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Resource Center for Plutonium**

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

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PLUTONIUM INFORMATION RESOURCE

ELECTRONIC RESOURCE LIBRARY

Electronic Resource Library

Pls: Mr. G. Huffman; K Ruddy, Ph.D., Amarillo College; D. Cluff, Ph.D., Texas Tech University

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

Summary of activities for the reporting period:

- Amarillo College (AC) met established deliverables.
- Texas Tech University (TTU) continues development of the PuCAT citations database.

Texas Tech University (TTU) ERL activities:

- Retrieval sets from International Nuclear Information System (INIS) and National Technical Information Service (NTIS) on plutonium indicate that there are a total of 32,074 records from INIS from 1976 through March of 1997. Of this total 24,498 are in English. Other notable languages include: Chinese, Czechoslovakian, French, German, Japanese, Portuguese, and Russian. NTIS displays 7,744 records on plutonium for 1983 through 1997.
- The production sequence for moving citation retrieval sets through ProCite software into a final PDF electronic file bibliography was finalized. ProCite allows merging of retrieval sets, elimination of duplicate records, and production of formatted bibliographies that include all abstracts and indexing terms when such are available.
- TTU working with the Amarillo site and the Adobe help desk to correct a problem encountered with the Adobe Capture software.
- TTU working with both Silver Platter CD-ROM publisher and the Amarillo site to thoroughly test recently loaded beta software.
- Test files of various output types were delivered to Amarillo site.
- Relocation of the entire computer laboratory from the Library basement according to the renovation schedule for Tech Library made a check of all software and computers to ensure proper operation necessary.

Amarillo College (AC) ERL milestones and deliverables:

Deliverables on Tasks 1 - 4, 6 and 7 were met earlier than expected and reported in the 1997 2nd quarterly report. For Task 5 -- ERL collaboration throughout DOE-complex to establish cooperative linking for full-image titles is well under way. Milestone collaborative efforts with Los Alamos National Laboratory (LANL) and with the DOE Office of Scientific and Technical Information (OSTI) below indicate the kind of work accomplished in this area.

- Signed contract with OSTI for delivery of original paper documents on the topic of plutonium for scanning into the ERL COLLECTION.
- Received first delivery of OSTI documents from Oak Ridge, Tennessee., and entered them into scanning/conversion process to TIF (tagged information file, an industry standard graphic format) level for prioritization and review of Criteria Verification Team.
- Began collaboration with LANL Technical Library project "Library Without Walls" to establish a collection development network.
- Linked all ERL collection documents on on-line catalogs via Z39.50 interface.
- Registered ERL with OCLC on-line services, DOE offices and national labs.

- Contec of North America software installed and ERL site customization begun. Software tracks and accounts for requests of copyrighted materials with full cooperation from publishers and authors. It will be implemented in the Electronic Reserve Room private pages of the ERL.
- Scanned, processed and posted to the PuCore COLLECTION in the ERL a total of 12,000 electronic pages. The Document Exchange Laboratory (DEL) at Amarillo College expects to significantly exceed the goal of adding 16,700 electronic pages the ERL for FY97.
- Began loading, integrating and processing files received from TetroTEC Company in Washington, DC for electronic-file-to-electronic-file exchange into PDF (portable document format) files for Web processing.
- Working to obtain paper documents on the topic of plutonium from Department of Defense Technical Information Center (DTIC) database.
- Internet home pages were built with "hot-links" that assists the ERL with services for: (a) web site development, (a) content development, (c) research and development, and (d) the Document Exchange Laboratory.
- Customized software programs for ERL/DEL Site Management in these areas: (a) DEL collection Builder, an automated system for creating bibliographic citations for processing titles for the COLLECTION pages, and (b) ERL/DEL Document Processing Form, streamlines the document-scanning work flow, enabling staff to automatically generate FORMS for sets of documents.
- Hardware and software for establishing a fire wall to prevent unauthorized access to the ERL/DEL machines and programs was installed.
- Progress was made toward the implementation of an on-line, automated HELP system for the ERL pages. An on-line INDEX to the ERL pages is also in the planning stages.
- Plans to incorporate the Mixed Oxide Fuel Data Repository (MOXDAR) project into the ERL - FY98 were formalized.

ADVISORY FUNCTION

DOE SUPPORT

Multi-attribute Utility Analysis (MAUA) Team

PI: J.S. Dyer, Ph.D., The University of Texas at Austin

Analysis and Selection of Alternatives for the Disposition of Surplus Plutonium

Our primary goal was accomplished and we recently completed and forwarded a report titled, "Analysis and Selection of Alternatives for the Disposition of Surplus Plutonium," to the Center. With the generous help of Beth Perry, Information Resource Specialist for the Center, this report was revised and prepared for publication. It now appears on the Center's web site, and was distributed in paper format.

The results of our study were presented at the July International Workshop on Decision Analysis Applications in Madrid, Spain. Currently, we are preparing a brief version of the paper for publication in Operations Research. We are also planning to present the results at the Institute for Operations Research and Management Science and Decision Sciences Institute conferences during the Fall of 1997.

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 HE by Adsorption and Biodegradation on GAC

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

During this quarter, rapid small scale column tests (RSSCTs) and single component adsorption isotherms for RDX and HMX were completed. For the isotherms, seven different bottle point tests were conducted, using two different waters (deionized water buffered at pH 7, and uncontaminated perched aquifer groundwater from well PTX10-1007) and two different granular activated carbons (Calgon F400 and Northwestern LB-830). LB-830 is used now at Pantex.

Compound	GAC	Water/pH	K (mg/g)(L /mg) ^{1/n}	1/n
RDX	F400	deionized, pH 7	88.7	0.286
RDX	F400	groundwater, pH 8.3	129	0.348
RDX	LB-830	deionized, pH 7	124	0.212
RDX	LB-830	groundwater, pH 8.3	260	0.569
HMX	F400	deionized, pH 7	215	0.241
HMX	F400	groundwater, pH 8.3	318	0.367
HMX	LB-830	groundwater, pH 8.3	217	0.313

Figure 1

The isotherm data were fit to the linearized Freundlich isotherm equation ($\log q_e = \log K + (1/n)C_e$ where q_e is the equilibrium solid phase concentration (mg/g), C_e is the liquid concentration (mg/L)) and the isotherm parameters (K and 1/n) were calculated. These parameters are summarized in Figure 1. For each test, a minimum of 11 data points was used for parameter calculation. With the exception of the RDX in deionized water with LB-830, data fit was good ($R^2 > 0.87$).

As expected, HMX is more strongly adsorbed than RDX under similar conditions. However, some results apparently contradict results of RSSCTs performed earlier this summer. RSSCTs indicated that Calgon F400 was superior to Northwestern LB-830, while the isotherm experiments indicate the opposite. Additionally, both HMX and RDX were adsorbed to a greater extent from Pantex groundwater as compared to deionized water. This result contradicts numerous other studies that have shown lower adsorption of contaminants from natural waters due to competition between target contaminants and natural organic matter.

Further tests will be conducted to investigate these anomalous results. Possible explanations for the unexpected results are the pH of the solution, presence of anions or cations, or some sort of facilitated or enhanced adsorption. Additionally, multiple component isotherm studies are under way. Multi-component isotherm tests are being conducted to determine the impact of each chemical (RDX and HMX) on the adsorption of the other.

RSSCTs showed that the GAC currently used at Pantex (LB-830) is a good adsorbent, but that Calgon F400 performed better. The expected GAC service life would be 40-50% greater with F-400. At design operating conditions, the expected GAC service life is 97 days with LB-830 (vs. 139 for F400) for the first replacement and 160 days (vs. 227) for all subsequent replacements.

