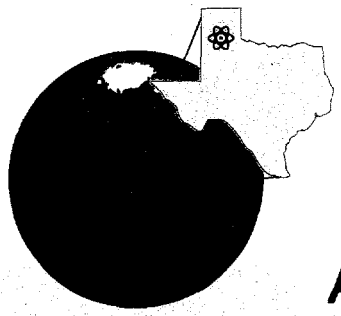

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Amarillo National Resource Center for Plutonium

A Higher Education Consortium of The Texas A&M University System, Texas Tech University, and The University of Texas System

Quarterly Technical Progress Report

August 1, 1997 though October 31, 1997

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CENTER PROGRAMS

PLUTONIUM INFORMATION RESOURCE

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TABLE OF CONTENTS

PLUTONIUM INFORMATION RESOURCE

ELECTRONIC RESOURCE LIBRARY

Electronic Resource Library

Co-PIs: D. Cluff, Ph.D., Texas Tech University ; G. Huffman, and K. Ruddy, Ph.D., Amarillo College

The Plutonium Information Resource task is known as the Electronic Resource Library (ERL), which is managed within Communication, Education, Training, and Community Involvement (CET&CI). Please see http://plutonium-erl.actx.edu.

Amarillo College (AC)

Deliverables were met for 3rd quarter 1997, and the deliverable of 17,600 pages for FY97 was exceeded with over 19,000 pages in the ERL collection by 10/31/97. Important collaborations and website enhancements continue. Negotiations are underway with American Nuclear Society, the editor of Nuclear Safety, Defense Technical Information Center and International Atomic Energy Association in Vienna, Austria to obtain relevant paper documents to digitize, i.e., conference proceedings and other copyright documents.

- Collaboration
  Continued collaboration with Lowell Langford at the U. S. Department of Energy Office of Scientific and Technical Information (OSTI) benefits both the ERL and OSTI's Info-Bridge project.
- Copyright Document Delivery
  Developed a program to deliver copyright documents as facsimiles and via U.S. mail.
- Electronic Digitization
  Added electronic pages to the ERL for a total of 19,000, exceeding goal of adding 17,600 electronic pages to the ERL for FY97. This translates to 975 titles, with a target of 1,100 for the year.
- Website Activity
  Web site handled over 15,000 hits from launch date, January 6, 1997 through October 31, 1997.
- Optimized all ERL-pdf (Image+text) files for ease of navigation on-line by loading updated Acrobat Exchange.
- Added "What's New?" link. This assists searchers in discovering the newest entries to the ERL Collection of full-text documents.
- Developed plan for links which takes into account "disappearing links" and interconnecting rich Internet sites pertinent to mission of ERL.
- Site Expansion
  Moved from the second floor of AC Library to a 900 sq. ft. space in the basement. Five additional Quality Assurance workstations were networked and six full-time temporary personnel were trained to increase production. Three shifts, 7 a.m. to 4 p.m., 4 p.m. to 11 p.m., and 11 p.m. to 7 a.m. are producing 15 to 25 ERL web-ready documents per day.

Texas Tech University (TTU)

Customizing of retrieval sets in the ProCite program and writing individual Biblio-Link configuration files necessary for accurate sortable citations are under development. Test files were delivered to AC.

ADVISORY FUNCTION

DOE SUPPORT

Multi-attribute Utility Analysis (MAUA) Team
PI: J.S. Dyer, Ph.D., The University of Texas at Austin

J. Butler, The University of Texas at Austin

Analysis and Selection of Alternatives for the Disposition of Surplus Plutonium

We prepared and submitted a brief version of our report, "Analysis and Selection of Alternatives for the Disposition of Surplus Plutonium", for publication in *Operations Research*, a leading journal in the field of decision analysis and operations research. We also plan to the present the results presentation at the Institute for Operations Research and Management Science and Decision Sciences Institute conferences in October and November, respectively.

We are also preparing for what we hope will be a follow up study analyzing the disposition selection problem from the Russian perspective.

ENVIRONMENTAL, PUBLIC HEALTH AND SAFETY

CURRENT ENVIRONMENTAL, HEALTH AND SAFETY

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

PI: G. E. Speitel Jr., Ph.D., P.E., The University of Texas at Austin

During the third quarter, progress continued on single and dual component adsorption isotherms. The focus has been on completing dual component isotherms, and on evaluating the results of previous single component isotherm experiments. Two granular activated carbons (GAC), Calgon F400 and Northwestern LB-830, were used for these studies. In the interests of providing relevant information for groundwater treatment at Pantex and to expedite future experiments, we have decided to do the bulk of our future work with Northwestern LB-830 (the GAC that is currently used in the Pantex groundwater treatment system).

Dual component isotherm tests have been completed to determine how HMX and RDX affect the adsorption of each other. Initial modeling, based on the Ideal Adsorbed Solution Theory (IAST) for multiple component adsorption, predicted that high concentrations of RDX (>20 mg/L) with moderate HMX concentrations (about 2,000 µg/L HMX) would reduce the amount of HMX that could be adsorbed. At much lower concentrations of RDX (about 2,000 µg/L) and moderate HMX concentrations (about 2,000 µg/L), IAST predicted that HMX adsorption would be affected relatively little; however, under these conditions, IAST predicted a significant decrease in adsorption of RDX. In both of these cases (high RDX with moderate HMX, and low RDX with moderate HMX), experimental results agreed fairly well with the model. In both cases, IAST slightly underpredicted the solid phase loading of the contaminant that was impacted by competitive adsorption. The remaining dual component isotherms are underway and are being conducted under conditions similar to those found in Pantex groundwater (i.e., similar initial RDX and HMX concentrations and similar pH).

Additional time during this quarter was spent on improving our current analytical capabilities. To achieve lower method detection limits for RDX and HMX in water, solid phase extraction (SPE) techniques were tested as an alternative to the salting-out extraction that is described in Method 8330. Two different SPE techniques were used. The first SPE technique had average recovery efficiencies of 56% for HMX and 58% for RDX (average of ten, 1-L replicate samples with 1 µg/L HMX and 1 µg/L RDX). Use of alternate solvents and conditioning procedures did not significantly improve these results. The second SPE technique resulted in 82% recovery for RDX and 78% recovery for HMX (average of two, 500-mL replicate samples with 5 µg/L HMX and 5 µg/L RDX), with fewer interference peaks. More testing will be conducted to determine the best technique. We have ordered a new Waters Alliance HPLC system with a photodiode array detector and a conductivity detector, and expect to take delivery by early December. This new analytical instrument should significantly reduce downtime and allow a much higher rate of sample analysis.

The next task that will be undertaken is the characterization of desorption of RDX and HMX from GAC. Preliminary work has been done to design desorption experiments. An initial literature review of potentially applicable methods was conducted. The method that will likely be used is a column method very similar to the small scale adsorption tests that were previously completed for this project.

Biodegradation of High Explosives

Co-PIs: R.L. Autenrieth, Ph.D.; J.S. Bonner, Ph.D., The Texas A&M University

The experiments performed earlier in the year showed that hexavalent chromium (Cr[VI]) inhibits the biodegradation of both RDX and HMX and the growth of the high explosive (HE) degrading cultures. The research of this quarter focused on quantifying growth inhibition by determining the inhibition coefficient, KI. Similarly, the effects of the presence of RDX on the HMX-degrading culture and HMX on the RDX-degrading culture were examined. Kinetics were based upon models with total carbon considered to be the substrate. Inhibition coefficients were determined for HMX and RDX by them-

selves with their respective cultures, and then combinations of HMX, RDX, and Cr(VI) were used to determine the inhibition coefficients for all constituents in those mixtures.

RDX-HMX Interactions

The presence of HMX (0.5, 1.0, 2.0, and 4.0 mg/L) inhibited the growth of the RDX-degrading culture, particularly at HMX levels of 1.0 mg/L and higher. Growth was non-existent when HMX was added at 4.0 mg/L. RDX transformation (from an initial concentration of 10 mg/L) over 3 days in all of the reactors with HMX present was between 28-30% compared to 39% in reactors with no HMX added. The presence of RDX (5,10,15, and 25 mg/L) inhibited the growth of the HMX-degrading culture, but the effect of RDX on HMX degradation remains unclear. In one set of initial-rate kinetic experiments, the rate of HMX transformation per unit of biomass increased with increasing RDX concentration. Models are being tested to determine KI. After 10 days, 40% of the HMX (initially at 1.0 mg/L) was transformed in reactors with no RDX added while only 28%, 28%, 26%, and 20% was transformed in the reactors with 5,10,15, and 25 mg/L RDX, respectively. The HMX-degrading culture also transformed RDX in these experiments with 10-day transformation percentages of 22%, 15%, 14%, and 11% in those same reactors.

HMX-Cr(VI) Interactions

The presence of Cr(VI) (1.0, 2.5, and 5.0 mg/L) affected the growth rate of the HMX-degrading culture. The growth at 1 and 2.5 mg/L Cr(VI) was comparable to reactors with no Cr(VI) present. After 10 days, HMX transformation percentages in all reactors were between 38% and 29% with less HMX transformation in reactors with higher initial amounts of Cr(VI). Initial-rate kinetic models are being tested.

RDX-Cr(VI) Interactions

The RDX-degrading culture revealed increasing levels of growth up to 2.5 mg/L Cr(VI). One recent experiment went beyond this concentration as the culture grew far better in the presence of 5.0 mg/L Cr(VI) than reactors with any other level of Cr(VI), including reactors with no Cr(VI) added. RDX transformation after 3 days (from an initial level of 10 mg/L) was 38% compared to 27%, 24%, and 27% in reactors with 1.0, 2.5, and 5.0 mg/L Cr(VI) respectively. Models are being tested to evaluate kinetic parameters and determine the mechanism of the interactions.

Above-Ground Treatment for Chromium Removal

Co-PIs: D.F. Lawler, Ph.D.; H.M. Liljestrand, Ph.D., The University of Texas at Austin

Tremendous gains were made this quarter in laboratory research on the remediation of Cr-contaminated groundwater through the use of ion exchange resins. Previous work at the University of Texas at Austin (UT) researched the use of anion exchange resins for the removal of Cr(VI) from Pantex groundwater. Current investigations have been conducted to compare the column treatment behavior of stryrene and acrylic based anion resins and to improve the performance of the original Cr(VI) treatment design. Through adjusting the system's operational pH, the predominant Cr(VI) species can be changed from chromate to bichromate. When operated in an environment dominated by the bichromate species, the selected anion resin's total exchange capacity is improved by a factor of 2.5. Through the appropriate pH adjustment of the treatment system, Cr(VI) column breakthrough is delayed and column run times are increased, requiring less frequent resin regeneration. All anion exchange column studies were conducted on Pantex groundwater from well PTX-08-1008.

Recent samples of Pantex groundwater indicate that the design of a combined system to treat trivalent and Cr(VI) may be prudent. Batch characterization and preliminary column studies on the removal of trivalent chromium from Pantex groundwater were completed in the summer of 1997. Due to pH fluctuations and competition effects from background cations, the information gained through the batch characterization studies could not be directly applied to predicting resin column performance. Three major structural classes of cation resins have been studied for column application in Cr(III) groundwater remediation. Pantex PTX-08-1009 well water was spiked with Cr(III) to serve as column influent source water. Strong-acid cation resins exhibited poor selectivity for Cr(III) in the presence of

background calcium concentrations. Weak-acid and chelating cation resins, on the other hand, performed much better than the strong-acid based resin and were not accompanied by exchange competition limitations. Attempts to regenerate the weak-acid and chelating structured resins with a conventional, mineral acid solution failed. However, through using an oxidizing regenerant solution, regeneration of these two resin types shows promise. Although similar in treatment and regeneration characteristics, the chelating cation resins outperformed the tested weak-acid resin.

A combined treatment system is currently in operation to investigate the simultaneous removal of Cr(VI) and Cr(III). The treatment system consists of two anion exchange columns in series for the treatment of Cr(VI), followed by a polishing cation exchange column for the removal of Cr(III). Since the majority of chromium detected in Pantex groundwater is in the hexavalent state, the final treatment system was designed to maximize Cr(VI) removal. Preliminary data analysis suggests the efficient recovery of both Cr(VI) and Cr(III) from Pantex groundwater. The graduate student working on this project is Mr. Joshua Norton.

