refined calculations to follow in the subsequent quarter.

Our study of transients in MOX-fueled VVER reactors is focused upon quantifying the sensitivity of key transient results (such as peak fuel temperature or total energy produced in the hottest pin during the transient) to uncertainties in nuclear data. If we succeed, then, for example, we will be able to predict the error in peak fuel temperature that would be caused by any given error in any nuclear constant, such as the delayed neutron decay constant in the nth delayed-neutron group in Pu-239. In this quarter we accomplished our objective of studying the relevant literature on sensitivity analysis in nonlinear transient problems, and we have...
decided upon the methodology that we expect to extend and apply to the MOX-transient problem. In the near future we will finalize detailed plans for the extension and application of this methodology; these plans must include which codes we will use for which parts of the transient calculations, and which codes must be written or modified.

Progress on the study of MOX fuel with burnable absorbers consisted mainly of a more precise definition of test problems to be used in a comparison of existing production methodologies against more precise treatments. We expect to make significantly further progress this summer.

Progress on the ORNL-funded task on "flexible" fuel cycles has been steady. In this quarter we did complete our primary scheduled deliverable, which was complete cross section tables for 10 different variants of Westinghouse assemblies. The tables were produced by the assembly transport code HELIOS, which was purchased by ORNL. (We have an account on an ORNL computer, which is where our HELIOS problems must be run.) We also performed an analysis that allowed us to see that we and ORNL and North Carolina State University had all been misinterpreting part of the HELIOS output. Our plan is for this analysis to be written as a joint Center-ORNL report. (This was requested by ORNL.)

Scoping Study for Issues of Particles, Aerosols, and Semivolatile Compounds in Plutonium Processing and Handling

William Marlow, Ph.D., Texas A&M University

The purpose of this one-year project is to identify areas of general plutonium processing operations in which development of fundamental understanding of particle and aerosol behavior would be useful. A particularly important objective of this work will be to contribute to the knowledge base which will help to minimize worker exposure. Since Los Alamos National Laboratory (LANL) is the center for development of these processing operations, this project's efforts are focusing upon their activities.

Initial discussions regarding work activities and responsible individuals at LANL were held with D. C. Christensen and L. Avens of the LANL Nuclear Materials Technology Division on 30 January at Texas A&M. Based upon that exchange of information, on 12 March, the Principal Investigator visited LANL with David Wannigman making arrangements. On the trip, discussions were held with four LANL staff members:

- Christopher James discussed current thinking on the preferred process for plutonium oxide formation and how it relates to worker exposure. The form of the particulate plutonium as a result of this oxidation as well as that due to water and carbon dioxide absorption was discussed along with particle sintering and the effects of temperature on particle size.
- Timothy George discussed plutonium oxide powder properties including bulk transport, decay-induced migration, particularly including resuspension, and experimental capabilities at LANL in his area.
- John McDonald discussed questions relating to the materials used for the gloves in glove boxes. He pointed out that little is known of the radiation aging of the glove material and that mechanical failures are the greatest problems leading to leaks.
- Gerald Schlapper discussed the safety activities of his group.

Following this visit, appropriate faculty at the University of Texas at Austin, Texas Tech University, and at Texas A&M were contacted and informed of the research opportunities suggested on the visit.

Special Nuclear Material Handling, Simulation and Robotics Design

Richard Volz, Ph.D., Louis Everett, Ph.D., and Jeffrey Trinkle, Ph.D., Texas A&M University

Alan Barhorst, Ph.D., Texas Tech University

George Kondraske, Ph.D., The University of Texas at Arlington

Weight and leak check system (WALS) simulation modification. Three students have been assigned to the task of updating the WALS TELEGRIP simulation. As of April 30, 1998, the simulation has been installed, and
coordination between Texas A&M University (TAMU) and Texas Tech University (TTU) has been established.

In the simulation obtained from Pantex, current coordinates have been tabulated and compared to the drawings of WALS as implemented at Pantex. The correctness of the measurement was verified between the students at TTU and TAMU. A copy of this table is attached. In the next quarter, the current simulation will be modified to align the simulation coordinates with the WALS drawing set.

The TELEGRIP model of the modified Celotex storage station was created as per the drawings obtained from the Pantex. The existing model of Celotex storage station in the WALS simulation was replaced with the new model. The necessary modifications were made in the Graphical Simulation Language (GSL) code to accommodate the changes arising out of the modified Celotex storage station.