Biodegradation of HE

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

The experiments performed in first quarter revealed that hexavalent chromium (Cr(VI)) inhibits the biodegradation of RDX and the growth of RDX degrading cultures. The optimum concentration of Cr(VI) for acclimation purposes was determined to be in the range of 1.0-1.5 mg/L Cr(VI) based on these preliminary experiments. The second quarter experiments on acclimated populations of Anderson Playa (RDX degrading culture) showed strong inhibition in the degradation of RDX at Cr(VI) concentrations of 1.0 mg/L, 2.5 mg/L, and above, although the growth at 1.0 mg/L and 2.5 mg/L was comparable to the reactors containing no chromium.

In the third quarter, the experiments were mainly directed towards determining the amount of Cr(VI) being taken up by the bacteria and the interactions of HMX and RDX in the presence of Cr(VI). As HMX and RDX can be co-contaminants at the Pantex facility, it is important to analyze the biodegradation in the presence of one another and Cr(VI).

In an eight day experiment, to evaluate the microbial uptake of Cr(VI), reactors containing 5.0 mg/L of RDX and different concentrations of Cr(VI) (0, 2.5 mg/L, 10 mg/L, 50mg/L) were monitored. The control contained 5.0 mg/L RDX and 10 mg/L Cr(VI). Chromium(VI) was added as potassium dichromate ($K_2Cr_2O_7$) from a stock solution of 1000 mg/L in water. Na_2EDTA was added to complex excess Cr(VI) to insure a soluble form of Cr(VI). Biomass was added from Oxoid reactors that had been spiked with the Anderson Playa culture. The growth of microorganisms and Cr(VI) and RDX concentrations were monitored with time. As in the previous experiments the growth in reactors containing 2.5mg/L of Cr(VI) was comparable to reactors containing no chromium whereas the growth at higher Cr(VI) concentrations was markedly inhibited. The Cr(VI) concentrations in reactors containing 2.5 mg/L and 10 mg/L were reduced to zero in 2 days whereas the Cr(VI) concentrations in reactors containing 50 mg/L Cr(VI) were reduced to zero in 6 days. The Cr(VI) concentration in the control was constant during the span of the experiment. On-going experiments are being performed to determine whether the microorganisms consumed all the added Cr(VI) or reduced Cr(VI) to some form not detectable using an IC. The redox is also being continuously monitored to check the conditions which might be favorable for the reduction of Cr(VI). The RDX degradation rates decreased as the concentration of Cr(VI) increased. The degradation was best in the reactors containing no Cr(VI).

In another experiment aimed to study the interactions of HMX on the degradation of RDX by Anderson Playa culture in the presence of Cr(VI), the degradation rates of RDX in the presence of HMX were markedly less than those observed in the absence of HMX. The HMX concentration remained constant throughout the experiment. The extent of RDX transformation in the presence of 1 mg/L HMX was observed to be 47.7% at 2.5 mg/L Cr(VI) but was reduced to 30.0% in 10 mg/L Cr(VI) reactors at the end of 8 days. The RDX transformation rates in reactors containing no HMX and 2.5 and 10.0 mg/L Cr(VI) were 99.0% and 95.5%, respectively.

Sensitive microprobes to be used for the continuous monitoring and condition optimization of redox potential, dissolved oxygen, and pH in soil slurry reactors have been obtained. Reactors are currently being monitored for redox and dissolved oxygen using an on-line data acquisition system to verify the range of these parameters that we have been working in and also determine the sensitivity of the probes.

Above-Ground Treatment for Cr Removal

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

Batch screening tests were completed last spring on cation exchange resin samples obtained from the nation's leading resin manufacturers. From the screening experiments, the two most promising resins were used in isotherm characterization studies. Of the two resins chosen for further investigation, one was of a strong acid structure and the other a chelating structure. These studies were performed using Cr(III)-spiked Pantex groundwater collected from well PM-20. Groundwater samples of

the pre-spiked PM-20 groundwater indicate current chromium concentrations at approximately 0.5 mg/L as Cr(VI). The isotherm studies were performed at an initial pH of 5.5 to avoid chromium hydroxide precipitation and at spiked Cr(III) concentrations that yielded the full isotherm characterization over a Cr(III) concentration range of 0-4.5 mg/L as Cr(III).

After the further isotherm characterization of the selected resins, the strong acid cation resin provided evidence of higher chromium adsorption capacity and was chosen for use in a series of column studies. Well PXT-08-1009 was used as the water source for the column studies. Cr(III) spiking resulted in an approximate increase of 0.5 mg/L as Cr(III) in the source water containing initial chromium concentrations of approximately 2.5 mg/L as Cr(VI) and trace amounts of Cr(III). While the batch isotherm experiments indicated favorable performance for chromium removal, data collected in two column studies showed poor competition for active adsorption sites in the presence of naturally occurring cations such as calcium and magnesium. With this knowledge gained, a new chelating cation resin, designed for heavy metal removal in the presence of calcium and magnesium, was obtained from a national resin manufacturer.

Although the first series of column studies using this newly obtained chelating resin is still in progress, some preliminary, qualitative conclusions can be made. For the resin under current examination, chromium (i.e., Cr(III)) competes well for active resin adsorption sites and is not displaced by natural groundwater cations. Preliminary data also suggest the limited removal of Cr(VI) within the column. Whether this phenomenon occurs through chromate reduction followed by Cr(III) ion exchange or through direct adsorption of Cr(VI) is not yet clear. Initial Cr(VI) removal is dependent on system pH: increasing removal with decreasing pH. Current measurements indicate the favorable removal of Cr(III) and the limited treatment of Cr(VI). The graduate student working on this project is Mr. Joshua Norton.

Chemical Models and Redox Chemistry of Cr

Pls: B. Batchelor, Ph.D., P.E.; E. Carraway, Ph.D., P.E.; M. Schlautman, Ph.D.; and B. Herbert, Texas A&M University

Standard procedure for measuring SRC (Soil Reduction Capacity) of Pantex soils based on their ability to reduce Cr(VI) was developed in this quarter. To determine optimum experimental conditions of the standard procedure, the effects of reaction temperature (room temperature and 60 C), types of reductants (FeSO_4 , Na_2SO_3 , $\text{Na}_2\text{S}_2\text{O}_4$, Na_2S), reduction time and oxidation time (1, 2, 4, 8 day) were investigated. Reaction temperature did not have any significant influence on the variation of SRC and the data obtained at room temperature were more consistent than those obtained at 60 C. Sodium dithionite ($\text{Na}_2\text{S}_2\text{O}_4$) was the most effective reagent for reducing Pantex soils and achieved near maximum results after 2 days reaction time. Measurement of the extent of reduction was conducted by measuring the extent to which the soils could reduce Cr(VI). Reduction of Cr(VI) was almost complete after 2 days reaction with dithionite. Therefore, two days reduction time (reaction with dithionite) and two days oxidation time (reaction with Cr(VI)) were chosen for the standard SRC test protocol. Applying the standard SRC test protocol, the intrinsic (no reduction step) SRC of Pantex soil was measured as 0.1 $\mu\text{eq/g}$ and the total SRC (with reduction step) was measured as 18.2 $\mu\text{eq/g}$. The intrinsic SRC of Pantex soil in place may be substantially higher than that measured in these experiments, because our soil samples may have been oxidized by atmospheric oxygen during storage.

Experiments were conducted to investigate reduction of RDX and Cr(VI) by zero valent iron (Fe^0) in solutions containing a single compound and both together. The initial concentration of 60 mg/l of RDX was completely removed in 12 hours using a 6% iron (Fe^0) to solid ratio. The reduction of Cr(VI) was found to be very fast even in the presence of 60 mg/l of RDX. The initial concentration of 2 mg/l of Cr(VI) was reduced to below detection limit in 40 minutes by 6% iron to solid ratio. The results showed no competition or inhibition processes during the simultaneous reduction of both contaminants. The results to the date indicate that simultaneous reduction of RDX and Cr(VI) is possible by zero-valent iron.