Chemical Models and Redox Chemistry of Chromium
Co-PIs: B. Batchelor, Ph.D., P.E.; E. Carraway, Ph.D., P.E.; M. Schlautman, Ph.D.; and B. Herbert, Texas A&M University

Continuous flow experiments using treated and untreated Pantex soil in columns were conducted to evaluate the ability of aquifer solids to reduce Cr(VI). The average breakthrough time and average reduction capacity of untreated Pantex soil was 23 min. and 0.03 (eq/g, respectively. The soil columns were treated with three reductants ($Na_2S_2O_4$, $FeSO_4$, $Na_2S_2O_4$ + $FeSO_4$) resulting in breakthrough times of 230, 260 and 230 hr, respectively. Reduction capacities were 16.6, 17.6 and 17.1 (eq/g for the three treatments. The relative behavior of the columns agrees with observations of the reactants in batch experiments. Preliminary experiments of vadose zone reduction showed SO_2 is a very effective reductant to reduce and immobilize Cr(VI) in the vadose zone giving 99% immobilization of Cr(VI).

Batch and column experiments were performed to examine the removal of Cr(VI) from water by two types of GAC: F400 and LB830. The performance of both GACs were greatly affected by pH changes over the range of 4 to 8 with higher Cr(VI) removals observed for the lower pH values. Initial breakthrough from the columns began at 23 bed volumes when the flow rate was 105 mL/hr at pH 7.5. After the columns were extracted by 0.01M Na_2HPO_4 and washed with water or 0.01N H_2SO_4, subsequent breakthroughs started at 10 and 87 bed volumes, respectively. After another extraction and washing with either water or acid, adsorption capacities for Cr(VI) were considerably reduced in water-washed column, but remained high in the acid-washed column.

Experiments were conducted on the reduction of a mixture of TCE (72 mg/L), Cr(VI) (20 mg/L), and 2,4-DNT (72 mg/L) by ZVMs (Fe^0 or Pd/Fe^0). The results show that reduction by Pd/Fe^0 is faster than by Fe^0 and the reduction of the components of the mixture is slower than of the contaminants singly. The slower reduction in mixed wastes indicates that competition or inhibition, perhaps by precipitated chromium solid phases, occurs at higher concentrations. Personnel changes and equipment downtime have delayed progress on RDX reduction experiments.

Feasibility of In-Situ Remediation of Residual High Explosives-Modeling
Co-PIs: D.C. McKinney, Ph.D. and G.E. Speitel Jr., Ph.D., P.E., University of Texas at Austin

The research being conducted at the University of Texas focuses on determining biological degradation rates through laboratory experiments and using these rates as an aid in obtaining a conceptual model simulating fate and transport of High Explosives.

During the third quarter, laboratory procedures were completed for radio-labeled HE degradation studies. The degradation studies were setup in batches to test various head space conditions and nutrient additions. The three head space compositions being tested are nitrogen (anaerobic), air (aerobic), and mixed (2-3% oxygen). The two nutrient additions being tested to identify limiting conditions are carbon and phosphate with nitrogen being supplied as the RDX degrades. The batch studies were setup in two sets. Set one is testing the three head space conditions with and without phosphate additions as well as controls. Set two is testing the addition of glucose, glucose with phos-

phate, and more controls. The analysis of set one is half completed with a current incubation time of 64 days. Set two has been setup and analysis will begin in early November.

Thus far, results are showing the greatest activity under anaerobic condition with activity in vials having a mixed head space escalating after conditions turned anaerobic. A 50% reduction of products in the ether phase has been seen under anaerobic conditions at 64 days of incubation. In addition, carbon dioxide production and degradation products partitioning into water are increasing correspondingly. Thus, results are suggesting that RDX is being completely metabolized.

Feasibility of In-Situ Remediation of Residual High Explosives-Laboratory

Co-PIs: K. Rainwater, Ph.D., P.E.; C. Heintz, Ph.D., P.E.; T. Mollhagen, Texas Tech University

V. Harkins; T. Musick; W. Medlock; Md. Shaheed, J. Bednarz; R. Peppel

Concentrations of HE in Soil Samples

All soil samples from Zone 12 and IW-2 were analyzed in the previous quarter for HMX, RDX, TNT parent compound concentrations as well as 1,3,5 TNB according to the Environmental Protection Agency (EPA) method SW 846-8330, with solvent extraction followed by high performance liquid chromatography (HPLC). The sample extracts were retained for future analyses for PETN and TATB. We are still trying to obtain a TATB standard from our analytical suppliers to allow final analysis for that HE. We are also negotiating with Dr. Ben Richardson of the Materials Technology group of Mason & Hanger to provide us with a small amount of relatively pure TATB. TATB and PETN are not part of the EPA method, so we will have to modify it to get best results when both standards are in hand.

Procurement of Additional Incubators for RABIT System. We were fortunate to receive additional end-of-year funding to purchase two additional incubators for our impedance system. This addition triples our sample handling capacity. The new incubators arrived in mid-October and were set up on-site by vendor representatives.

Evaluation of HE Tolerance by Metabolically Active Microorganisms in Zone 12 Soil Samples

As part of Todd Musickís thesis project, soil samples from Location 6 near Building 12-43, with known initial HE concentrations, were spiked with RDX to increase the HE content to two to four times the initial levels. This test was a preliminary attempt to determine whether increased HE concentrations were toxic to the microorganisms. RABIT test results indicated no impact on metabolic activity in the range of concentrations tested.

Evaluation of Heterotrophic Microbial Flora in Soil Samples

Using the Whitley's broth recovered from the samples tested in the RABIT, isolation and characterization of the heterotrophic microbes present in the soil samples already tested for metabolic activity. In addition, we are also examining surface soil samples from the ditch downstream of Building 12-43 that had very high HE concentrations. These tests employ the Biolog and spiral plating devices and techniques developed in previous work funded by the Center.

Design of Microcosm Tests

With the expansion of the RABIT system, we redirected our testing for selection of microbial enhancements to the RABIT device rather than the soil microcosms originally scheduled. The RABIT system allows us to do faster experiments with smaller amounts of soil and chemical amendments to screen the possible carbon, nitrogen, and phosphorous sources. These tests utilize soil from depths of 30ft or less and are underway. The soil microcosms for later conventional tests have been designed to allow long-term tests (up to three months) and some replication while living within the limits of the available soils. The microcosm tests should begin in the next quarter.

FUTURE ENVIRONMENTAL, HEALTH AND SAFETY

Risk Characterization for a Mixed-Oxide Fuel Facility

Co-PIs: R. Charbeneau, Ph.D., P.E.; D. Maidment, Ph.D., P.E., The University of Texas at Austin; D. Barnes, Ph.D., P.E., Amarillo National Resource Center for Plutonium

The purpose of this project is to develop the database framework for characterization of environmental risks from a mixed-oxide (MOX) fuel processing facility at Pantex, and to develop and analyze potential pathways for human and ecological exposures. Through the development of the database and pathway analyses, information gaps will be identified so that additional research may be initiated in a timely fashion, and informed decisions may ultimately be made.

During the third quarter the following objectives have been addressed:

- Work to continue to refine the time lines and action plans for completing the screening level calculations for the bounding pathways was completed. Target completion for the screening analysis is prior to the DOE presentation of its draft Environmental Impact Statement (EIS). DOE expects to present its draft EIS during the First Quarter 1998.
- Screening calculations have been completed for several accident scenarios. The scenarios include:
  - an instantaneous release to the atmosphere and transport by air dispersion followed by deposition.
  - accumulation of the deposited particulates in a playa and recharge to the groundwater.
  - Deposition by air dispersion on Lake Meredith and ingestion of drinking water from the Lake supply.
- Screening calculations have been completed for several routine releases identified for the proposed Plutonium Conversion facility and the proposed MOX Fuel Fabrication. The scenarios include atmospheric releases of weapons-grade plutonium (Pu) and tritium and human inhalation exposure.

During the fourth quarter the following objectives have been addressed:

- A briefing workshop will be held with regulators from the TNRCC to present the interim results of the risk characterization project. The workshop will provide an opportunity for the regulators to continue to provide input on the study. Preparations for the workshop presentations were completed during the third quarter.
- Briefings will be held with Pantex management and an open public workshop will also be held. These workshops will provide an opportunity for the facility and the public to provide input on the study. Preparations for the workshop presentations were completed during the third quarter.
- Additional work has been conducted on the spatial database with experiments to connect tabular data to the available maps. Additional environmental data will be collected from the facility to continue this effort during the fourth quarter.

Development of a Monitoring Station for Estimating Interplaya Recharge

PI: B.R. Scanlon, Ph.D., Bureau of Economic Geology, The University of Texas at Austin

The original thermocouple psychrometers purchased and calibrated for this project had the wrong gauge wire; therefore, these psychrometers were returned to the manufacturer and replaced by 50 new psychrometers. These psychrometers were calibrated in the laboratory by using sodium chloride solutions of known osmotic potential and at three different temperatures to bracket expected temperatures in the field. We compared two calibration procedures, one using only the 2-second voltage reading and the other using 100 readings. The two calibration equations were very similar, and use of the 2-second reading will minimize data analysis.

Bill Mullican visited Pantex, and an interplaya location was chosen for the monitoring station. Don Reddell visited the Bureau to discuss drilling and instrument installation procedures. NEPA workplans have been developed for the drilling and sampling and have been submitted to DOE. We have tentatively set the date of November 15 to drill and install the monitoring station, assuming that we receive permission from DOE by that time.

Mobilization and Uptake of Actinides and Heavy Metal Analogs by Agricultural Plants

PI: L. R. Hossner, The Texas A&M University

Research during this period has concentrated on the calculation of transfer coefficients for Cr and uranium (U) and mechanisms of uptake and translocation of Cr. Root crops like turnip and beet accumulate more Cr than leaf crops and have a higher transfer coefficient. Addition of chelates doubled the transfer coefficient of some plants. Sunflower had the highest Cr(III) and U transfer coefficients with or without added chelate. Addition of chelates increased the Cr(III) transfer coefficient of sunflower by more than five fold. Addition of chelates had little effect on U accumulation. Sunflower is an effective accumulator of both Cr and U. Data collected during this period support the hypothesis that metal harvest (metal concentration x plant biomass) can be increased by chelates and that some plant species can be used as accumulators of both Cr and U.

Analysis of plant organs has indicated a lack of metal transfer from roots to shoots. Heavy metals, such as Cr, cause the accumulation of anthocyanin in the hypocotyl sections of the stem in soybean. This response has been reported in other plants with other metals (Cd) and with other stressful stimuli (salt stress, heat shock). Anthocyanin accumulation is also related to a specific gene responding to the external stimuli. RNA extraction from Cr-treated, heat-shocked, and control seedlings has been accomplished, and transfer to nitrocellulose membranes has been successful. Northern hybridization of the probe with the presumable, induced mRNAs is still in progress. Our most urgent, immediate goal is to assess how well the PCR-generated probe is suited to detecting the gene response from both Cr-and heat-treated sunflower seedlings.

Chromium (III) chloride and Fe(III)Cl_3 had a slight stimulatory affect, increasing the ferric chelate reductase activity (FCR) to about 5 µg/gFW/hr, in *Brassica juncea* and cucumber at the higher Cr concentrations. Cr(III)$(NO_3)_3$ dramatically increased the apparent activity to near 20 µg/gFW/hr. A series of assays on *B. juncea* were performed in citrate-phosphate buffers and, as predicted, the low pH solutions produced bright red stained roots and higher activities, although the maximum activity (at pH 2.3) was 7 µg/gFW/hr. This stimulation (dubbed "the acid affect") results from loss of root mass at low pH. A more refined experiment revealed that the FCR activity of this strain of *B. Juncea* has a broad pH optimum with a maximum activity (at 24.5°C) at around pH 5.1. We hypothesize that Cr(III) (and possibly nitrate ions) stimulate FCR activity explaining why some older reports suggesting Cr enhanced plant growth.

EPR spectra of treated plants indicated the presence of $Cr(OH)_3$ in or on the root but not in the shoot. The roots of plants grown in $CrCl_3$ were greenish-blue, similar to the color of $Cr(OH)_3$. Scanning electron micrographs (SEM) of root sections grown in $CrCl_3$ and plants grown in the control revealed a difference in the root surfaces. The $CrCl_3$ treated root surface was covered with small spherical particles indicating precipitated $Cr(OH)_3$ on the surface of the root. There is strong evidence that Cr^{3+} is precipitating in or on the roots of plants grown in the presence of dissolved Cr^{3+}. The mobilization of Cr^{3+} from $Cr(OH)_3$ is very slow in the presence of plant produced ligands such as citrate, oxalate and muginеic acid. Therefore, it is unlikely that the plant can mobilize significant amounts of Cr from $Cr(OH)_3$. There is a preliminary indication that Cr-oxalate and Cr-citrate are absorbed by the plant and Cr-citrate is transported to the leaves, and that Cr-EDTA is not taken up by the plant as an intact complex.