TheManual Operation Station (MOS) is currently being modeled. In this first phase of MOS modeling, the details of what is to be modeled for simulation realism is being established. Initially it was thought that Pro Engineer (tm) would be better suited for drawing the MOS then it would be imported into the TELEGRIP simulation. This turned out to be only marginally easier with respect to modeling the system so it was decided to do all modeling in the CAD environment provided in TELEGRIP.

Changes made to the current components of the WALS simulation:

- The operator room wall has been modified.
- The conveyor system has been deleted per the current drawing set.
- The Celotex storage station has been modified.

Demonstration of design tools for programming automation tasks. The programming of automation tasks can greatly be simplified if the sense of touch can be added to the system as one of the feedback. The advantages of having the touch sensing can be enjoyed in one way if the system is able to detect if the force signal was caused due to an edge touching a surface, surface touching a surface, or a point touching a surface. This way the system can be programmed to achieve a type of contact rather than moving to a particular position and orientation. This is analogous to the way the human acts and it is naturally extensible to different types of parts.

This study aims at determining the contact formation types. These contacts occur when the object grasped by an automation agent such as a robot interacts with its work environment.

During the first quarter, previous work in the related area has been examined and a strategy for determining the contact formations in a more complete form has been decided. It has been decided to achieve this goal using the feedback of force data alone to dispense with errors due to uncertainties in position and velocity data. The following procedure will be attempted in order to accomplish this goal.

The force sensor signals from the robot’s end effector are classified into discrete robot symbols, termed single-ended contact formations (SECF), which qualitatively describes how the grasped object touching its environment. An assembly operation can be represented as a sequence of these discrete symbols. So the SECF is used as the qualitative state that drives the assembly skill.

The classification of the force signals into SECF is accomplished using fuzzy logic classifiers or a neural network. The classification depends on the position and orientation of the force cones in three-dimensional space. If the orientation of the grasped object with respect to the robot’s end effector is changed after the training data is collected, a mapping of this data is required to successfully classify the SECF.

There are two ways of achieving such a mapping. One approach is re-training the network without collecting all of the new data and making the system operate with original efficiency. If the relation between the relative change in orientation of the force cones with respect to the relative change in orientation of the grasped object can be derived, then the
inverse of this mapping can be applied to the original training data and retrain the network off-line.

A second approach is to map the force signals before inputting them to the neural network. This will make the orientation changes transparent to the previously trained neural network. This approach is different from the first approach in that instead of retraining the network, the inverse mapping is applied to the force signals from in real time.

Add contact/impact model & system compliance to simulation testbed. The work for incorporating a simulation for motions of moveable objects in contacts has been extended from the FY97 to the first quarter of FY98, and has been completed. An impulse-based dynamic model has been devised, and is used to predict the motions (i.e., by computing the accelerations) of bodies before and after their collisions. Simulation depends very much on correct collision checking between colliding bodies, and this is done through a general-purpose collision-detection package (called C-Space Tool Kit) from Sandia National Laboratory.

A real-time animation has been carried out for a simple model of pit-dropping-to-the-ground for several time steps by taking into account the effect of impact. The simulation capabilities are marginal due to the limitation in contact-determination capability.

Neuromotor workload measurement. Funding of the FY98 project at UT did not commence until April 1998. However, a student (Mr. Swaminathan Chandrasekaran) had been recruited (prior to finalization of contractual matters) to work on software development for the stand-alone neuromotor workload measurement package, which is our prime deliverable. We originally anticipated delivering a working version by Month 8; however, this may be delayed until Month 10 due to the contract start-up delays.

A preliminary graphical user interface for the software measurement tool has been defined and an initial draft of a design document/operator's manual has been started. Also, a development tool for programming the package in JAVA has been acquired. The programming of selected subfunctions of the overall package is underway, in part to learn this programming environment and in part to achieve progress toward realizing the software required for the overall system. Finally, Mr. Chandrasekaran has prepared a plan for completion of a Master's thesis directly related to the development and evaluation of the neuromotor workload measurement package.