Feasibility of In-Situ Remediation of Residual HE-Modeling

Pls: D.C. McKinney, Ph.D. and G.E. Speitel Jr., Ph.D., P.E., University of Texas at Austin

Soil cores from two locations, Building 12 and IW-2, were obtained from the Pantex site, and several soil depths were tested to determine the level of RDX contamination. The main goal was to determine which soil depth or depths to use for the study. The results from Building 12 showed RDX contamination as high as 10.3 mg/kg with an average of about 9 mg/kg over a 15-foot section. These data were consistent with average RDX levels of 10.5 mg/kg obtained by the contract lab that analyzed samples over the same 15-foot section. Data obtained from location IW-2 showed very small traces of RDX; most samples were under 1 mg/Kg. Therefore, soil samples from Building 12 between 55 to 70 feet were selected for kinetic experiments with ^{14}C -radiolabeled RDX, because the history of RDX contamination increases the probability of RDX degraders being present in the soil.

At this time, methods development is complete, initial control experiments have been run, and the radiochemical experiments have just been set up. A variety of experimental conditions are being explored involving a range of electron acceptor and nutrient concentrations. The duration of these experiments is unclear, and will depend on the rate of RDX biodegradation. We anticipate that data will be collected over the next several months and that a progress report will be completed by the end of FY 1997.

The fate and transport of RDX is being modeled with UTCHEM, a three-dimensional chemical flood simulator developed by the Center for Petroleum and Geosystems Engineering at the University of Texas at Austin. UTCHEM describes dispersive, diffusive and advective transport of chemicals in the vadose and/or saturated zone. Adsorption, vapor/liquid partitioning, and biodegradation reactions are also simulated by the model. Work on modeling to date has included making small modifications to the computer code and setting up and testing of Pantex site test simulations.

Two code modifications have been made to adapt UTCHEM to conditions at the Pantex site. First, changes were made to allow for the partitioning of oxygen between the air and aqueous phase. Partitioning between the aqueous phase and air phase may seem fundamental; however, since UTCHEM was originally designed for enhanced oil recovery, vapor/liquid partitioning had been limited to gas/oil. The same partitioning capability was extended to model air/water partitioning. Second, the adsorption capabilities of UTCHEM are being improved to allow higher adsorption capacities of RDX in the vadose zone.

A one dimensional base case input file has been developed to test these modifications and simulate conditions at the Pantex site on a smaller scale. The one dimensional base case allows for shorter run times and provides a simplified data set to analyze. The grid system for this input file was taken from a previous model that simulated soil vapor extraction of TCE in Pantex soil. By using this grid system, future modifications can easily be made to test soil enhancement techniques by pumping different nutrients into the soil. Reservoir properties were obtained from the Pantex annual report dated May 1996 and from studies conducted by Kendrick. Such properties include porosity, permeability, and initial water saturation.

Simulations of RDX transport and biodegradation will be performed in the fall of 1997. Since experimental results may not be available yet, simplified biodegradation kinetics will be used to allow modeling to proceed. For the initial case, first order transformation of RDX followed by first-order mineralization of reaction products will be assumed. The work done by Dr. Douglas Young at the University of Arizona suggests that a first order decay rate can be used to simulate the biotransformation of RDX.

Feasibility of In-Situ Remediation of Residual HE-Laboratory

*Pls: K. Rainwater, Ph.D., P.E.; C. Heintz, Ph.D., P.E.; T. Mollhagen, Texas Tech University
V. Harkins; T. Musick; W. Medlock, K. Van Hooser; Md. Shaheed, J. Bednarz*

Concentrations of HE in Soil Samples

HMX, RDX, TNT parent compound concentrations as well as 1,3,5 TNB were analyzed in 70 selected soil samples from Zone 12. The analytical method was EPA SW 846-8330, with solvent extraction followed by high performance liquid chromatography (HPLC). The sample sites were locations 6 (0-30 ft depth) and 10 (0-125 ft) near Building 12-43, and injection well IW-2 (0-256 ft) near the northeast corner of Zone 12. The results of these analyses were reported in a deliverable dated July 21, 1997. RDX was most prevalent in the samples near Building 12-43, with concentrations ranging from almost 50 mg/kg at the surface to 6 mg/kg at 125 ft. The analytical results compare well with values reported by the environmental contractors employed by the Battelle Environmental Restoration (ER) group. The analytical results were delayed as we awaited the delivery of commercial standards for both PETN and TATB. The TATB standard has still not been delivered. The sample extracts were retained for future analyses for PETN and TATB.

Determination of Metabolic Activity in Soil Samples

Soil samples that have been analyzed by impedance microbiology to ascertain the presence of viable microbes included 45 samples from Locations 6, 7, and 10 near Building 12-43 and IW-2. Both direct and indirect impedance testing has been performed on all samples. Sites with measurable activity are candidates for in situ remediation. We currently are probing only for heterotrophs and have found indications of metabolic activity from areas known to be contaminated with HE to depth of 125 ft. As warranted, further studies on chemical and physical requirements for stimulation of the biota will be undertaken. We will use this information next to design experiments with the impedance system and conventional microcosms to investigate stimulation of HE degradation in the soil.

Evaluation of Heterotrophic Microbial Flora in Soil Samples

Using the Whitley's broth recovered from the samples tested in the RABIT, we are beginning the portion of the project concerned with the isolation and characterization of the heterotrophic microbes present in the soil samples already tested for metabolic activity. Mr. Ruurd Peppel, a student from the Van Hall Institute in The Netherlands, will arrive in Lubbock on August 11 to join in this phase of the project.

Ecological Risk

Co-Pls: J. W. Bickham, Texas A&M University; R. J. Baker, Texas Tech University

During the past quarter we continued to investigate the genetic characteristics of wildlife populations exposed to environmental contaminants. The overall objectives of these studies are to determine how wildlife populations respond genetically to pollution and to perfect and validate the genetic procedures for use in risk assessment. The benefits to DOE of these studies include having a better understanding of the long-term (chronic) ecological effects of pollution at various DOE facilities being studied as well as the capability to employ cutting-edge genetic assays in ongoing or planned ecological risk assessments. By this, DOE will be better able to address the present regulatory requirements regarding risk assessments, as well as anticipated changes to these requirements in the near future.

A Masters thesis was completed this spring which examined the effects of nitroaromatic compounds and radiation on somatic tissues of white-footed mice and prairie voles. The field work was conducted at a DOE and DOD site in Missouri (Weldon Springs Training area) selected for its similarity in actual and potential contamination to Pantex. Both species showed evidence of somatic effects in spleen cells as measured by flow cytometry. A manuscript is currently being prepared for submission.

Population genetic studies to assess heritable genetic effects are presently underway in the prairie voles from the same location. Genetic variation in these populations are being assessed by sequencing a portion of the mitochondrial genome. Preliminary results have indicated that the genetic diversity was lower in radiation-exposed animals than in vole from reference sites. No differences were found between TNT exposed and reference populations.

A third study has been completed which addresses population genetic effects resulting from radiation exposure in aquatic organisms. That study was conducted on Eastern mosquitofish taken from two contaminated ponds and two reference ponds at another DOE site, the Savannah River Site in South Carolina. This study was designed to test the hypothesis that specific genetic markers (previously studied in Western mosquitofish). For this study, adult female eastern mosquitofish (*Gambusia holbrooki*) were collected from two radionuclide-contaminated and two reference sites in and around the U.S. Department of Energy's Savannah River Site (SRS). DNA was analyzed by the randomly amplified polymorphic DNA (RAPD) technique in order to determine if the differences in population genetic structure between the contaminated and reference sites. A previous study used the RAPD technique to examine population genetic structure of western mosquitofish (*G. affinis*) living in radionuclide-contaminated ponds at the Oak Ridge National Laboratory (ORNL). In the ORNL study, it was found that there were certain RAPD markers which were present in radionuclide-contaminated western mosquitofish (*Gambusia affinis*) populations at a higher frequency than in reference populations (these markers will be referred to as "contaminant-indicative markers"). This and other evidence suggested that these may be markers of loci which impart a selective advantage in contaminated habitats. In the present study, it was found that similar contaminant-indicative markers were present in the contaminated SRS populations at a higher frequency than in the reference populations. In addition, Southern blotting revealed that the SRS *G. holbrooki* contaminant-indicative markers were homologous to the ORNL *G. affinis* contaminant-indicative markers.