POLLUTION PREVENTION AND POLLUTION AVOIDANCE

New Polymers and Extractants for Plutonium Separations

PI: R.A. Bartsch, Ph.D., Texas Tech University

Attendant to any method for the disposition of surplus weapons Pu is the generation of Pu-contaminated wastes. The most frequently used process for Pu recovery from a wide range of materials involves dissolution in concentrated nitric acid and selective recovery of the Pu by sorption with a special, ion-exchange resin. Although the commercial anion-exchange resin currently utilized in the full-scale recovery process at Los Alamos National Laboratory (LANL) removes Pu effectively, the rate of Pu sorption onto the insoluble resin much slower than desired. This problem is being addressed with new bifunctional anion-exchange resins which are prepared at TTU and evaluated at LANL. The new resins are produced by reaction of a commercial polymer with alkylating agents which possess a positively charged group, such that the product resin contains two anion-exchange sites in proximity rather than the isolated anion-exchange sites found in currently utilized commercial resin. Evaluation of the new bifunctional anion-exchange resins has revealed a much more rapid removal of Pu from 7M and 9M nitric acid solution compared with the presently employed commercial resin. In addition, the overall level of Pu recovery is higher with the new bifunctional anion-exchange resins.

During the reporting period, new bifunctional anion-exchange resins were prepared by reactions of Reillex HP™ macroporous poly(4-vinylpyridine) resins with 21 and 18% crosslinking and a course form of Reillex™ 402 poly(4-vinylpyridine) resin with (5-bromopentyl)trimethylammonium bromide in methanol at 100 °C in a pressure reactor. These new resins were prepared for comparison of their Pu-sorbing behavior with that of analogous bifunctional anion-exchange resins synthesized from 25%-crosslinked Reillex HP™ resin which had been evaluated earlier. Through these experiments the influence of the physical form of the starting poly(4-vinylpyridine) resin upon the Pu-sorption behavior of the bifunctional anion-exchange resins was determined. It was found that a lower level of crosslinking in the initial macroporous poly(4-vinylpyridine) polymer produces bifunctional anion-exchange resins for which the rate of Pu sorption from 7M nitric acid is increased. Bifunctional anion-exchange resins prepared from Reillex™ 402 resin were found to sorb Pu less efficiently from concentrated nitric acid solutions than those derived from the Reillex HP™ macroporous resins. Efforts are currently underway to determine the effect of varying the level of alkylation of the poly(4-vinylpyridine) resins upon their Pu sorption behavior. Once this factor has been assessed, larger amounts of the most appropriate bifunctional anion-exchange resin will be prepared for evaluation at LANL in a column configuration instead of the single-stage sorption studies which are being employed for the current testing.

For preparation of larger quantities of the bifunctional anion-exchange resins for bench-scale testing at LANL, an efficient method for the synthesis of the alkylating agent, (5-bromopentyl)trimethylammonium bromide, was needed. A problem has been the formation of the unwanted disubstitution product together with the desired monosubstitution product from reaction of trimethylamine with 1,5-dibromopentane in acetone or ethanol. A synthetic procedure has been discovered using a different solvent from which the monosubstituted product precipitates as soon as it forms thus preventing over-reaction to form the disubstituted product.

Publications and Presentations

R.A. Bartsch, TTU; J.S. Kim, TTU; J. Nam, TTU; S.F. Marsh, LANL; G.D. Jarvinen, LANL. "New Bifunctional Anion-Exchange Resins for Plutonium Separations", Plutonium Futures - The Science, Santa Fe, NM, August 25-27, 1997.

Alternative Uses for High Explosives
PI: C. G. Willson, The University of Texas at Austin

Part 1: Diamond Generation by Explosive Compression of Buckminsterfullerene

At the time of the last quarterly report, two (samples one and two) of five three-dimensional shots had been opened and the contents analyzed. Since the last report, the remaining three shots have been opened. The carbon to metal loading in these three shots (three, four, and 5) wasfivevaried to investigate the effects of higher metal loadings on quenching. One of the shots (five) was also seeded with diamond particles.

Analysis of shots three and four proved more difficult than shots one and two due to the higher metal loading. During detonation, metal contained within the sample chamber becomes molten and fuses with the chamber wall. As a result, the carbon sample is trapped in the resulting metal network. Dissolution of the metal is required to allow for sample recovery. Various solvents have been tested on model systems to determine their effectiveness in dissolving stainless steel. These solvent systems tested include: nitric and hydrofluoric acid; sulfuric acid; hydrochloric acid; and hydrochloric acid with ferric chloride and a platinum wire catalyst. It was found that boiling hydrochloric acid caused the most degradation in the stainless steel. This solvent was tested on one of the previously analyzed shots (one) to establish a sample recovery protocol and to test all processing steps. Shots three and four are now being dissolved by this method. We will continue to explore alternative methods for sample recovery.

The carbon sample from shot five was easily recovered and no acid treatment was required. Analysis of this sample showed strong diamond peaks in x-ray diffraction, confirming that diamond was able to withstand the compression / heating of the detonation.

Part 2: Demonstration Burn for Energy Recovery

Testing was done at Pantex on the formation of pellets by using the polymer filler as the binding agent. The polymer was reduced to a fine powder by slurrying in n-butyl acetate. Ground explosive was added to provide a mixture that was 90/10 (wt/wt) polymer/explosive. Water was added to the mixture to yield beads of polymer/explosive mix. Further cooling of this material provided a final product in the form of thin sheets. Based on these experiments, a 10% HMX/90% polyphenyline oxide product can be readily produced. Several batches of material with ratios of 5%, 10%, 15%, and 20% HMX/polyphenyline oxide will be produced and submitted for sensitivity testing.

Officials from the city of the Center are excited about conducting a full scale 1000 lb. test burn as soon as possible. Unfortunately, production of the fuel pellets remains a low priority at the Pantex.

COMMUNICATION, EDUCATION, TRAINING, AND COMMUNITY INVOLVEMENT

PROGRAM IMPLEMENTATION

Program Management

Co-PIs: E. Zounar, Ph.D., B. Perry, C. Dixon, S. Floyd, and E. Harle, Amarillo National Resource Center for Plutonium

Communication, Education, and Training has been changed to Communication, Education, Training, and Community Involvement (CET&CI). It is responsible for Task 1 and Task 4. The size of the CET&CI staff has stabilized at eight plus two graduate assistants in the education department.

Program management has been engaged in the following:

- 9/9-11/97 Conducted peer review of proposals submitted for FY98.
- 9/24/97 Non-research budget approval.
- 10/29/97 Research budget approval.
- October Published ANRCP-1997-2 "An Automated System for Chemical Analysis of Airborne Particles Based on Corona-Free Electrostatic Collection" (Liu and Dasgupta, Texas Tech University).
- Graduate Education, Training, and Science Information and Resource Center program analysis.

External Communications

During the quarter, communication program personnel continued to heighten external communications efforts on DOE-related issues of importance to the Amarillo community.

- The Governor's office of the state of Texas has asked the Center to perform a risk characterization study that evaluates possible new missions for the Pantex. External communication activities this quarter included:

  Presentations

  8/1/97 Agriculture representatives

  8/7/97 Pantex Plant representatives

  8/12/97 Serious Texans Against Nuclear Dumping, the Peace Farm, and Pantex Neighbors and Landowners

  Print Media

  8/1/97 Press release to *Amarillo Globe News* requesting public input to the study.

  8/3/97 Article titled "Plutonium Center tapped for Study of Pantex Options" ran in *Amarillo Globe News*.

  8/3/97 Questionnaire ran in the *Panhandle Herald* and *Amarillo Globe News* seeking public comment.

  Non-Print Media

  8/5/97 KFDA and KVII interviews stating public input is sought on the study.

- The Speakers Bureau presented 30 speeches for the first three quarters, an increase of 6 over the first three quarters in FY96. Presentations for the quarter included:

  8/5/97 "From Nuclear Weapons to Electric Energy " (Desk & Derrick Club of 74)

  9/22/97 Amarillo Board of Realtors (audience of 100)

9/23/97	Pantex Plant Physics Group (audience of 20)
10/16/97	Sons of the American Revolution (audience of 20)
10/29/97	"The Plutonium Paradox: Trash or Treasure" (general audience of 163)

- Published a set of eight nuclear fact sheets. Distribution approximates 7,500.
- The Center's web site at http://www.pu.org has been accessed 49,674 times since it was launched 11/95. The site is continuously monitored and evaluated. It continues to be developed and currently includes items such as information on mixed-oxide fuel, the FY97 second quarter report, procedures for publishing technical documents, nuclear fact sheets, and comments to DOE.
- The Center received 73 newspaper hits for the first three quarters of FY 97. This is 62 more articles than the entire previous fiscal year. The Center received 22 other media hits which included 4 hits with television coverage on all three local stations. Compare this to a total of 4 media hits for the entire previous fiscal year. For the reporting period, media coverage included the following:

8-9/97	Public Service Announcements on the Center.
8/4/97, 8/13/97, & 9/5/97	Various KGNC radio interviews.
9/28/97	Press release on Dr. C. Grant Willson, University of Texas at Austin re-searcher and recent winner of the Malcolm Pruitt Award ran in *Amarillo Globe News* and in *Austin American Statesman* on 9/29/97.
9/28/97	Announcement of the appointment of Dr. Dale Klein, Executive Director and Chairman of the Board of the Center to the Radiation Safety Board by Texas Governor George W. Bush ran in the *Amarillo Globe News.*
10/9/97	"Study Offers Hope Gallium Problems in MOX Fuel can be Controlled" ran in Nuclear Waste News.
10/30/97	"UT Professor Discusses Benefits of Plutonium" ran in *Amarillo Globe News* following the 10/29/97 presentation by Dr. Maxey.

Exhibit Program

The Center's exhibit program consists of the Pu Past, Present, and Future exhibit; the Center's skyline exhibit; and a recent addition, a mobile tabletop exhibit.

- Pu Past, Present, and Future exhibit is being updated and will be completed by 12/1/97. The objective of this exhibit is to inform a general audience about Pu, disposition alternatives, the Pantex Plant, and the Center. The exhibit has been located at the Amarillo International Airport in a high traffic throughway since 12/96. Amarillo airport officials estimated that 455,607 passengers boarded airplanes in 1996.

  During October, passenger and visitor behavior was observed at random at the exhibit over an eight-day period. Observations revealed that 50 people passed by the exhibit every 15 minutes; 1 person stopped to look at the exhibit every 17 minutes; 1 person touched the exhibit every 16 minutes; 1 person interacted with the computers every 29 minutes; and nobody viewed the videos.

  A distribution record of brochures and newsletters has been maintained since 2/97. From 2-9/97, 407 brochures and 527 newsletters have been taken which equates to 1.7 brochures and 2.2 newsletters taken daily. Over the eight-month period, newsletters were consistently taken more frequently than brochures.
- The objective of the Center's skyline exhibit is to inform the various audiences who attend exhibit events about the Center's mission, the research projects undertaken by the Center, and the or-

ganization of the Center. The Center's brochure, newsletters, fact sheets, and informational videos are part of the exhibit. For this reporting period, over 750 pieces of literature were carried away; more than 1,090 people visited the exhibit; and 66 more people asked to receive newsletters.

Interest in the Center's exhibit program has heightened over the past two quarters by the presence of the exhibit at the following events:

9/13-18/97	Tri-State Fair, Amarillo, TX
9/19/97	University of Texas Nuclear Engineering Day, Austin, TX
9/27/97	Panhandle Area Math and Science Conference, West Texas A&M University (WTAMU) campus, Canyon, TX
10/6-8/97	Farmer-Stockman Show, Lubbock, TX

Education Activities

- As a result of encouragement from the Center, Amarillo Independent School District has decided to participate in JASON IX during the 1997-1998 school year. Eighty-two (82) teachers at 5 middle schools have committed to implementation of the project. This number represents 2,525 students who will participate in the curriculum and local field experiences and, who will attend an interactive broadcast during 3/98. The JASON Project uses advanced curricular and technological approaches to excite and engage millions of students and educators throughout the world in science and technology (reference http://www.jasonproject.org/JASON/HTML/).
- 9/25/97 - "Math, Science Teachers to Attend Conference at WTAMU Campus Saturday" appeared in *The Canyon News* in anticipation of The Panhandle Area Mathematics and Science Conference which was held 9/27/97 at WTAMU.