Storage

Conductivity Monitoring for Detection of Leaks of Double-Walled Plutonium Containers

William Marlow, Ph.D., Texas A&M University

The preamplifiers that were ordered in the first quarter, as discussed in the last quarterly report, arrived in March 1998. We believe that they will work but because of the high gain of the cathode preamp, we are having problems with background noise. The geometry of the detector plays vital roles in both the ion collection efficiency and the reduction of magnetic field pickup. A parallel plate configuration was analyzed as a candidate for detector form. While this geometry was favorable for creating an acceptable electric field, the cathode was unacceptably susceptible to magnetic fields. A parallel wire geometry was investigated but was not successful because of the lack of an effective electric field. Because of the practical difficulties in shielding of magnetic fields, we are investigating other anode/cathode geometries rather than concentrating on shielding of the magnetic fields at this time. Specifically, multiple parallel wire configurations are used elsewhere in detectors and variants on this geometry will be the focus of our efforts during the May-July quarter.
Development and Characterization of Plutonium Storage Containers

David Boyle, Ph.D., and Theodore Parrish, Ph.D., Texas A&M University
Darryl James, Ph.D., Texas Tech University
Hsiang Yeh, Ph.D., and Houshang Masudi, Ph.D., Prairie View A&M University
Sheldon Landsberger, Ph.D., The University of Texas

This research develops and validates a set of analysis tools that will allow Pantex and State of Texas officials to evaluate the suitability and expected performance of new plutonium container designs in a timely and consistent fashion. Initially, this work is focused on examining the thermal, mechanical, chemical, and neutronic performance of the Pantex-designed AL-R8 (SI) container for plutonium pits.

Dr. Boyle's activities during this first quarter centered on coordinating the specific work plans of the listed co-PIs with the current and expected needs of Pantex. He organized a series of meetings at the Pantex site, traveled in the company of each co-PI to these meetings, and participated in explaining the research plans and determining the priorities and data needs of Pantex officials. In addition, throughout the period he met separately with most of the co-PIs and their research teams to review initial project directions and ensure understanding of the critical container issues. He obtained detailed drawings and specifications for the containers and arranged for the shipment of prototype AL-R8 (SI) containers to experimental laboratories at UT, TTU, TAMU, and PVAMU. During this period, DOE formally decided to employ the AL-R8 (SI) for storage of surplus pits. In addition, Pantex implemented recent changes to the AL-R8 (SI) design, lengthening the bottom portion of the sealed insert by one inch and revising slightly the shape and valve arrangement of the lid. These design changes should have minimal impact on the modeling/validation process underway at each university. However, the desirability of obtaining the revised container lids for some future experiments is under evaluation.

A brief summary of activities conducted under each specific analysis area follows.

Corrosion and Chemical Interactions. In February, Bill Moddeman from Pantex visited UT to brief the project team on previous corrosion studies conducted on the AL-R8 (SI) containers and beryllium cladding at Pantex. The stainless steel may be vulnerable to chloride attack generated from the organic packing material, Celotex. Throughout the month of February, graduate students conducted research in the library pertaining to stainless steels and conferred with Dr. Harovel Wheat on the design of experiments for and conduct of the corrosion study. Celotex samples were received near the end of March from the Pantex supplier. An AL-R8 (SI) container and a drum of Celotex arrived at UT in the first week of April. In the following week, Celotex extraction procedures were received from Bill Moddeman. In early April we prepared dry Celotex samples for Neutron Activation Analysis (NAA). The results of the NAA procedure show that chlorine is present in Celotex, and it is easily detected by this procedure. Identical samples underwent elemental analysis using different methods (EDS, SEM, etc.) to establish consistency in the data. Reflux extraction of Celotex and subsequent NAA tests are scheduled to occur in the first week of May. In the following months, the Celotex will be further analyzed for chlorine content, and some samples will be sent out for fluorine analysis. Celotex extract will be prepared for corrosion tests.

Thermal Analysis. A newly hired Master's level graduate student began work on this project and is searching for a company that will fabricate the shell for a pit thermal simulator. This process has gone slowly because companies with the capability to fabricate the required stainless steel spherical shells are generally not interested in fabricating a one-of-a-kind article. Prof. James recently made contact with a small Texas foundry, and he expects to resolve the pit simulator problem shortly. The needed components for the data acquisition system are in place or have been ordered. The research team is putting together an experiment plan to determine where temperature measurements will be made throughout the container and how the back fill gas (Argon at 550 torr) can best be
introduced and monitored for pressure. The sealed insert in the AL-R8 (SI) container shipped to TTU did not include the pit-holding fixture. Including this fixture in the experimental set up is important because conduction through the fixture is potentially the dominant mode of heat transfer. Dr. Boyle has been informed of this need and is working to provide TTU with a pit-holding fixture.