A final study is examining population genetics of barn swallows exposed to mixed urban and industrial wastes in and near Gary, IN. Genetic variation in these populations is being determined using the RAPD technique as well as microsattellites. This study is currently underway and data are being collected.

Publications and Presentations

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FUTURE ENVIRONMENTAL, HEALTH AND SAFETY

Risk Characterization for a MOX Fuel Facility

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., the Center

The purpose of this project is to develop the database framework for characterization of environmental risks from a MOX fuel processing facility at the Pantex Plant, and to develop and analyze potential pathways for human and ecological exposures. Through the development of the database and path-

way 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 second quarter the following objectives have been addressed:

- Work 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 Department of Energy (DOE) presentation of its draft Environmental Impact Statement (EIS). The DOE expects to present its draft EIS during the First Quarter 1998.
- Regional coverage of the area within a 50 mile radius of the Plant have been finalized in the ArcView Geographic Information System (GIS). These coverages include:
 1. the 1:250,000 scale raster image maps (the USGS topographic maps), the 1:24,000 scale raster image maps for the near-site vicinity,
 2. a coverage of land use and land cover,
 3. a coverage of surface soil type from the STATSGO soil database,
 4. a coverage of surface vegetation has been developed from available digital sources. Further refinement of this coverage is expected with input and data from the Agricultural Group,
 5. A coverage of census information from the 1990 census, and
 6. A coverage including the features of the regional aquifer system from the Texas Natural Resource Conservation Commission (TNRCC).
- The digital line graph coverage of the roads, railways and hydrologic features previously developed are being recompiled to reflect the 50-mile radius extent of the regional coverage.
- Digital facility drawings were received from the Plant personnel late in the first quarter. Processing of these drawings for use in the GIS is complete.
- During the quarter a briefing workshop was held with regulators from the TNRCC and other State agencies to present the action plan for the risk characterization project. The workshop provided an opportunity for the regulators to provide input on the study.
 1. Screening calculations have been initiated for several scenarios. The scenarios include:
 2. an instantaneous release to the atmosphere and transport by air dispersion followed by deposition.
 3. accumulation of the deposited particulates in a playa and recharge to the groundwater.
 4. terrestrial food chain pathways based on the deposition on plants and uptake by cattle.

Development of a Monitoring Station for Estimating Interplaya Recharge

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

Fifty thermocouple psychrometers were calibrated in the laboratory 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. Material for installation of the thermocouple psychrometers has been ordered, including gravel, sand, epoxy, and bentonite. Sample containers for collection of soil samples for water content, water potential, chloride, and stable isotopes were also obtained. Bill Mullican will visit the Pantex Plant to determine the optimal location for the monitoring station in an interplaya setting. Soil samples will be collected at this time also to determine the appropriate type of time domain reflectometry probe that should be used to monitor water contents. If the soil is highly conductive a coated TDR probe may be required to minimize signal attenuation.

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

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

Several approaches were evaluated to determine the effects of organic acid on Cr uptake and transport by clover, including (i) induction of organic acid accumulation under nutrient deficiency (Fe or P) conditions; (ii) addition of organic acid to nutrient solution; and (iii) addition of organic acid to plants through the stem using a syringe injection system. We have completed the plant culture, sample collection and analysis. Data processing and analysis are underway. The results from this experiment will determine whether organic acid enhances Cr uptake and transport from root to shoot and will shed light on the mechanism of Cr uptake and translocation.

Plant culture and sample collection phases of an experiment addressing kinetics of Cr uptake and translocation by plants were completed. About 500 samples have been collected. Sample processing and analysis are in progress. Previous experiments have indicated that Cr uptake and translocation differ greatly among plant species and Cr sources. Chromium uptake and distribution between shoot and root are being determined for a fixed period of time using four Cr(III) sources (Cr-citrate, Cr-oxalate, Cr-EDTA, Cr-DTPA) and plants with high and low uptake and translocation potentials as determined in previous experiments. We will also calculate kinetic constants of Cr uptake and translocation for these Cr sources and plants. The results from this experiment will help explain the differences in Cr uptake and translocation among plant species and Cr sources and give us clues about Cr uptake system associated with the various plants and Cr sources.

Experiments comparing the sensitivity of two *Brassica juncea* strains reveal no difference in either whole-plant weight, or root growth to varying chromate concentrations. Root length was a more sensitive indicator of chromate toxicity than whole plant weight. Research into the physiology of ferric chelate reductase (FCR) activity in *Brassica* is continuing. Some plants had much higher activity than others, suggesting that this is a genetically determined trait that is not shared identically by the plant population we are using. These results support our hypothesis that elevated FCR activity is not a likely explanation for why some strains have the ability to accumulate certain metals.

Anthocyanin accumulation due to Cr in hypocotyl sections of the soybean stem is similar to that reported in other plants as a result of metal accumulation and stressful stimuli (salt stress). It has also been shown that anthocyanin accumulation is related to a specific gene responding to the external stimuli. In soybean, this gene has been isolated, identified and characterized and is referred to as GmGST-26. Objectives of this quarterly research effort have been to quantify the anthocyanin content, to clone GmGST-26, and to determine if induction by heavy metals, particularly Cr, is a characteristic of GmGST-26. Amplification of a segment of the target gene was successful with PCR, and a radioactive probe has been prepared. RNA extraction from Cr-treated and control seedlings has been accomplished and transfer to a nitrocellulose membrane was successful. Northern hybridization of the probe with the presumable induced mRNA is in progress. DNA sequencing of the PCR-generated probe to determine its homology with native GmGST-26 is underway.

Presentations and Publications

L.R. Hossner, TAMU; R.H. Leoppert, TAMU; R.J. Newton, TAMU; P.J. Szaniszlo, UT-Austin. "Qualitative and Quantitative Determinations of Phytosiderophores by High-Performance Liquid Chromatography" August, 1997. Manuscript

L.R. Hossner, TAMU; R.H. Leoppert, TAMU; R.J. Newton, TAMU; P.J. Szaniszlo, UT-Austin. "Mobilization and Uptake of Actinides and Heavy Metal Analogs by Agriculture Crops: Uranium Uptake by Plants from the Brassican Family and High Biomass Crops" August, 1997

L.R. Hossner, TAMU; R.H. Leoppert, TAMU; R.J. Newton, TAMU; P.J. Szaniszlo, UT-Austin. "Phytoaccumulation of Chromium, Uranium, and Plutonium in Plant Systems" August, 1997. Literature Review

POLLUTION PREVENTION AND POLLUTION AVOIDANCE

Alternative Uses for HE

PI: C. G. Willson, The University of Texas at Austin

Part 1: Diamond Generation by Explosive Compression of Buckminsterfullerene

Since the last quarterly report, five three-dimensional shots have been detonated at the Pantex facility. All five of the samples were successfully recovered, proving the recoverability and reproducibility of the work piece design. Our system reproducibly subjects samples to higher pressure, several hundreds of Gpa, than any of which we are aware. The composition of the five samples was chosen to provide information on the effects of quenching materials on yield. Nickel and Cobalt were investigated with varying particle size and varying metal/Buckeyball ratio. The remaining shot contained both a quench material and "diamond seeds".

To date, two sample containers have been opened and the compression products analyzed. It was determined by X-ray diffraction and Raman spectroscopy that a conversion of buckminsterfullerene to graphite was accomplished in the first detonation with no diamond formed. The products of the second detonation, however, appear to contain both graphite and a substance which exhibits a diamond peak in Raman spectroscopy. The preliminary X-ray diffraction analysis is inconclusive because the strong reflection from nickel oxide obscures the region of the diamond reflection. We are now running the analysis in a way that improves the signal to noise in hope of resolving a clear diamond reflection. The sample is heterogeneous having both black and clear particles. We have arranged access to micro-Raman spectroscopy at AMD in Austin which will allow us to acquire Raman spectra of the different components of the sample..