  Approximately 800 teachers from the Texas Panhandle, South Plains, and Tri-State area participated in the conference with teachers who have received the Texas Presidential Award for outstanding teaching in mathematics or science. Both the Middle School Science Resource Manual and the High School Computer-Based Physics Manual were presented and made available during discussions at this conference. The Center reported a $5,000 award to support this conference last quarter.
- The Traveling Chemistry Road Show has been staffed and plans are in place for a 2/1/98 start.
- During the quarter, the following awards were made:

$72,488	Panhandle Information Network in order to provide (a) teacher training in curriculum integration of technology and technical support of the Internet system through training consultants, (b) the development of training manuals by Region XVI Education Service Center, and (c) four months of dial-up Internet access for teachers to Instructional Trainers and Technical Trainers during Fall 1997.
$3,000	The University of Texas Student Chapter of the ANS to co-sponsor the 1998 Western Regional Conference in March, 1998.
$5,600	The Texas A&M University (TAMU) PACES-on-Tour Program to provide the student chapter of the Society of Mexican-American Engineers and Scientists an opportunity to visit schools in the Texas Panhandle and encourage students to (a) graduate from high school, (b) reflect on the opportunities of a college education, and (c) consider the value of mathematics, science, and engineering as fields of study.

COMMUNICATION PROGRAM

Science Information And Resource Center

Co-PIs: Z.D. Curry, Ph.D.; M. Gentry, Ph.D., Texas Tech University

The development of the exhibit on the story of Pu continued. Investigators met in Amarillo with the Center's Education Program Manager and with an energy information center consultant for exhibit text and graphics. The outcomes of this meeting were: (a) recommendation to consolidate the nuclear and environmental exhibits into one exhibit with multiple structures (approximately five); (b) decision that investigators would receive approved copy for exhibit text and graphics by November 1, 1997; and (c) decision that investigators would obtain videos from Los Alamos and Sandia for possible inclusion into the exhibit. Deliverable date for the exhibit is 1/15/98.

EDUCATION PROGRAM

K-16 Science And Mathematics Education

PI: J. Kelley, West Texas A&M University

All scheduled activities for this project were completed during 1/97 as scheduled. The formal survey (needs analysis) scheduled for submission in 8/97 was canceled since there were no significant changes in information submitted on a previous survey. This decision terminates the activity on this project.

West Texas Environmental Project for Integrative Studies in Science and Mathematics

Co-PIs: R. Powell, Ph.D., Texas Tech University; J. Kelley, West Texas A&M University

Conduct teacher advisory panel meeting

On 8/7, the West Texas Environmental Project (WTEP) conducted an all-day teacher advisory panel meeting on the 1997 summer institute and field trip. Purposes of the meeting were to (a) brainstorm and explore ways for strengthening future projects if funding is made available, (b) consider the infusion of video and computer technology into the field studies portion of the project, and (c) begin planning the 1998 project on the Ogallala Aquifer (contingent upon funding). Seven teachers representing Amarillo, Hereford, Perryton, Floydada, and Lubbock, as well as the FY 98 WTAMU representative, attended the meeting.

Conduct site visits for follow-up evaluation and research interviews

In order to collect data for research on and evaluation of WTEP, site visits to teachers' classrooms began on 9/15/97, and will continue through 11/10/97. All teachers who participated in the 1997 WTEP are being observed in their classrooms, and are being interviewed. All interviews are being taped and transcribed. For site visits, a two-hour observation of typical classroom teaching is undertaken. Following this observation, each teacher and the WTEP PI carry on a taped conversation. Each conversation follows a structured protocol that inquires into teachers' perspectives of the project, and asks (a) how they project elements of the project are being implemented in their classrooms if at all, and (b) what they think will strengthen the project in future years. Results of this research and evaluation study will be compiled into a research report that will be presented at two national conferences.

Initiate curriculum development

During the summer institute, teachers in the WTEP were organized into grade-specific groups for curriculum development. One high school group, two middle school groups, and one elementary group were organized. Teachers in the various groups have been corresponding with each other to carry out their curriculum development responsibilities. They also are making plans to complete their curriculum development activities at the November follow-up conference.

Secondary School Physics Curriculum
Co-PIs: J.P. Spears, West Texas A&M University; T.C. Ahern, Ph.D., Texas Tech University

Physics teachers who attended the second summer workshop for Computers in Physics presented samples of their work and discussed the use of physics simulations in their classrooms at the WTAMU Mathematics and Science Teachers Conference on 9/27/97.

At this time, simulations contributed by the workshop teachers are being converted to PC format. Explanations and worksheets for each are being completed for inclusion in the final version of the Physics Manual due 1/98.

Middle School Science Resource Manual
Co-PIs: G. Skoog, Texas Tech University; T. Brasher, West Texas A & M University

Three workshops were conducted for teachers on the use and application of the Science Resource Manual. Two were conducted for 40 teachers during the Panhandle Regional Mathematics and Science conference held at West Texas A&M University (9/97). The third was conducted for 12 teachers at the Conference for the Advancement of Science Teaching in Texas in Fort Worth (10/18/97). Feedback indicates that teachers are using the manual and sharing the activities with other teachers.

Building Foundations for Foundations Mathematics and Science Success
Co-PIs: G. Mann, Ph.D., West Texas A&M University; R. Powell, Ph.D., Texas Tech University

The Amarillo Independent School District again had five schools participating in the Cool School component of the project. (Cool School was formerly known as SuperSaturday. The name was changed due to a conflict with Gifted and Talented SuperSaturdays.)

9/21/97	Cool School event announced in *Amarillo Globe News.*
9/25/97	"WTAMU Education Majors Assist with Cool School" ran in *The Canyon News.*
10/1/97	Feature article titled "Students Learn Through Hands-on Workshops" ran in the *Amarillo Globe News.*

A second cohort of WTAMU student teachers (interns) received training and access to mathematics curriculum materials. Preliminary evaluation findings appear to show that the interns trained in the project performed better than was anticipated. This shows that the training and access to effective curricular materials provided are a strength of the project and will affect mathematical and science instruction in the Texas Panhandle far beyond the duration of the project.

The principal investigator of the project has examined evaluation instruments designed to measure the effectiveness of the project. It appears that the instruments were well-conceived and that good information will be provided at the conclusion of the project.

This data base will provide other researchers with information needed to assess the impact of other Center projects. The database will be made available to Center personnel after the Fall 1997 student participants are added to the database.

The project stipulated that a student need's assessment would be conducted to identify classes offered in project school sites. School coordinators administered an interest inventory to school personnel to identify topics that interest students. Classes were created to respond to the interests identified in those questionnaires and instructors were recruited with expertise in those areas.

Texas Pre-Freshman Engineering Program (TexPREP)
Co-PIs: C.N. Kellogg, Texas Tech University; T. Jones, Amarillo College

The 1997 sessions of AmarilloPREP and TexPREP-Lubbock concluded on 7/25/97. A total of 189 students, 109 at the Amarillo site and 80 at the Lubbock site, successfully completed the program. Of the total number of students, 100 were 1st year students, 52 were 2nd year students, and 37 were 3rd year students.

The TexPREP-Lubbock site did not submit demographic data. At the Amarillo site, 54 were 1st year students, 33 were 2nd year students, and 22 were 3rd year students. Sixty three (63) students were female and 46 were male. Fifteen (15) students were African American, 17 were Asian, 30 were White, and 47 were Hispanic. The largest subgroup (29) was female Hispanic. This supports the trend throughout the first, second, and third-year students that female Hispanics are the largest subgroup of students.

Progress continued on trying to increase the number of respondents to the annual follow-up survey conducted on each of the TexPREP sites across the state. Investigators worked through the TTU Ex-Students Association to help identify and locate former TexPREP students who have attended Texas Tech University. In addition, investigators conducted extensive Internet searches with little success.

The follow-up for the survey of College Eligible students, those who graduated from high school 5-6/97 or previous to that year, was pursued diligently during August. AmarilloPREP attained a 94% response (141 out of 151 college eligible students); TexPREP-Lubbock attained a response of 14.8% (52 out of 350). The Amarillo site reported on years 1990 - 1994. One hundred seven (107) students are attending college and of these, 51 are taking courses in engineering and science. This is 36% of those students who responded to the College Eligible survey. Of the same 141 respondents, 6 were college graduates, 4 in engineering (.03%) and 2 in science (.014%). The year with the highest rate of college attendance was 1992 followed by 1991 and 1990 respectively. College enrollment dropped from 23 in 1990 to 6 in 1993 and 6 in 1994 showing a downward trend in college enrollment. TexPREP-Lubbock did not submit survey data.

Several meetings were conducted toward the goal of increasing permanent support for the TexPREP Lubbock program. Investigators met with the recently appointed Vice Chancellor to consider the impact of the TexPREP program on recruiting and diversity.

The Directors meeting was held at the University of Texas at San Antonio 10/24/97. Director of AmarilloPREP reported the success of the 1997 Panhandle sites to the coordinator of the statewide TexPREP program, the other site directors, and visiting directors from the HACU effort toward Nationalization of PREP.

TRAINING

Plutonium Reference Book

Co-PIs: D.C. Hoffman, Seaborg Institute for Transactinium Science; M.A. Fox, The University of Texas at Austin

Pending funding resolution. Project has not yet commenced.

NUCLEAR AND OTHER MATERIAL STUDIES

PROGRAM IMPLEMENTATION

Coordination and Technical Information Support for Nuclear Group Activities

PI: P. Nelson, Ph.D., P.E., The Texas A&M University

D. Boyle, Ph.D.; G. Alexander, M.A.; I. Carron, Ph.D.; M. Payton, The Texas A&M University

Nuclear Group administrative activities for the current reporting period provided both technical and information support to Center staff and to the investigators of the various subprojects.

In the area of coordination and technical support, Dr. Paul Nelson represented the Nuclear Group at the Center's Governing Board meetings and participated in several technical planning meetings and conference calls in preparation for and during the FY98 proposal process. Dr. Nelson, with assistance from Ms. Alexander and Mrs. Payton, coordinated with the Center's Nuclear Program Manager Dr. Carl Beard in the logistical and administrative processing and technical peer review of FY98 proposals from researchers.

Dr. Igor Carron was also involved in numerous project coordination efforts this quarter, most notably organizational collaboration with the Moscow Engineering Physics Institute (MEPhI) on the NATO (Norht Atlantic Treaty Organization) Advanced Research Workshop on Safety Issues Associated with Plutonium Involvement in Nuclear Fuel Cycles: Volga '97. This meeting was held September 2-6, 1997, near Moscow, and was attended by approximately 90 experts from six countries.

Dr. Carron was also Involved in writing a proposal to NATO's new Science for Peace Program that would involve universities represented by the Center, INSTN (the educational training branch of the French CEA), Russia's Moscow Engineering Physics Institute (MEPhI) and Institute of Nuclear Power and Engineering (INPE), and two universities from the Ukraine. The goal of this proposal is to set up a program in Russia and in the Ukraine on nuclear materials safety management in order to establish the seed for a culture of safety in nuclear activities in these two countries.

Activities related to technical information support included three updates of the Nuclear Group Calendar of Conferences located at http://trinity.tamu.edu/~igor/hi.html (August 4, September 11, and October 27). and expansion of the Nuclear Group Technical Working Documents series by three reports.

Providing timely information to investigators involved in various Nuclear Group activities remains a central and primary function of this subproject. This aim is also the primary responsibility of Dr. Carron. Activities during the present reporting period included:

- Interacting with the ERL and Center personnel on ERL activities regarding documents to be included in the ERL's collection;
- Providing the Center's Environmental Task Force with documents on mixed oxide fabrication facilities;
- Providing principal investigator Dr. Ron Hart with references on irradiation of beryllium; and
- Continuing work in support of specialists studying the water-reactor option for disposition of excess weapons-grade Pu by compiling a comprehensive list and historical background of critical experiments using Pu as a component mixed-oxide fuel.