Mechanical Analysis. During this period, the literature review was conducted and background information on the AL-R8 (SI) storage container and its overall reliability were obtained. Additionally, tasks to meet the long-term project objectives were developed and finalized. Information on bolts was also collected. The literature review revealed that the design of containers for storage of nuclear materials has been the subject of investigation for safety and reliability considerations for many years. The designers believe that the stresses arising from dynamic loading are of particular importance. Progress was also made in the area of Finite Element Analysis, in element selection, mesh generation and refinement. The graduate research assistants began familiarization runs with the ANSYS Finite Element code. As a result, a simplified FE model of the container has been constructed and tested under static loading.

Criticality and Shielding. The literature search to ascertain storage container testing and documentation requirements for licensing has begun. Late arrival of the AL-R8 (SI) container has slowed the start of the effort somewhat. The container was received in April and measurements/properties needed for developing an MCNP model have been recorded. An MCNP model is being formulated and will be tested shortly against our preliminary gamma ray source experiments. A gamma ray detection system using a high efficiency NaI detector has been assembled and calibrated. The research team has obtained several gamma ray sources and have performed preliminary counting measurements with the sources placed inside the container. These initial measurements did not include the pit-holding fixture. However, a pit-holding fixture has been obtained recently and will be included in future experiments. A neutron detection system (using BF3 counters) is being assembled. Several neutron sources have also been located for use. The Cf-252 source currently available is too weak. However, Dr. Parish located another source on campus (at the Cyclotron) that is expected to be strong enough for our purposes. He expects to start preliminary neutron counting next quarter.

Other Research Activities

1. Presentations:
   b) “Center Storage Container Program,” Boyle, 24 February 1998, Center Board of Governors Meeting, Amarillo, Texas.
   c) “Three-Dimensional Thermal Model of Plutonium Storage Facility,” James, April 1998, Center Board of Governors Meeting, Amarillo, Texas.

A Feasibility Study for the Storage of Plutonium Pits in Non-Partitioned Warehouse Facilities

Darryl James, Ph.D., and Siva Parameswaran, Ph.D., Texas Tech University

The interface between AutoHexa and HEAD3d has been tested and verified to work on two different simplified grids. The computational domain for Room 121 in building 12-116 has been assembled. There are a total of 504 AL-R8 containers in three rows of fourteen racks in Room 121. Each rack consists of two six packs stacked vertically. The air handler units are currently being balanced in building 12-116. When the units have been balanced, the volume flow rates exiting the eight diffusers and entering the return air will be measured as this information is needed in the simulations to be performed. A second domain is being generated that has four return air grills, one in each corner of the room; currently the return air is located in diagonally opposite corners of the room.

Other Research Activities

Presentations: Presentation was given to Pantex personnel in January 1998 to discuss the modeling of Room 121. Presentation was
Nuclear and Other Material Studies

given to the Center Coordinating Board in April 1998.

Development of a Two-Equation Model for Turbulent Prandtl Number for Buoyant Flows and its Validation Against Experimental Data and Direct Numerical Simulation Results

Siva Parameswaran, Ph.D., and Darryl James, Ph.D., Texas Tech University

Kenneth Ball, Ph.D., The University of Texas

This project was initiated in April and is aimed at improving the turbulence models used in the HEAD3D code. The existing k-ε model is inadequate to predict buoyant flows which are important for thermal simulations of plutonium storage facilities. This effort will modify the existing k-ε model and replace the constant Prandtl number with a two-equation heat transfer model. These advanced turbulent models for momentum and heat transfer will be validated against the experimental and direct numerical simulation results.

In April, a meeting was held at The University of Texas among the involved researchers to discuss the scope and duration of the project, as well as to determine the division of effort among the participants. A project schedule and budget was developed. In addition, consultations were held with Dr. David Boyle (Texas A&M University) to ensure this activity was well coordinated with other ongoing Center-sponsored storage projects.
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