It was also discovered that the steel sample holders exhibited tremendous hardness after detonation, especially in the inner regions of the work piece, near the sample cavity. Cutting a single work piece open destroyed all of the hardened steel saw blades in our machine shop! We are currently examining the cross sections of the steel work pieces at Texas Tech with a microhardness apparatus to map the hardness as a function of position and examining the morphology of the material by scanning electron microscopy. The machine shop at UT Austin has received a new shipment of saw blades and the three remaining samples are currently being opened and analyzed. Plans for future detonations with carbon samples will depend on the outcome of the analyses currently underway. We do plan to conduct at least one attempt directed toward compressively synthesizing Carbon Nitride.

Part 2: Demonstration Burn for Energy Recovery

A meeting was held at Pantex on 6/12/97 to make plans for production of a 1000 lb. batch of fuel pellets consisting of waste thermoplastic polymer and ground TATB. It was decided that the fuel pellets will be formed using an inexpensive epoxy as the binding agent. A batch of this formulation (without explosive) was prepared at the University of Texas and a successfully test burn was conducted at the facility in Center, Texas. Officials from the city of Center are excited about conducting a full scale 1000 lb. test burn as soon as possible. Unfortunately, production of the fuel pellets has relatively low priority at the Pantex facility and we are told that work on the fuel formulation will probably not begin until October.

COMMUNICATION, EDUCATION, AND TRAINING

PROGRAM IMPLEMENTATION

Program Management

PI: E. Zounar, Ph.D., Amarillo National Resource Center for Plutonium

Co-PIs: E. Harle; C. Dixon; and B. Perry, Amarillo National Resource Center for Plutonium

Communication, Education, and Training (CET) is responsible for Task 1, Task 4, and training. CET is divided into Center programs, awards, and grant-funded research projects. The size of the CET Center staff is projected to reach ten by the end of FY 1997; it is currently eight plus two graduate assistants in the education department - an overall increase of two over the previous quarter. One employee was promoted to the position of Community Liaison.

Program management has been engaged in the following:

- FY98 Continuation Application development and submission.
- Proposal process evaluation, revision, development, and implementation for FY 98.
- Publication policy development for general publications and technical publications, review, and approval.
- Performance of human resource needs analysis within CET and development of position descriptions for Training Program Manager and Science Information and Resource Center Program Manager.

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

- Continued to operate the Center's Speakers Bureau and prepared speeches and presentations including the following:
 - 5/7/97 North Amarillo Lion's Club on environmental issues which was announced on 5/6/97 in the *Amarillo Globe News*.
 - 5/9/97 Golden K Kiwanis Club of Amarillo on environmental issues.
 - 6/3/97 Canyon, Texas Rotary Club on mixed oxide fuel.
 - 6/5/97 Panhandle 2000 organization on mixed oxide fuel.
 - 7/25/97 Texas Pre-freshman Engineering Students on engineering, a career.
- Published Volume III, Issue III of the Center's newsletter with a distribution of 4,500 which includes 3,000 Pantex personnel. Newsletters (200) were delivered to the central library for distribution to branch libraries.
- Continued development of the Center's web site at <http://www.pu.org>. Refer to the appended section for CET for the news release "...Publishes Technical Document on Plutonium Disposition." The news release illustrates the movement toward placing the Center's technical publications on the Center's web site.
- For the reporting period, media coverage included the following:
 - 5/19, 5/20, 5/21/97 Television channel 10 three-part series on mixed oxide fuel.
 - 6/3/97 National Public Radio (Chicago WBEZ) debate on mixed oxide fuel.
- Efforts of communication personnel included development and initial implementation of a risk characterization communication plan in response to a request from the Texas Governor's office to evaluate possible new Pantex Plant missions. The Center's study focuses on health and safety, waste management and environmental issues.

The Center's exhibit received heightened attention this quarter at the following events:

- 5/22/97 Agriculture Days in Bushland, Texas attended by 240 area farmers and other agriculture industry people.
- 6/12/97 Environmental Impact Statement Scoping Hearings in Amarillo, attended by approximately 325 people.
- 6/17/97 Panhandle Human Resources Manager's Seminar, Amarillo attended by approximately 50 people.
- 7/9-11/97 Texas State Future Farmers of America (FFA) Convention attended by approximately 6,500 FFA students, teachers, and sponsors.
- 7/24/97 Summer Crops Field Days in Etter, Texas.
- 7/31/97 State/Public Employee Recognition Event at Amarillo College Business and Industry Center, attended by more than 200 teachers, professors, politicians, personnel from various state agencies, and families of selected state employees.

The purpose of the 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 organization of the Center. Interest levels vary depending upon the event but observations continue to reveal the importance of the exhibit at public events.

During this quarter, K-16 education program personnel were engaged in a number of exciting programmatic activities and events.

- Facilitated on 5/1/97 a JASON Broadcast Field Trip for six Amarillo Independent School District teachers at Clark County Independent School District, North Las Vegas Community College. The field trip allowed teachers to observe a live broadcast of the JASON program, a program that encourages students to engage in science and technology, and decide whether or not to bring JASON to Amarillo.
- Attended 5/7/97 open house of the Fannin Middle School Discovery Lab. The lab was made possible by a \$40,000 contribution from this Center and matching funds from the Amarillo Independent School District. The purpose of the lab is to facilitate student learning of mathematics and science through the use of technology and by interdisciplinary teaching. Approximately 640 students will have access to the lab. Television channels 4, 7, and 10 covered the event. Refer to the appended section for CET to see "World of Discovery," *Amarillo Globe News*.
- Attended 5/15/97 reception to recognize four junior and senior students at Caprock High School who participated in the Advanced Technology Lab pilot project. These students will receive college credit for their advanced research work in the lab. Refer to the appended section for CET to see the press release "Research at the Rock." Twenty-five students are expected to participate during Fall 1997.

During the quarter, the following awards were made:

- \$5,000 Amarillo Area Center for Advanced Learning in support of the Environmental Laboratory project.
- \$5,000 Panhandle Area Mathematics and Science Conference which allows educators in the Panhandle and South Plains to meet and share their teaching expertise.
- \$5,000 Student Research Conference at West Texas A&M University in support of research and professional development among university students.
- \$400 Horace Mann Middle School, Amarillo to support Summer Science Camp for students in grades 6 - 8. See "Students Learn from Mock Hazardous Meltdown Activity" from *Amarillo Daily News* in the appended section for CET.

COMMUNICATION PROGRAM

Science Information And Resource Center

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

During the reporting period:

- Development of exhibit #1 continued. Investigators met in Amarillo with the Education Program Manager of the Center three times during this quarter. Included in the first meeting was Dr. Lee Peddicord, Texas A&M University System; in the second meeting, Greg Shuman, Interim Director of the Discovery Center; and in the third meeting, John Rhoades, Director of the Bradbury Science Museum. Exhibit text was revised following each of the first two meetings. After the third meeting, the decision was made to extend the delivery dates for exhibits #1 and #2 and contract with an exhibit writing agency to finalize text.
- The design of the exhibit "structure" was finalized and approved. When text is completed, and the number of display units can be determined, investigators will obtain cost estimates from fabricators.
- Concept for exhibit #2 on environmental issues was completed and presented.

Comments: After meeting with a consultant, the team decided to contract with an exhibit writing firm to finalize text. As a result, the delivery date for both exhibits has been extended to January 15, 1998. The new date should provide adequate time for completion, assuming that the exhibit writing firm and the fabricator are able to accommodate the time frame.

Distribution Count for Plutonium Exhibit		
Date	Newsletter	Brochure
5/7/97	50	39
5/29/97	63	40
6/29/97	13	40
7/28/97	58	38
Totals:	184	157

Figure 2

Amarillo National Resource Center program personnel have been implementing the exhibit plan for the Plutonium Transportable Exhibit (Plutonium Past, Present, and Future) which is the partnership exhibit between the Center and Pantex (Mason & Hanger). For the reporting period, the display remained at the Amarillo Airport due to its popularity. Refer to the following chart for an indication of the numbers of newsletters and brochures taken by passers-by.