Ms. Alexander continued editorial work on the proceedings of the NATO Advanced Research Workshop on Nuclear Materials Safety Management, held in Amarillo last March, and the Moscow Engineering Physics Institute FY 1996 final report. Both documents were slated for publication during the current reporting period. However, the MEPhI report was delayed due to a lengthy but necessary technical review process, and the NATO proceedings were delayed primarily due to difficulties in obtaining appropriate translations of contributions from international workshop participants. Both documents are now near completion. Ms. Alexander has also been assigned editorial responsibility for the

proceedings of the NATO Advanced Research Workshop on Safety Issues Associated with Plutonium Involvement in Nuclear Fuel Cycles: Volga '97 (as described above).

INTERNATIONAL STUDIES

Support of Russian Activities

PI: P. Nelson, Ph.D., P.E., The Texas A&M University

Activities in support of international studies (formerly support of US/Russian joint studies) has included participation in technical meetings, several conference presentations, and other interactions with our counterparts at the Moscow Engineering Physics Institute (MEPhI).

Technical Meetings

Dr. K. L. Peddicord attended the presentations by MOX Team USA during the visit to Amarillo on August 7, 1997.

Five researchers from the Center participated in a meeting of the US-Russia Joint Technical Working Group on Water Reactor Options for Disposition of Weapons Plutonium, held August 25-27 in Oak Ridge, Tennessee. Drs. Marvin Adams and Igor Carron from Texas A&M University (TAMU), Dr. Musa Yavuz from the University of Texas, and graduate research assistants Georgeta Radulescu and Hatice Akkurt all gave presentations to the assembled US-Russian team. There was much progress at the meeting, including the approval of detailed plans for the US-Russia team's work in the next fiscal year. These plans include the Center continuing in its role of collaborating with ORNL to conduct the US portion of the research.

Conference Presentations

Dr. K. L. Peddicord also presented a paper as part of the NATO Advanced Research Workshop on Safety Issues Associated with Plutonium Involvement in Nuclear Fuel Cycles: Volga '97, September 2-6, 1997, on the MOX fuel performance evaluation project funded by the Center. This conference was held near Moscow, Russia

Moscow Engineering Physics Institute (MEPhI) Master of Science Program in Nuclear Materials Management

During a NATO-sponsored visit to Russia in September, Dr. D. R. Boyle met with the MEPhI investigators for the MS course project and reviewed the status of their effort. Reasonable progress has been made on the specialized courses being funded by the Center. In spite of the serious illness of Dr. V. Khromov, the principal investigator for the effort, his team started the initial class on schedule this fall. This first group of students are working towards the new Master of Science in Nuclear Materials Protection, Control, and Accounting. With continued funding, MEPhI hopes to be able to start a class next fall working towards the new Master of Science in Nuclear Materials Management.

Expert Visit

During September and October, Dr. Boyle has coordinated travel arrangements and participated in preparations for the pending official visit of Dr. Alexander M. Dmitriev, Deputy Chairman of Gosatomnadzor, the Nuclear and Radiation Safety Authority of the Russian Federation.

STORAGE: FACILITY DESIGNS

A Feasibility Study for the Storage of Plutonium Pits in a Warehouse

Co-PIs: D.L. James, Ph.D., S. Parameswaran, Ph.D., Texas Tech University

The full computational domain for phase III was originally proposed to include twenty two stacks on either side of a walkspace. Each stack contains sixteen containers, giving a total of 704 AT-400A containers in the computational domain. The computational domain is divided into sub-domains, and each sub-domain is divided into a number of cells. The velocity, temperature, and pressure data is com-

puted on a cell basis. We have discovered that the current software used to discretize the computational domain has a limit on the number of sub-domains used when building the full computational domain. The proposed phase III domain exceeds this sub-domain limit by more than a factor of two.

The partial phase III domain that was reported in the last quarterly report has been extended to include 4 1/2 stacks resulting in seventy-two AT-400A containers on either side of the walkspace for a total of 144 AT-400A containers in this partial domain. A simulation has been performed for air flow entering through the ceiling at a constant rate of 1 m/s and exiting through the floor. An additional simulation will be run with the flow entering through the floor at a constant rate of 1 m/s and exiting through the ceiling. Comparisons of the resulting temperature distribution will be made in order to determine which inlet condition provides fewer hot spots.

Note that we purchased new software this quarter that does not have the sub-domain number limitations and are currently working to integrate this software with our CFD code.

Automation, Robotics, and Tele-Operation

PIs: A. Barhorst, Ph.D., Texas Tech University; D. Volz, Ph.D., The Texas A&M University; G. Kondraske, Ph.D., The University of Texas at Arlington.

Co-PIs: J. Macedo, Ph.D., W. Kolarik, Ph.D., M. Parten, Ph.D., and J. Wolstad, Ph.D., Texas Tech University; J Trinkle, Ph.D., L. Everett, Ph.D., The Texas A&M University; S. V. Sreenivasan, Ph.D., The University of Texas at Austin

The project is on schedule. Students are in the process of defending theses this fall and interaction with Pantex Engineers has been mutually beneficial. The funding for this year appears to be completely spent. The work being completed is of first quality and will be published in the leading journals in the respective fields of the researchers.

In what follows the progress for this quarter reporting period will be presented by school. Projects not explicitly reported are to be shown as in progress and on schedule; most of the projects will be completed by the end of the project fiscal year as stated in the milestone log. Following the progress updates will be a milestone update.

Texas A&M University

Add contact/impact model & system compliance to simulation testbed:

The TELEGRIP software can simulate the motions of robotic devices in the virtual world, but it cannot simulate the motions of these devices when then are in contact with moveable objects in the environment. The new software has remedied this deficiency through predicting the motions (i.e., by computing the accelerations) of bodies before and after their collision. Then, the simulation can be performed by using integration steps with the accelerations.

However, since we need the integration steps which are valid only before, during, and after the moment of an impact of a rigid body with another (e.g., when the pit drops and hits the ground.), we have introduced a special model for computing those accelerations.

The simulation of motions after the impact is being done by introducing a specific impact model (impulsive-based dynamic model) upon the detection of a collision between two bodies, and the purpose of this model is to predict the motion after the impact.

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 collection of position, force, and other relevant data has been observed during the simulation for the purpose including a feature to allow the user to set up scenarios and to apply motions and/or forces to bodies in the virtual world through user-friendly mouse actions in the future.

Use of VR Capabilities for simulation and remote viewing

Rotational movement have been added to the capabilities of the 3-D remote vision system that has already been created for use in the remote viewing system. This was achieved by adding rotations to

the end effector of the robot arm, since control of the arm has been directly tied to the motions of the head-mounted display. On the robot arm, two camera and auto-focus/auto-convergence system has been mounted to provide stereo images which are relayed to the user who wears the VR4 head-mounted display. Then, motion tracking of the user's head is relayed to the robot to position the cameras where the user is looking. The rotations are only applied in the direction that can facilitate the straight orientation of the object been seen with the cameras. This aspect of rotations is being tested to give maximum comfort to the user. This has been implemented to give the user a more realistic view of the environment.

Two Analog-to-Digital converters have been purchased. They are for the purpose of displaying the graphics on the VR4 helmet. Geiger readings being captured from below the robot are passed as InterAgent objects and are displayed on the screen of the SGI machine. These are to be displayed on the VR helmet with the help of the Analog-to-Digital converters.

Architecture for Storage System Construction Set:

The draft report on design of the architecture for SSCS was prepared, being finalized for submission. Expected time of submission is Aug. 15. Basically, SSCS is a capability through which we can define relationships between storage system components, which will lead to faster development of storage system simulations. The original architecture of SSCS was modified, to provide the user with the capabilities for adding new storage system component types to the library and defining their constraints. Although this was possible in the original design, it required additional C++ modules to be written by user. The modified architecture allows this to be carried out through graphical interface of SSCS. The report is being modified to include the design changes.

The preliminary graphical interface for SSCS was developed and its initial integration with Telegrip carried out.

Detecting environment changes:

The objective of this component of the project is to investigate a means to determine changes in a working environment. For example to determine changes in position of Storage containers in a vault. The method will sense object position and compute the geometric transformation between current and previous position/orientation (the pose).

This objective is being met by visually capturing the robot's working environment using a stationary camera positioned to cover the desired scene. Camera images taken after the robot performs a task form the initial pose reference for the objects. Whenever changes need to be determined, the camera takes another image of the scene and the data is processed to determine pose changes. Pose identification is performed by recognizing key points on the containers. To aid this process, reflectors are placed on the containers. After each container's key points are identified, the pose is calculated. The new poses are finally compared with those obtained from the reference image to identify the motion transformations.

At the present time, images can be captured, and the key points identified. The positions of the key points relative to the video frame of reference can be determined. What remains is to convert these positions into pose estimates.

Texas Tech University

Interface Design–Ergonomic Evaluation of Display Formats and Visual Enhancement Cues for Three-Dimensional Teleoperational Task:

Preparation for the Experiment (completed)

A pilot experiment was performed to evaluate the experimental procedures and protocol, and training subjects. A final copy of Sung Ha Park's dissertation proposal was distributed to his dissertation committee for approval. Members of the dissertation committee are: Dr. Jeff Woldstad (chair - Industrial Engineering); Dr. James Smith (Industrial Engineering);

Dr. Jerry Ramsey (Industrial Engineering); Dr. Patricia DeLuca (Psychology); and Dr. Peter Westfall (Information Systems and Quantitative Sciences). On October 24, 1997, Mr. Park successfully defended his dissertation proposal before this committee and received final approval for conducting the proposed experiment. In addition, the proposed experiment formally approved by the human subjects Institutional Review Board at Texas Tech University.

Data Collection (in progress)

Data collection for this project has begun. Final preparations for the experiment took longer than anticipated, however, we still anticipate finishing the data collection component to this project during the upcoming quarter.

Safety and Reliability:

The self-assessment of survival (reliability) project demonstration unit has been completed to the point of functional demonstration. In its current state, it contains a physical sensor, a data collection module, prediction and calculation models, and computer interface screens. The hardware and software are integrated with Labwindows hardware and software, respectively. Initial operations utilize an exponential smoothing model, with basic neural network model research on-going.

The project demonstration unit is an integral part of Mr. H. Lu's doctoral research program. Mr. Lu plans to defend his research work sometime in December or January.

Once Mr. Lu's work is completed and defended, Task 1.C will be completed.

As an extension and application of this research, starting in January, this technology will be applied to human reliability, as a part of "Human Reliability and safety for Safe Handling and Long-Term Storage of Nuclear Components" - co-PIs W. Kolarik, J. Woldstad, and I. Hamilton.

Add contact/impact model & system compliance to simulation testbed:

One Ph.D. and two M.S. theses are being completed or defended at the time of this writing. In these projects the theory and algorithms needed to completely model the frictional contact/impact of robots and machines (flexible and rigid) as they interact with a work space are being developed and verified. In the Ph.D. thesis the tools needed to model the impact of multiple flexible bodies are being fine-tuned and experimentally verified. In the first MS thesis the problem of predicting the motion of an object being manipulated by a robotic hand is addressed. Numerical studies are provided. Finally the last MS thesis examines the problems associated to modeling flexible bodies in closed kinematic loops, where the loop closure occurs in the domain of the flexible members; experimental verification is provided. All these tools will allow the precise modeling of the interaction of machines with the payload and environment; which has ultimate application in the machine/ control design and safety and hazard analysis.

Development of Nondestructive Assay Methods

PI: N. M. Abdurrahman, Ph.D., The University of Texas at Austin

Co-PI: B. W. Wehring, Ph.D., The University of Texas at Austin

Ayman Hawari, Raul Radulescu

During this quarter the setup and testing of the neutron generator and the slowing down time spectrometer continued. Several issues were addressed and completed:

1. The vacuum system for the generator was improved by the installation of a new ion pump. This enabled us to reach vacuum levels of around 1.2×10^{-6} Torr on routine bases. The value of the vacuum rises to around 4×10^{-6} Torr upon the introduction of deuterium into the system.
2. A new circulating cooler was installed for cooling the turbo pump and the bending magnet. The closed loop cooling system was tested and is functioning successfully.

3. A complete interlocking/radiation monitoring system was installed and successfully tested. The system prevents operation if a radiation level above 20 mrem/hr is reached and/or if a person attempts to enter the high radiation area during operation.
4. Prepared and filed the application for certification to operate the neutron generator. In September of 1997 NETL was granted the required State of Texas certification for the operation of the neutron generator. This allowed us to test the operation of the neutron generator, and successful generation of a deuterium beam was achieved.
5. Currently we are preparing for the initial generation of a pulsed neutron "beam". We plan to test the pulsing system, install beam diagnostic devices (e.g., faraday cups and quartz viewing windows), and a neutron target during the month of November, 1997. Our data acquisition system is also being prepared for testing (this includes the radiation detectors, electronics, a digital oscilloscope, and a computer). The pictures below show the slowing down time spectrometry setup including the graphite pile as of October 31, 1997.