EDUCATION PROGRAM

K-16 Science And Mathematics Education

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

All activities for this project were completed in January 1997 as scheduled. Results of a formal survey (needs analysis) will be submitted by August 1997.

Integrative Studies In Science And Mathematics

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

This project is known as the West Texas Environmental Project (WTEP). WTEP is a teacher enhancement project to engage K-12 teachers in experiential, integrative, and site-based learning activi-

ties. These activities focus on the interface between environment, and science and mathematics curricula. As an experiential project, teachers are involved in proactive and problem-solving activities based on contemporary writings in environmental sustainability, ecology of semi-arid lands, and contemporary agricultural practices on these lands. As an integrative project, teachers are introduced to and become proficient at developing classroom learning activities that are theme-based (e.g., sustainability of the Ogallala aquifer), and that clearly and explicitly unify various traditional subject areas (e.g., science, mathematics, humanities, political science, and so on). Integrative curriculum development and instruction is only now being implemented in selected schools across the nation. As a site-based project, teachers take part in an extensive field expedition to critically explore agricultural and societal practices that threaten environmental, societal, and agricultural sustainability.

The WTEP field trip for teachers was conducted during June 17 - June 27. Refer to the appended section for CET to see "Science Teachers to Spend Two Weeks in a Lab without Walls."

- Preparation Sessions June 17 - June 20.

The WTEP teacher workshop and Field Trip began on June 17, 1997 at West Texas A&M University in the Jack B. Kelley Student Center. Thirty teachers attended a four-day workshop during which they (a) prepared for the field trip, (b) met in curriculum groups; (c) learned about integrative curriculum development, statistical applications, and water sampling; and (d) learned from guest speakers about issues related to sustainability. Speakers for the sessions were:

1. Mike Harter: Historical & Geological Perspective
2. Dr. Duane Rosa, Professor of Economics at West Texas A&M University spoke on Economics and Environmental Sustainability
3. Dr. Dave Barnes, Program Manager for Environment, Safety, and Health at the Amarillo National Resource Center for Plutonium presented "Groundwater and groundwater contamination: Educating the public."
4. Dr. B.A. Stewart, Head of the Center for Dryland Agriculture at West Texas A&M University spoke on Aquifers

The teachers came from Texas schools in Amarillo, Lubbock, Bushland, Perryton, Plainview, Sonora, Floydada, Abilene, Canyon, San Antonio, Hereford, and Waco. One teacher represented Pensacola, Florida.

During the workshop, teachers were individually interviewed. The interview questions were designed so that a post interview could reveal changes that might occur in the individuals.

- Field Trip June 21 - June 27. Zounar and Harle from the Amarillo National Resource Center for Plutonium attended the field trip. It was an extraordinary experience to watch teachers collect and record data through photographs, sketches, and journals along a 2,000 mile route.

Day One: Saturday, June 21, 1997 Headwaters and Headworks from Canyon to Tucumcari, NM

The field trip began with a caravan of three large vans. Each van had a CB radio so the teachers were in constant audio contact. This communication system allowed interactions among the teachers concerning the roadside flora and fauna, geologic formations, land practices, and various other topics. Teachers were assigned vans according to their teaching levels in order to promote lively conversations among passengers. The first day's theme was "On Headwaters and Headworks" with stops scheduled at The Canadian River, Rita Blanca National Grasslands, Bueyeros Mission, Canadian River (water sampling), Conchas River (water sampling), Conchas Lake (tour of dam facilities, observation of headworks of Tucumcari Irrigation Project), and Tucumcari, NM (hotel).

Day two: Sunday, June 22 Legislated Sharing and Sustainability from Tucumcari to Pampa

The caravan left the hotel at 4:30 AM and traveled to the Caprock Amphitheater near San Jon, NM to observe sunrise over the Caprock rim. The caravan traveled to the Logan, NM Dam site, then to Lake Meredith to tour facilities of the Canadian River Municipal Water Authority. Teachers sampled water at several sites along the route. The last site of the day was Adobe Walls Historical Monument, the site of a battle between buffalo hunters and the Plains Indians. This was an example of area natives fighting for their sustainability - and losing.

Day three: Monday, June 23 Sustainability, Stewardship, and Survival: Capitalism and Social Inequity

The group left Pampa at 7:30 AM to enter the Red River Basin via Clarendon TX. It stopped at the Whiteflat (ruins) for observations and discussions about the demise of small towns. The next stop was the White River Lake (tour of White River Municipal Water Authority), followed by a guided visit to Leuders, TX via caravan and CB radio by Mary Vandeventer. Leuders is another example of lost sustainability. It is a ghost town. From Leuders, the caravan traveled to Ericksdahl, TX Lutheran Church where Wilbur Jensen presented "Farming History, Equity, and Sustainability." The group spent the night in Albany, a bustling rural town, where participants compared Albany and Leuders, and visited historical sites.

Day four: Tuesday, June 24 Ethics of Sharing Water: From Survival and Stewardship to Environmental Sustainability from Albany to Lamesa, TX

From Albany, the caravan traveled to J.B. Thomas Reservoir and Colorado River Municipal Water Authority (water sampling). From this point, the group ascended the Caprock and entered Llano Estacado mesa near the eastern border of Dawson County. Harvey Everheart, manager of the Mesa Underground Water Conservation District presented information and conducted a tour of a farm near Lamesa.

Day five: Wednesday, June 25 The "Naturalness" of Artificiality: Understanding Postmodern Agricultural Stewardship."

The group left Lamesa at 7:30 AM and arrived at a cotton farm between Brownfield and Levelland, TX. Don Mimms, owner of the farm, explained irrigation systems, underground water, and survival. After leaving the farm, the caravan traveled to Muleshoe National Wildlife Refuge and observed "natural" playa lakes and then, traveled to Hereford to hear Jim Steiert's discussion of Playa Lake issues.

Wrap-Up

The closing sessions were held on June 26 and 27 in the Education and Administration Building at Texas Tech University. The groups worked on curriculum development and visited the High Plains Underground Water District office and the City of Lubbock's water purification plant. After final synthesizing activities and curriculum presentations, the workshop/field trip ended.

- Follow-up

The teachers will further develop their curriculum modules and implement the material in their classrooms during the Fall semester. The Principal Investigators and assistants will visit each teacher in his/her classroom to observe and continue the research model started at the beginning of the session. During the visit, each teacher will participate in a closing interview. The pre- and post-field trip interview data will be help to evaluate the WTEP.

The teachers will stay in close contact with one another in order to further develop and refine curricula and teaching techniques. The teachers will meet again in late fall on the Texas Tech University campus to produce field-tested curricula.

Secondary School Physics Curriculum

PI: J.P. Spears, West Texas A&M University; T.C. Ahern, Ph.D., Texas Tech University

The revised version of the physics curriculum manual was delivered in June. Dr. Ahern and Ms. Spears are currently writing sections to provide users of the manual with information on the design of instruction and simulations. The revised version includes simulations in addition to those in the first version.

The Physics Teachers Network home page at <http://nemo.educ.ttu.edu> was redesigned to include on-line use of the manual, an FTP site that allows for downloading of curricular material, LiveCard demonstration of on-line stacks, and an ongoing mediated conference. The web site will function as a continual source of instructional information for secondary physics teachers.

The first Computers in Physics Workshop for area teachers was held July 21-25 for four area physics teachers. During the workshop, the teachers were trained in the design and development of computer-based instruction. After training, these teachers joined the core network group (made up of teachers who were trained in 1996) and their students will join the area-wide physics student network.

Planning for the second Computers in Physics Workshop was completed and the dates for the workshop were set.

Middle School Science Resource Manual

PIs: G. Skoog, Texas Tech University; T. Brasher, West Texas A & M University

During the period May 1-May 30, emphasis was given to recruiting participants and preparing for a June 2-6, 1997 workshop on the use of the Middle School Science Resource Manual in Canyon, Texas. Thirty-six teachers participated. Evaluation data were collected and analyzed, and the written report was submitted.