Computationally, we focused our MCNP work on modeling realistically our experimental setup in order to use the results as a benchmark to guide our laboratory work. This work is currently completed and we have started our analysis of the results. Our objective is to combine the results of these calculations with experimental measurements before the end of 1997.

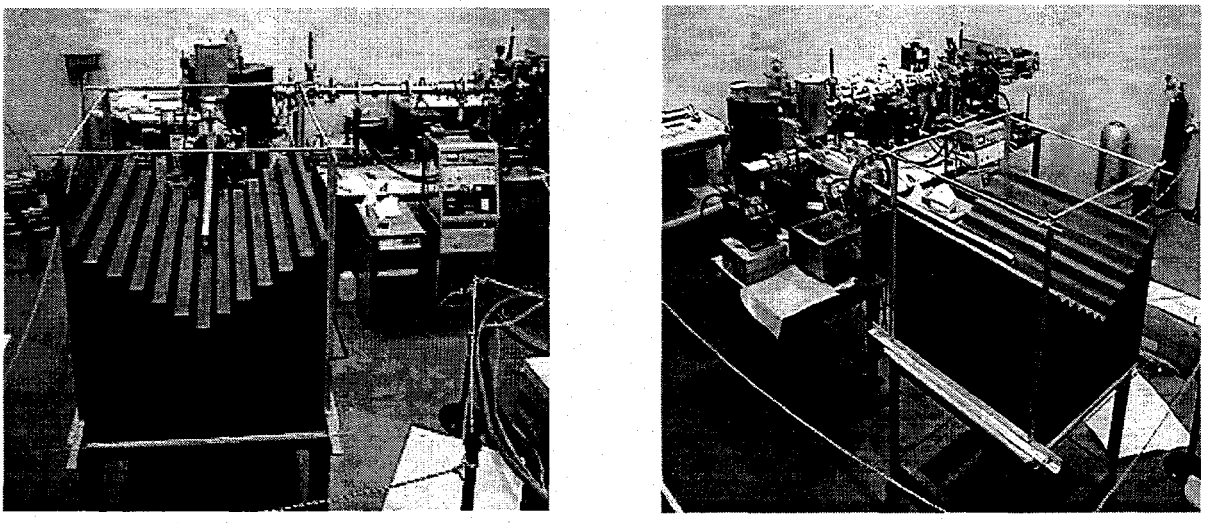

Figure 1. The Slowing Down Time Spectrometer facility setup including showing the neutron generator and the graphite pile currently under construction at the Nuclear Engineering Teaching Laboratory of The University of Texas at Austin.

STORAGE: FACILITY ANALYSIS

Aircraft Overflight

PIs: .C. Rock, The Texas A&M University ; M.T. McNerney, The University of Texas at Austin

Our effort this quarter focused on two areas: refinement of estimates used in current (and future) models, and refinements of the models themselves. Improved probabilities and rates for accident analyses in the SWEIS were captured in the deliverable report mentioned below. Model improvements are being documented in the form of a tutorial on the statistics contained within DOE Standard 3014-96: *Accident Analysis for Aircraft Crash into Hazardous Facilities.*

As part of the refinement of estimates, we reviewed the data contained within the support document for DOE Std 3014-96. We excluded retired aircraft and recomputed Pantex crash rates based on aircraft currently flying in Amarillo airspace. The results appear in "Improving Aircraft Accident Forecast-

ing for an Integrated Plutonium Storage Facility", a deliverable intended to help the Pantex Aircraft SAR contractor refine aircraft accident evaluations at Pantex. Further refinement of military crash rates is possible. To this end, we are reviewing the Sandia Lab files of Air Force accident data assembled by Y. T. Lin. Unfortunately, we have his data in hard copy only, not in a computer format that would streamline necessary sorting and analysis. We are examining the possibility of obtaining the data directly from the military.

We focused our model refinement efforts this quarter on developing alternative impact frequency and release frequency models which allow for more realistic assessments of these rare events. These are documented in the tutorial report listed under the first milestone, below. We continue to examine skid models with stochastic elements in order to produce skid distance distributions, allowing the development of confidence intervals.

Publications and Presentations

A review draft "Improving Aircraft Accident Forecasting for an Integrated Plutonium Storage Facility" has been sent to Dr. Carl Beard in Oct. 97 and the final to Ms Gia Alexander Nov. 97 for processing. We expect on-time delivery to the Center to meet our promised Jan 98 schedule. This report should be forwarded to Terry Zimmerman for his use in managing the Pantex Aircraft SAR contract.

Mathematical derivations for "A Tutorial On Using Bayes Rule for Aircraft Accident Modeling" are now substantially complete. We expect submission not later than Jan 98 in form of peer reviewable journal article. The title may change. One option is: "Accident Analysis for Aircraft Crash into Hazardous Facilities: A Statistical Primer".

"Bounding Model for Aircraft Skid Distance". Due to new understanding of the problem, this intended journal article needs some additional work. Anticipate Mar 98.

"The Modified Four-Factor Model" — partially complete; expected delivery in June 1998. This manuscript will extend the concepts found in the Tutorial paper from point estimates to density function estimates.

Aerosol Dispersal Analysis

PI: D. Klein, Ph.D., The University of Texas at Austin

Co-PI: S. Manson, Ph.D., The University of Texas at Austin

This research has been undertaken to augment the computational models currently used to perform safety analyses of the PANTEX cell facilities. In the event of a contained chemical explosive transient during disassembly activities, there is some concern that a release of Pu aerosols may result. The computational modeling of some accident scenarios has been limited by the one-dimensional approach of the MELCOR code. This approach may be adequate in narrow rampways and through leakage sites, but the flow in the cell room itself is clearly multidimensional. This flow controls the mixing of particulates and the air, and hence is crucial to modeling aerosol transport. Furthermore, depressurization of the cell room is accomplished over relatively long times (>10 seconds), by both the leakage of air to the environment, and the cooling of hot gases through natural convection to the cell walls. This natural convection heat transfer is also multidimensional in character. Thus, this research effort will apply modern computational techniques to post-explosion transient flow in cell facilities.

In the past quarter, research efforts have centered on the completion of the final stage of this research effort. A doctoral dissertation entitled "Numerical Analysis of Two-Dimensional Natural Convection Heat Transfer Following a Contained Explosion" is now in production, and is expected to be completed in December, 1997. This document is approximately 60% complete.

STORAGE: STORAGE/SHIPPING CONTAINERS

Radiation Degradation

Co-PIs: R.R. Hart, The Texas A&M University; K. Ünlü, The University of Texas at Austin; G.O. Carlisle, West Texas A&M University

The investigation into material problems in stainless steel that may result from high fluence alpha particle irradiation continued this quarter. The efforts were concentrated on preparation of additional samples and the improvement of the techniques employed.

A new batch of SS-316 samples were prepared for implantation with high fluence He-3 ions. The aim is to assess differences observed in the surface structure of the samples during previous work. Special emphasis was placed on eliminating auxillary effects, like cleaning agents, that might contribute to the generation of residue like structures on the sample surface. One of the objectives this quarter has been on improving the depth resolution of the UT-NDP facility. For this purpose a partially depleted surface barrier detector (Ortec Ultra series) was tested. Work is on going to install different type of detectors and to compare the results for better resolution using a reference sample.

The electron microscopy part of the study progressed with emphasis on optimizing the operating parameters of the TEM sample preparation and choosing an electrolyte that gives good results for TEM observations. A number of samples were prepared for SEM and they will be implanted with He-3 ions. Currently the implantation of He-3 ions into the new set of samples has been somewhat slowed down due to temporary dedication of implantation facility to Ga work.

Publications and Presentations

An Internal Technical Working Document (ITWD) entitled "Electron Microscopy Study of Stainless Steel Radiation Damage Due to Long-Term Irradiation by Alpha Particles Emitted from Plutonium" was submitted in July 1997. This report includes preliminary SEM and TEM observations of implanted and unimplanted stainless steel samples.

A Paper entitled "Alpha Radiation Damage in Plutonium Encapsulating Materials," by Kenan Ünlü, Mehmet Saglam, Ron R. Hart and John Shipp was presented at the Plutonium Future-The Science Conference, Santa Fe, New Mexico, August 25-27, 1997 [Plutonium Futures-The Science Conference Transactions, LA-13338-C, 123 (1997)]

Air Monitoring

Co-PIs: H.M. Liljestrand, Ph.D., The University of Texas at Austin; P.K. Dasgupta, Ph.D., Texas Tech University

During the previous reporting quarter, we had fabricated combined aerosol collection and analysis system. The current quarter was earmarked for evaluation of the combined system. We have completed the performance evaluation and the system is capable of conducting sensitive measurement.

Evaluation of the combined system was conducted by sampling Ce(III) containing test aerosols. Ce(III) aerosol was generated in laboratory, as explained in the February report. In order to generate low concentrations of Ce(III) in various aerosol size and concentration, supporting matrix such as sodium sulfate was used in the aerosol generating solution. Tested aerosols contained particles in the size range of 0.2 – 1 μm mass median aerodynamic diameter. The Ce (III) concentration of the tested aerosol was in the range of 50 pg/m^3 – 7.5 ng/m^3. Blank aerosol was generated by nebulizing pure water with zero air (from AADCO 737 Pure Air Generator). Fine tuning of the coupled system reduced noise levels to a minimum and thus we could get very good detection limit. Calculated detection limit for aerosol Ce(III) measurement is 15 pg/m^3 with an air sampling rate of 10 L/min combined with sample concentration for five minutes. Increasing aerosol sampling rate and concentrating the sample for longer duration will of course further decrease the detection limit. The response is near linear in the range of tested aerosol concentrations and can be fitted in to an equation. Day to day variations of the aerosol analysis is better than 5% and includes the variations in aerosol generation.

In-house performance evaluation of the combined aerosol collection analysis system is now complete. Sensitive, reliable aerosol measurements can be made with the combined system.

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

PI: William H. Marlow, The Texas A&M University

The Ludlum electrometer board which was delivered and implemented in the measurement system, as reported in the last Quarterly Report, failed to provide consistent results. Consequently, it has been replaced by two Canberra preamplifiers. Though not ideal because the distances from the detection electrodes to the preamplifiers are longer than normally used, this setup does function as required. In addition, we have corrected persistent problems with external noise, atmospheric leaks in the chamber lid, and some problems of geometry related to alpha source location and ionization current detection. Using this system, we have measured the ionic and the electronic pulses originating from alpha decays and the results are similar to what was calculated and reported earlier by Lu and Marlow under this project (*Technical Summary: Feasibility Study of Conductivity Monitoring for Leak Detection in Double-Walled Plutonium Containers*, ANRCP-NG-ITWD-97-05). Measurements following from the resolution of these problems have revealed the expected high dependence on the electron scavenging capabilities of atmospheric air and a dependence on the separation of electrodes relative to the alpha source.

We are preparing to measure the ionic and electronic pulses simultaneously, in the presence of atmospheric air and in pure argon, and to modify electrode geometries. With the information developed from these measurements, we will determine the experimental parameters required to complete the model of Lu and Marlow in fulfillment of the Deliverable originally scheduled for completion in October, 1997. Finally, these results will also enable us to collaborate with Sandia in the design of a demonstration system for measuring container leaks as originally specified for the November, 1997 Milestone.

DISPOSITION: WATER REACTOR OPTIONS

Mixed-Oxide Fuel Fabrication: Gallium Removal and Interactions with Zircalloy Cladding

Co-PIs: N. M. Abdurrahman, The University of Texas at Austin; M. L. Adams, The Texas A&M University

There was considerable activity on the gallium-removal task this quarter. All of the quarter's milestones on FTIR analysis and surface area measurements have been achieved. The Center researchers presented papers at conferences in August and October, describing recent experimental results from a simple thermal process that was first suggested by LANL researchers and then enhanced by the Center researchers. (See a later section for more details on experimental results obtained during the quarter.) The Texas A&M team has been conducting three to four gallium-removal experiments per week, then using BET to analyze surface area and pore size and FT-IR and AA for elemental analysis. Selected samples have been sent to Texas Tech University for additional analysis using ICP. A tubular furnace suitable for gallium collection has been repaired and is now ready for use. A preliminary design for a furnace collector is prepared and it will be presented to LANL in the next meeting for the approval of LANL researchers.

Progress continued on beam-driven studies of the interaction of Ga with fuel cladding. A Zirc-IV sample has been implanted in two areas with 100 keV Ga ions to fluences of 5E17/cm2. The sample was maintained at a prototypical temperature of 400 C during the implantations. One area is to be implanted with an additional fluence of 140 keV Zr ions to produce lattice displacements equivalent to those produced by fission fragments during reactor irradiation. However, we are still experiencing difficulties obtaining the high intensity Zr ion beam needed. In this regard, work is continuing on ion source modifications. Also, computer modeling of fission-fragment-induced lattice displacements in zircaloy is continuing.

Publications and Presentations

The paper, "Solid/Gas Phase Catalytic Reduction for the Clean Separation of Gallium from Gallium Oxide/Plutonium Oxide" was written by C.V. Philip, W.W. Pitt, K. Chung, and R.G. Anthony of Texas A&M University, was presented at the 'Plutonium Futures - the Science' Topical Conference on Pu and actinides, Hilton of Santa Fe, NM. August 25- 27, 97. The experimental results were presented indicating gallium can be removed from Pu by a simple thermal process. The findings describe the new process, which is an enhancement of a process first suggested by Los Alamos National Laboratory researchers. The paper indicates the new process is "cleaner, simpler, and more efficient than those based on existing techniques under evaluation."

Dr. R. G. Anthony attended the meeting "Tenth Symposium on separation science and technology for Energy Applications", Park Vista Hotel & Convention Center, Gatlinburg, Tennessee, October 20 - 24, 1997 and presented a second paper also titled "Solid/Gas Phase Catalytic Reduction for the Clean Separation of Gallium from Gallium Oxide/Plutonium Oxide". The latest data of Ga Removal project was included in the presentation. All the milestones on FTIR analysis and surface area measurements were reached as in the Task plan.

Amarillo researchers, C. V. Philip, R. G. Anthony, R. M. Roundhill and Carl Beard attended a meeting at Los Alamos National Laboratory on September 19, 1997 and discussed the designs of 'Gallium Collector' and the Horizontal Rotary Furnace. The work Texas A&M University needed shifting in the objectives to meet the new goals. Nine samples from 'Ga Removal Experiments' were sent to Texas Tech for ICP analysis.

Personnel Changes: Professor W. Wilson Pitt retired on August 31, 97. Dr. Rayford. G. Anthony, Charles D. Holland Professor and Head of department of Chemical Engineering, has replaced Prof. Pitt as the senior member of the research team. Dr. Sivaraj Chokkaram joined on August 15 as a post doctoral research associate (100% effort). Venkat Tulasi , an Electrical Engineering graduate student (20 hours/week) has joined the group on September 1, 1997. Dr. C. V. Philip and Christopher Krampitz, a Chemical Engineering undergraduate student, are continuing.

Results from Gallium Removal Experiments:

1. Safe gas (6%H2 in argon) removes gallium from 10% Ga_2O_3 in CeO_2 mixture at 900°C and metallic Ga Collects on Copper wire. The gas stream should be free of any Oxygen. Even traces of oxygen interfere with Ga Removal efficiency.

2. Ga droplets collected on Copper wire is an alloy with copper. $CuGa_2$ has a melting point of 550. Melting point of CuGa is 650°C. Since the melting point of 'Ga Cu alloy droplet is around 650°C and from the phase diagram we can conclude that CuGa is the main product formed at 900°C. The AA analysis at Texas A&M University showed 40% wt. Ga and 60% wt. Cu in the CuGa alloy bead. The ICP results from Texas Tech will be used to verify the results.

3. The CuGa alloy droplets have very high viscosity at 900°C and even vigorous shaking fails to drop the smaller droplets from Cu wire tips. As the weight of droplets increases above one hundred milligrams, it falls of >from the copper wire.

4. CeO_2 is probably reduced to Ce_2O_3 by the reducing the gas (6%H2 in argon) in the presence of Ga_2O_3. The color of the oxide mixture changes to dark gray. After cooling, the reduced oxide reacts wit air violently releasing heat forming a yellowish white residue. When CeO_2 is heated alone in 6%H2 in argon no color change was observed. Since Ce chemistry is less relevant to the objectives of the project, the details of Ce chemistry is receiving a lower priority

5. The surface area and pore size distribution of samples from Ga removal experiment are being measured using Micromeritic ASAP 2000 surface area pore size analyzer. Based on the limited number of samples analyzed, an average reduction in surface area from 16 m/g to low as 6 M/g was observed for the CeO_2 matrix left after Ga removal.

6. The diffuse reflectance accessory (DRIFT) is installed in Nicolet Magna 560 FT-IR spectrometer. Powder samples (100 mg) are filled in samples cups and the mid-range FT-IR spectrum of samples scanned. The work is only in its initial stage.

Mixed-Oxide Use In Reactors:
Water Reactor Options for Disposition of Weapons Plutonium
Co-PIs: N. M. Abdurrahman, The University of Texas at Austin; M. L. Adams, The Texas A&M University

The Center collaboration continued in the joint US/Russian effort to develop the capability to use weapons-derived MOX fuel in Russian VVER-1000s. Five Center researchers joined a six-member team from Russia and many researchers from ORNL at a meeting in Oak Ridge Aug. 24-28. The team discussed the joint team's code-benchmarking efforts of the past year and finalized plans for the coming year, which include further benchmarking, a beginning look at analysis of transients, and the preliminary design of a VVER-1000 lead test assembly. The Center researchers gave six presentations at the meeting, which were very well received. The joint team asked the Center researchers to further develop the SAXTON and ESADA benchmarks, focusing on the difficult problem of power distributions, and a great deal of progress was made on this effort during the remainder of the quarter.

During the last quarter, the Center project to study thermally-driven gallium-cladding interactions made substantial progress in experiment preparations. The full Phase III experiment is now expected to begin in February 1998. The 1/2 scale prototype in operation at the Nuclear Science Center has provided valuable operational and safety data. A heat transfer modeling program has been written and is being compared to the prototype data. The lead-bismuth cooling system is exceeding expectations. A cladding compatibility test is scheduled to begin in late November. The experiment data acquisition program and instrumentation have been improved for greater flexibility and capabilities. Using supplemental funding provided by ORNL, the power supply and a set of six heaters have been ordered for an expected delivery date in early December. The final experiment matrix has been determined in collaboration with ORNL. LANL is preparing to press pellets (which will use cerium as a surrogate for Pu) for delivery in late January, 1998.

The Center water-reactor team began work on "flexible fuel cycles" during the quarter. (This work is funded by a direct contract from ORNL.) Work began October 1, and by October 31 a detailed HELIOS model of a Westinghouse UO_2-fueled PWR assembly had been developed and debugged. HELIOS is the code chosen by ORNL as the primary assembly-level transport code for this project. The Center researchers compared HELIOS results against those from CASMO-3, and found small discrepancies that are completely consistent with results obtained by previous researchers working with these codes. Also, work started on building the MOX assembly model that would be needed for the project. Finally, the transport code WIMS-7 was received and successfully installed. This code has been chosen (in a collaborative decision with ORNL) for some of the assembly-level calculations for this task.

The task on studying the feasibility of using a reactor to simultaneously generate electricity, burn weapons-grade MOX fuel, and produce tritium was completed early in the quarter. The final report of the project is being prepared as a Center report and will also be submitted to a technical conference in the near future. The conclusion of the study was that MOX fuel could probably be utilized in a tritium-producing PWR with no adverse effects.

Mixed-Oxide Use in Reactors: Mixed Oxide Fuel Evaluation
PI: K. L. Peddicord, The Texas A&M University

This quarter the work on the project has shifted to direct collaboration with Belgonucléaire in Brussels, Belgium. The documentation for the work permit for John Alvis which had been submitted to Belgian federal authorities was approved. On September 9, 1997, Mr. Alvis took up residency in Brussels. This was in accordance with the Memorandum of Agreement between Belgonucléaire and the Texas Engineering Experiment Station signed earlier this year. At Belgonucléaire, he is working principally with Marc Lippens who is in charge of fuel performance modeling. The modeling work is based on

irradiation data owned by Belgonucléaire from tests the company has conducted in-house and in co-operation with international partners. The first phase of the work is dealing with low temperature fission gas release at high burnups. Mr. Alvis' work will be to develop high burnup thermal models for oxide fuel. In exchange, BN will provide the COMETHE fuel performance code for five years to analyze the behavior of weapons MOX fuel in light water reactors.

Because of the delay in the issuing of the work permit, the milestone/deliverable list of the Task Plan has been revised accordingly to reflect the timetable for the work in Belgium and is shown below.

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 work this past quarter has been to initiate the development of models of the thermal behavior of oxide fuel at high burnups typical of current LWR's. These models will be used for the subsequent thermal and mechanical analysis.

A significant point was reached during this Quarter on September 9, 1997, when John Alvis took up residence in Brussels, Belgium, to work directly with Belgonucléaire (BN). This came after a lengthy process in which he had to submit voluminous paperwork to the Belgian federal authorities to receive his work permit. At Belgonucléaire, he is interacting with Marc Lippens who directs the fuel performance modeling group at BN. At this point the project moved into the phase of developing models for the thermal behavior of oxide fuel at high burnups. The initial work is focusing on high burnup, low temperature cases and identifying the impact of current thermal models on fission gas release under these conditions. This will provide a basis for high burnup thermal model development.

Three additional activities related to the project were initiated during the quarter. Two students, Pavel Medvedev who is studying for his Ph.D., and Phillipe Bellanger, who is working towards his M.S., are receiving financial support from the Department of Nuclear Engineering and are working on topics related to MOX fuel performance evaluation. The three topics of investigation are:

Conducting a detailed review of the fission process and the fission product spectrum of uranium-225 and Pu-239 fission. This will provide a rigorous physical basis for assessing differences in behavior between UO_2 and MOX fuel.

Identifying and collecting literature of work done in France on MOX fuel performance modeling with a particular emphasis on the METEOR/TRANSURANUS code system. This will provide a basis of comparison with the COMETHE code. Emphasis is being given to articles and reports published in French. Contact has been established with Electricité de France and the Commissariat à l'énergie atomique.

Identifying and collecting literature of work done in Russia on UO_2 fuel performance modeling with a particular emphasis on the START code. This information will be helpful in modeling the behavior of weapons MOX fuel in VVER-1000 reactors . Emphasis is being given to articles and reports published in Russian. Contact has been established with the Kurchatov Research Centre and the Bochvar Institute of Inorganic Materials which are the lead organizations in Russia on fuel element modeling.

Now that John Alvis is at Belgonucléaire, the milestone/deliverable list of the Task Plan can be revised in accordance with the new schedule.

DISPOSITION: NON-PROLIFERATION/TRANSPORTATION

Transportation Analyses: Transportation of Mixed-Oxide Fuel

PI: H.S. Mahmassani, Ph.D., The University of Texas at Austin

The general objectives of the Transportation Analysis effort under the Nuclear Project is the identification and study of transportation-related issues that arrive in conjunction with the disposal of spent Pu. These issues are integrally related to the identification and quantification of the various sources and types of risks that accompany the movement of radioactive materials. These include risks that arise from the behavior of the materials transported, and that of the storage containers used, as well as the

interaction of these with external risk sources associated with vehicular reliability, traffic conditions and possible external threats. Several components of this overall project are addressing the source of these risks, but not all. The second major element of the transportation analysis is the development of strategic and related algorithmic procedures to incorporate these risks in decision-making regarding route selection before the shipment is sent, as well as regarding route modification in real-time as the conditions that affect these risks and their consequences change, to the extent that information becomes available. A third and equally important element pertains to the manner in which associated risks associated with a particular shipment are framed, communicated to and perceived by the population likely to be involved in the process of route selection and/or consequence management.

The present study aspires to be comprehensive in its outlook and scope, but has had to limit its focus to specific risk elements, and to the development and adaptation of modeling methodologies with specific application to the transport of spent Pu. A major aspect of this effort is to identify and characterize the vast and complex regulatory framework applicable to the transport of radioactive substances, and incorporate these considerations in any mathematical or algorithmic set of decision support procedures. In addition, the project has all along sought to complement the existing set of tools developed by DOE and its laboratories, such as TRANSNET and RADTRAN, by expanding the ruleset underlying route selection and evaluation to recognize different types and/or levels of risks, as well as the dynamic nature of these risks.