Treasure Brasher will present lesson plans from the manual at the Panhandle Regional Mathematics and Science Conference in September at West Texas A&M University and at the Conference for the Advancement of Science Teaching in Texas in October at Fort Worth, Texas. Look for the Science Manual in the Electronic Resource Library (Task 1) at <http://plutonium-erl.actx.edu>.

Foundations Mathematics And Science Success

PI: G. Mann, Ph.D., West Texas A&M University; R. Powell, Ph.D., Texas Tech University

This project was initiated on January 15, 1997 with the purpose of (a) improving elementary students' mathematical and science literacy, (b) improving future teachers' knowledge and understanding of instructional planning and delivery of mathematical and science content, (c) promoting elementary students interest in pursuing a career in a field related to mathematics and science.

The project's primary activities were completed January - March and provided:

- hands-on-science and mathematics classes to elementary students in the Caprock cluster of the Amarillo Independent School District and elementary students in the Panhandle Independent School District.
- training for future teachers at West Texas A&M University in these methods of instruction and opportunities to practice these strategies with participating students under the supervision of professional teachers.

The SuperSaturday Sessions serviced 492 students at six different school sites. Fourteen undergraduate teacher education students at West Texas A&M University worked as aides to Master Teachers who in turn, mentored on instructional planning and delivery.

The InterSession Camp serviced 211 students at four different school sites. The undergraduates in teacher education who worked as aides in the SuperSaturday sessions were the teachers during the InterSession camps. They received training and worked under the direction of Master Teachers.

The project will be replicated during the Fall of 1997 in the same schools. Currently, project personnel and school officials from the Amarillo Independent School District and the Panhandle Independent School District are planning for the Fall activities using procedures which were successful during the Spring, 1997 school term. The project will continue to serve one more school than was specified in the proposal.

Texas Pre-Freshman Engineering Program (TexPREP)

Pls: C.N. Kellogg, Texas Tech University; T. Jones, Amarillo College

Finalizing faculty and staff, curriculum and room assignments for Amarillo PREP '97 and TexPREP-Lubbock were the priorities during May. Parent meetings were held on both sites to inform the parents about the prep program and to provide scheduling information and an opportunity for the Job Training Partnership Act/Summer Youth Education and Training program staff to talk to interested students and parents. Speaker invitations were mailed and field trip requests were made of various area industries. Organizing field trips and speaker lists continued through the first weeks of June.

One hundred twenty-eight (128) Amarillo PREP students and 104 Lubbock PREP students began their eight-week TexPREP classes on June 2 on the Amarillo College and Texas Tech University campuses, respectively. Placement testing and orientation were completed the first day. Classes began on June 3rd.

June and July were spent in intensive classroom activity Monday through Thursday, usually beginning with a guest speaker at 9:00 a.m.

Field trips were provided Friday, June 6, 13, 20, 27, July 11 and 18. Both sites participated in extended field trips: a trip to the Waste Isolation Pilot Plant in Carlsbad, New Mexico for the second-year participants; and a trip to Palo Verde, Yucca Mountain site, the Grand Canyon and Hoover Dam in Arizona and Nevada for third-year participants.

Amarillo PREP graduation for the 109 students that completed the program was held on July 25, 1997. Dr. Lee Peddicord, Associate Vice Chancellor for Strategic Programs, Department of Nuclear Engineering, Texas A&M University and Representative David Swinford for the 87th district of Texas, addressed the graduates.

The Lubbock PREP graduation was held on July 25, 1997 for 80 graduates.

TRAINING

Plutonium Reference Book

Pls: 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.

CET APPENDIX

**For More Information Contact:
Cathy Dixon – (806) 376-5533**

**June 19, 1997
For Immediate Release**

Amarillo National Resource Center for Plutonium Publishes Technical Document on Plutonium Disposition

The Amarillo National Resource Center for Plutonium has published findings from a two-year study requested by the U.S. Department of Energy that evaluates the options for disposing of surplus plutonium from dismantled nuclear weapons.

The paper, titled "Evaluation of Alternatives for the Disposition of Surplus Weapons-Usable Plutonium," was written by James S. Dyer and John C. Butler of The University of Texas at Austin, Thomas Edmunds of Lawrence Livermore National Laboratory, and Jianmin Jia of Chinese University of Hong Kong. The work was funded by the Amarillo National Resource Center for Plutonium at the request of the U.S. Department of Energy's Office of Fissile Materials Disposition.

Although the Center has several major technical documents to its credit, the newly published paper on the evaluation of plutonium disposition alternatives is important to the Center not only for the scope of the work but also because of the involvement of Center staff located in Amarillo. Beth Perry, the Center's new information resource specialist, compiled, edited, and coordinated the printing of the paper.

This technical document is on the Center's web site, found at <http://www.pu.org/main/reports/reports.html>. Anyone with Internet access can download the complete document and store it on their hard drive or print some or all of the pages for their own files.

"The work published in this document is valuable not only to the U.S. Department

-more-

Plutonium Resource Center Publishes Paper

p. 2

of Energy, but also to Amarillo-area residents who are seeking fact-based knowledge about possible new missions at Pantex,” said Bill Harris, director of the Center. “By including the document on our web site, we are making our information available to homes, businesses, and schools.”

The technical document evaluates the alternatives for plutonium disposition that were considered by the DOE as it developed a permanent disposition plan for surplus plutonium from nuclear weapons. The work was requested by DOE to provide an independent evaluation. By working with DOE, Center researchers gained access to representatives of the National Security Council, the U.S. Department of State, and the White House Office of Science and Technology.

The DOE considered several different disposition options before settling on two plans that will be initiated. This dual-track plan calls for the conversion of plutonium triggers or “pits” to oxide form, blending plutonium oxide with uranium oxide, then pressing the oxides into fuel pellets for nuclear power plants. The other track is to mix some of the surplus (that not suitable for fuel) into molten glass and storing the hardened logs in an underground repository.

The Amarillo National Resource Center for Plutonium is a higher-education consortium of The Texas A&M University System, Texas Tech University, and The University of Texas System. The Center’s mission is to serve the Texas Panhandle, the State of Texas, and the U.S. Department of Energy by conducting scientific and technical research; advising decision-makers; and providing information on nuclear weapons materials and related environmental, health, safety, and nonproliferation issues while building academic excellence in science and technology.

EXTRA

AMARILLO WEST

A Weekly Section Serving West Amarillo

June 4, 1997

World of discovery

Fannin Middle School launches Discovery Lab



Henry Briggs/Globe-News

Fannin students Christina Ince, left, and Melissa McWilliams show Effie Harle an atomic model of plutonium students made.

By DAVID SMALL
Globe-News Feature Writer

Students at James W. Fannin Middle School now have a world of technology at their fingertips to help them pursue excellence in math and science.

Several Fannin faculty members have worked to transform one of the school's classrooms into the Fannin Discovery Lab, a computerized learning laboratory complete with Internet access, rooftop weather equipment for atmospheric data interpretation, multimedia presentation software and a host of math- and science-oriented software packages.

The new lab comes courtesy of a \$40,000 grant from the Amarillo National Resource Center for Plutonium and a matching grant from the Amarillo Independent School District, according to a release from the Resource Center.

Fannin Principal Elaine Vinyard said the new lab, which boasts 15 state-of-the-art personal computers offering both Macintosh and IBM-compatible formats, will be used as part of an integrated curriculum at all grade levels, including sixth through eighth.

"We wanted something that specifically targets the math and science curriculums, and this (lab) will help us do that," she said.

Vinyard said the rooftop weather equipment includes several probes that can measure atmospheric data such as dissolved oxygen and radioactivity. The data can be used by science students at all



Fannin seventh-grade science teacher David Nilsche examines the Discovery Lab's new weather equipment with students Bjork and Jo Beth Harris.

Henry Burza/Globe-News

grade levels, she said.