Each project task is discussed separately in the following sections.

Modeling for Safe Routing

PI: H. S. Mahmassani, The University of Texas at Austin

During the period August 1 to October 31, 1997, the effort at UT-Austin focused on completing a report describing the a priori routing algorithm for strategic nuclear materials developed as part of *this* study. The model enables more thorough risk assessment of potential highway routes than existing procedures. Unlike the current routing models, HIGHWAYS, that is used by the Department of Energy, this routing algorithm can find the shortest-cost route in a network where cost may be specified as the travel time, population density, or any other user-defined non-negative "cost" function. A second advantage of this model over the current HIGHWAYS models is that it permits travel times and population densities to vary over the day. Curfews, or avoidance of large cities during certain hours of the day, and waiting at nodes are also incorporated in the TDLCP algorithm.

The report describes a test application of the model to a real highway network extending from the Pantex Plant in Amarillo, Texas to the Savannah River Site in Aiken, South Carolina. In this example, cost was defined as the residential population living within one mile of a highway link.

The report completed in this period has been submitted for review.

Publications and Presentations

Ms. Elise Miller-Hooks and Hani S. Mahmassani paper titled "A Priori Least Expected time Paths in Stochastic Time-Varying Networks," was presented at the INFORMS Dallas Fall Meeting, Dallas, Texas, October, 1997.

Ms. Elise Miller-Hooks and Hani S. Mahmassani paper titled "Optimal Routing of Hazardous Materials in Stochastic, Time-Varying Transportation Networks," was accepted by the Transportation Research Board for presentation at the 77th Annual Meeting of the Transportation Research Board in Washington D.C. in January of 1998 and publication in the Transportation Research Record.

A final report, "Routing Criteria and Models for Radioactive Material: A Review, co-authored by Laurie A. Bowler and Hani S. Mahmassani, Technical Report # ANRCP-NG-TWD-97-8 was published as part of the Amarillo National Resource Center for Plutonium Nuclear Group Internal Teaching Working Documents, September 9, 1997.

Ms. Laurie Bowler, under the supervision of Hani S. Mahmassani and Chandler W. Stolp, completed her thesis report "Routing of Radioactive Shipments in Networks with Time-Varying Costs and Curfews," August 1997.

Modeling for Safe Routing

PI: Paul Nelson, Ph.D., The Texas A&M University

All work on this task was completed in July 1997 with the publication of the following final report: "Risk Analysis of Shipping Plutonium Pits and Mixed-oxide Fuel," A. B. Caldwell, Texas A&M University, July 3, 1997. (ANRCP-NG-ITWD-97-07).

Application of Existing Codes and Techniques

Co-PIs: R. Radha, Ph.D., and Z. Huque, Ph.D. Prairie View A&M University

Progress has continued on Transportation Analysis and application of codes and techniques. During the period of August 1 to October 31, 1997, Mr. R. Santappan, a graduate student in Civil Engineering at PVAMU, used the TRANSNET program and especially the Highway Program to determine safe routing. The results were compared with an alternative mode of transportation. This comparison included the evaluation of Highway Program results with the results obtained using Railroad Routing model-Interline.

Efforts continue to estimate the population along the selected route and population exposure to potential radiation by considering a corridor width along the route. This evaluation will enable avoiding dense population areas and keeping potential impact on the population as low as possible due to transportation of Pu pits and mixed oxide fuels along the selected routes. The planned completion date for Master's thesis by the graduate student is Summer 1998.

Investigation of Neural and Fuzzy Logic Analysis Techniques for Surety Issues in Transportation of Nuclear Materials

PI: D.C. Wunsch, II, Ph.D., S. Texas Tech University

Few training techniques are available for neural networks with fuzzy number weights, inputs, and outputs. Typically, fuzzy number neural networks are difficult to train because of the many a-cut constraints implied by fuzzy weights. Introduction of a weight representative that simplifies the constraint questions was developed. A constrained form of back propagation was then developed for fuzzy number neural networks. Weight representation allowed use of the additional a-cut constraints during a weight update. A paper titled "Training Fuzzy Number Neural Networks Using Constrained Backpropogation," by Dunyak, J. and Wunsch, D., was produced as a result of this research effort which was submitted to and is currently under review by the 1998 World Conference on Computational Intelligence.

A new theory of independent fuzzy probabilities, that addresses limitations of both fuzzy fault trees and Zadeh's fuzzy extension of probability is underway. In contrast to the fuzzy fault tree approach, the new theory is complete since it assigns a fuzzy probability to every event. In the case of a probability theory built from independent events, Zadeh's extension is not consistent with fuzzy fault trees, whereas the new extension is also consistent. A paper titled "Safety Analysis of Redundant Systems Using Fuzzy Probability Theory, co-authored by Dunyak, J., Saad, I. W. and Wunsch, D., was presented and published in the Proceedings of the High Consequence Safety Symposium II at Sandia Laboratory which details this new theory.

Milestone & Deliverables for this period: 1) "Safety Analysis of Redundant Systems Using Fuzzy Probability Theory," by James Dunyak, Ihab W. Saad and Donald Wunsch, published in the Proceedings of the High Consequence Safety Symposium II at Sandia Laboratory; and 2) Training Fuzzy Number Neural Networks Using Constrained Backpropagation," by James and Donald Wunsch, was submitted to the 1998 World Conference on Computational Intelligence, and is currently under review.

Development of Source Term Components for Formulation and Initial Release of Plutonium- containing Aerosol for Conditions and Effects Not Treated by Existing Models for Transportation Incidents

Co-PIs: W. H. Marlow, Ph.D., and Y. A. Hassan, Ph.D. Texas A&M University

Identification of cases to validate and assess the coupling between the particles with the fluid phase has been determined. The routines to present the patterns of the flows have also been identified. The progress toward determining the Pu particle patterns is continuing.

DISPOSITION: GEOLOGIC DISPOSAL

Immobilization: "Can-In-Canister" Option

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A paper detailing the glass system-level approximate thermal modeling effort (completed during the quarter ending 30 April 1997) was presented at the 1997 National Heat Transfer Conference held in Baltimore, Maryland in August. The paper has also been submitted for publication to the ASME Journal of Heat Transfer, and is currently in review.

High-temperature experiments with molten glass have continued. Flow visualization experiments were conducted to obtain air flow patterns around the falling glass jet. An apparatus was constructed to use thermocouples to obtain temperature measurements in the molten glass jet at various axial locations. Temperature profiles are being obtained for a glass jet with an inlet temperature of 1050 deg. C. A procedure for making mechanical test samples of the surrogate DWPF glass is under development. Preliminary mechanical test samples have been made to determine the optimum fabrication process to minimize void content. Data on the high temperature experiments were presented at the ASM/TMS 1997 Materials Week, Indianapolis, Indiana in September.

Progress continued on the room temperature experiments using silicone oil (Dow Corning 200 Fluid) with a viscosity of 60,000 cSt. Using a high speed camera (2000 frames per second, 8 seconds recording time), frequency and velocity measurements were performed. A wide range of mass flow rates was considered (5 to 35 g/s). No significant changes in the jet velocity at the landing region could be observed, consistent with the observation that the jet has reached a freely falling state. The average velocity was found to be 4.8 m/s with a range of uncertainty of plus or minus 0.4 m/s, whereas the Torricelli limit is approximately 5.8 m/s. From this it can be inferred that viscous drag plays a role in the velocity development. In another series of experiments, the oscillation frequency of the jet at the landing region was measured as a function of the mass flow rate. (The jet oscillates in a spiraling manner due to a viscous buckling instability.) The jet frequency decreases with increases in the mass flow rate, and can be described by a power law relation: $\log(f) = \log(C) + n \log(\text{mass flow rate})$, where f is the frequency in Hz, C is a constant equal to 635.9, n is the power law exponent and is equal to −0.3988, and the mass flow rate is measured in g/s. The above relation was found for a jet height-to-inlet diameter ratio of 142.

The computational fluid dynamics and heat transfer software package FLOW-3D (Flow Science, Inc.) was used to perform detailed modeling of the analogous fluid jet. Both 2-D and 3-D computational models have been developed, which predict the spiraling frequency of the landing jet with less than 10% error for the test cases considered. Now that the accuracy of these models has been quantitatively verified, their robustness will be investigated, and the physical conditions in the models will be gradually modified to approach the actual can-in-canister molten glass conditions.

Ceramic Materials for Immobilization of Plutonium

PI: A. Clearfield, Texas A&M University

Analysis of several phases of barium zirconate loaded with varying amounts of hafnium seems to indicate a limit of approximately seven percent hafnium substitution for zirconium. These samples were

synthesized by solid state methods. Further experiments will be carried out with "dirty" zirconium oxide to determine if the seven percent limitation is produced by the synthetic method. Due to the apparent low substitution limit of hafnium in the zirconate phase, experiments with gadolinium as the neutron sorber have proceeded. Initial synthesis indicates at least a ten percent substitution of gadolinium for zirconium in the zirconate phase. Further experiments with higher gadolinium loadings have been completed and are in the process of being analyzed by powder X-ray diffraction. It is interesting to note that the Gd substituted samples are gray in color rather than the white expected for oxides. The source of this coloration has not yet been determined. We have also begun experiments using gadolinium in the zirconolite phase. Two syntheses, one calculated for ten percent Gd substitution in the Zr site, the other for substitution in the Ti sites, have been completed and X-ray data collected. the determinate of the siting of the gadolinium in the lattice is being pursued by Rietveld refinement based on the X-ray powder patterns. The sample in which Gd substituted for Zr was pure white while substitution for Ti yielded yellow products.

Disposal: Disposition in Deep Boreholes

Co-PIs: R.T. Johns, Ph.D., and M.M. Sharma, Ph.D., The University of Texas at Austin

Research activities in this quarter focused on the completion of a conference paper and its presentation. The paper - Effect of Pre-Test Pressures and Temperature on Drill Stem Test Interpretation - was accepted and presented this fall at the Society of Petroleum Engineers (SPE) conference in San Antonio, Texas. A second paper - Interpretation of Sequential Hydraulic Tests in Low-Transmisivity Fractured Media - was submitted to *Water Resources Research*. This last paper presents a new analytical solution for the interpretation of low-permeability hydraulic tests in potential nuclear waste repositories and demonstrates the use of the solution on real test data from a hydraulic test in Switzerland.

Future Work

The project is scheduled to close on December 31st of this year. A final report will be written that details the results and conclusions from this project.

ACRONYMS

3-D	Three Dimensional
AC	Amarillo College
ANCRP	Amarillo National Resource Center for Plutonium
BN	Belgonucléaire
CET	Communication, Education, and Training
CET&CI	Communication, Education, Training, and Community Involvement
Cr	Chromium
DOE	U.S. Department of Energy
DRIFT	Diffuse Reflectance Accessory
EIS	Environmental Impact Statement
EPA	Environmental Protection Agency
EPR	Electron Paramagnetic Resonance
ERL	Electronic Resource Library
FCR	Ferric Chelate Ruductase
FLOW	Flow Science, Inc.
FY	Fiscal Year
GAC	Granular Activated Carbon
HE	High Explosives
HPLC	High Performance Liquid Chromatography
IAST	Ideal Adsorbed Solution Theory
INPE	Institute of Nuclear Power and Engineering
INSTN	Education Training Branch of the French CEA
ITWD	Internal Technical Working Document
KFDA	Channel 10–Amarillo, Texas
KGNC	Radio 97.9–Amarillo, Texas
KVII	Channel 7–Amarillo, Texas
LANL	Los Alamos National Laboratory
LWR	Light Water Reactor
MAUA	Multi-attribute Utility Analysis
MEPhi	Russia's Moscow Engineering Physics Institute
MOX	Mixed-Oxide Fuel
NATO	North Atlantic Treaty Organization
NG	Nuclear Group
OSTI	Office of Scientific and Technical Information
PANTEX	Pantex Plant
Pu	Plutonium
PVAMU	Prairie View A&M University
RNA	Ribonucleic Acid
SPE	Solid phase extraction
SSCS	Storage System Construction Set
TAMU	Texas A&M University
TexPREP	Texas Pre-Freshman Engineering Program
TNT	Ammonium Nitrate Explosive
TTU	Texas Tech University
U	Uranium
UT	The University of Texas at Austin
UT-NDP	The University of Texas at Austin-Neutron Depth Profile Facility
VR	Virtual Reality
WT	West Texas A&M University
WTAMU	West Texas A&M University
WTEP	West Texas Environmental Project

INDEX