"While eighth grade studies how weather affects the environment, seventh grade will study how weather affects plant and animal life," she said.

Eighth-grade science instructor Peter Sample said an exciting software feature in the lab is a geographical information system (GIS) software package.

The software is used by farmers, engineers, agronomists and other professionals to produce geographical maps detailing plant types, soil types, moisture levels and a variety of other information as it changes across a large geographical area.

The package will enable science students to use real-life data to see how professionals plan projects based on environmental data. The result will be an increased interest in learning.

"If studies are tied to actual (math and science) applications, students are more interested in it," he said.

Seventh-grade math instructor Cheryl Dutton said spreadsheet and database software will enable math

students to use math skills to manipulate scientific data.

"On spreadsheets, students will learn to write formulas to manipulate their data," she said. "That's where the math comes in."

Vinyard said writing, publishing and multimedia presentation software in the lab will let students prepare reports and presentations to communicate their classroom findings.

"One of the things students need to learn is to communicate what they learn to others," she said. "They retain best when they teach it to someone else."

Vinyard said students' first task will be to explore the software packages in the lab and write instruction sheets, which will be evaluated by fellow students.

Students and faculty at Fannin began exploring the lab's software during an open house for the public on May 7. Effie Harle, education program manager for the Resource Center, said students' enthusi-

asm during the open house spoke for itself.

"The thing I find exciting is watching these students work," Harle said. "No one has to say it's time to get quiet and go to work. Everyone (here) is excited and ready to learn."

Harle said the Resource Center provided the grant funds because it has a vested interest in boosting excellence in math and science.

"We're very interested in the future work force," she said. "We know that technology is part of that. The younger we can get people started, the better off we'll be."

The Resource Center is a consortium of The Texas A&M University System, Texas Tech University and The University of Texas System.

According to the news release, the center's mission is to serve the Texas Panhandle, the state of Texas and the U.S. Department of Energy by conducting scientific and technical research, advising decision-makers and providing information on nuclear weapons materials and related environmental, health, safety and nonproliferation issues while building academic excellence in science and technology.

Fannin computer literacy teacher Janice Johnson, science teachers David Nische and Peter Sample, and librarian Julie Greene collaborated to design the Discovery Lab.

We wanted something that specifically targets the math and science curriculums, and this (lab) will help us do that.

James W. Fannin Middle School principal
Elaine Vinyard

**For More Information Contact:
Wes Reeves – (806) 376-5533**

**May 14, 1997
For Immediate Release**

“Research at the Rock” to Feature Research Findings of Caprock Seniors

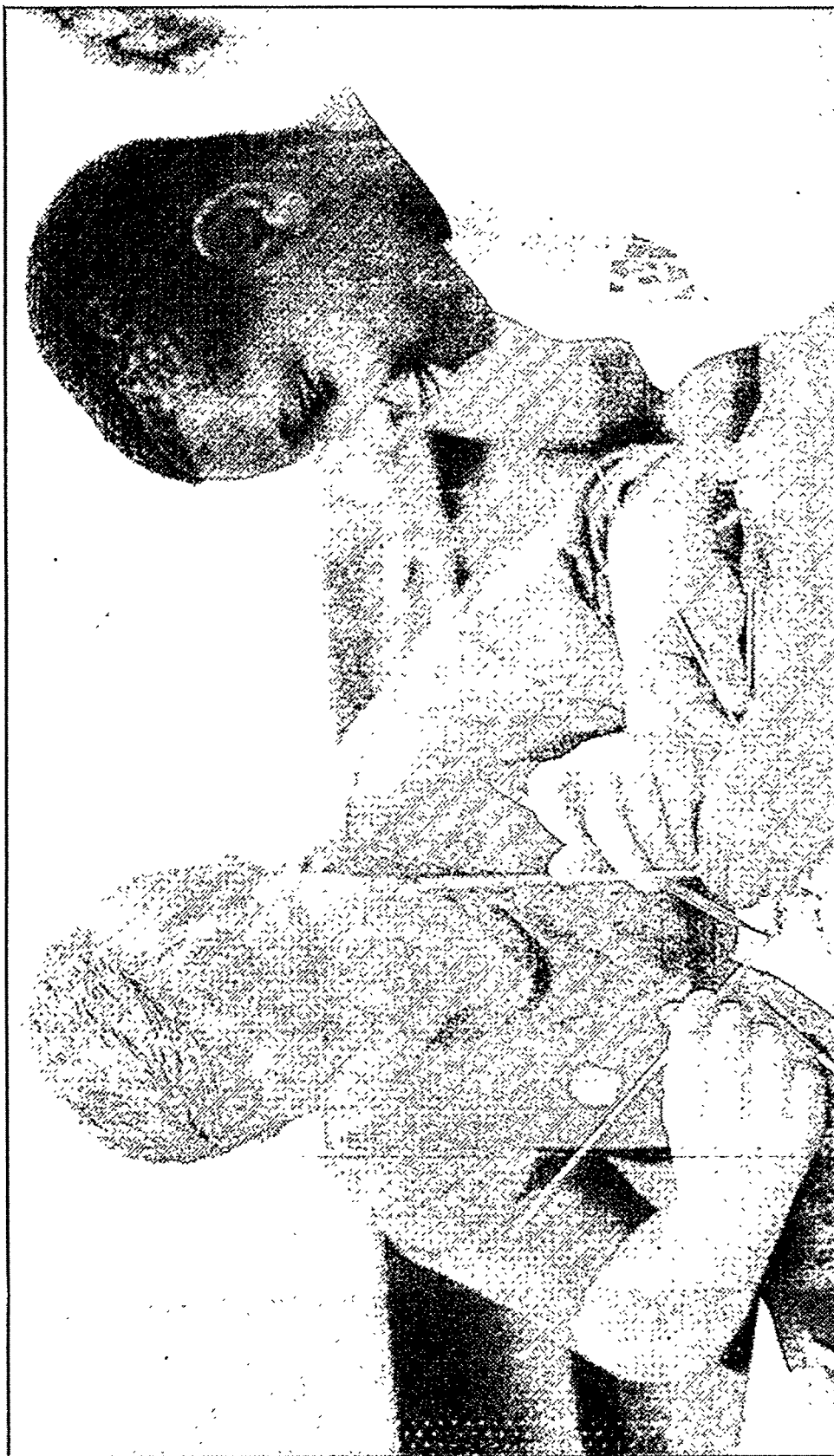
Four Caprock High School seniors will present their senior research projects during “Research at the Rock,” a special presentation scheduled for 7 p.m. Thursday at the Amarillo Independent School District Educational Support Center, 7200 W. Interstate 40. The presentations will be presented in the board room on the first floor.

Students presenting research are Martine Apodaca, Don Caviness, Christi Johnson, and Heather Slemph. Apodaca will present “Plutonium: The Fuel of the Future.” Caviness will present “The Possibilities, Implications and Future of the Search for Life on Mars.” Johnson’s presentation will be on “Tibial Stress Syndrome: Shin Splints,” and Slemph will present “An Overview of Virology.”

All four of the Caprock seniors researched their findings in the school’s new research lab that is made up of computers with Internet access. The lab was made possible through a grant from the Amarillo National Resource Center for Plutonium.

The Amarillo National Resource Center for Plutonium is a higher-education consortium of The Texas A&M University System, Texas Tech University, and The University of Texas System. The Center’s mission is serve the Texas Panhandle, the State of Texas, and the U.S. Department of Energy by conducting scientific and technical research; advising decision-makers; and providing information on nuclear weapons materials and related environmental, health, safety, and nonproliferation issues while building academic excellence in science and technology.

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Lab teammates Art Acord, left, and Colby Campbell attempt to remove "hazardous contamination" from a chocolate chip cookie during a science experiment recently. Both boys are sixth-graders. Karen D. Smith/ Globe-News

**For More Information Contact:
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**June 3, 1997
For Immediate Release**

Science Teachers To Spend Two Weeks In A Lab Without Walls

In a lab where the students are the teachers, all the rules are different.

Instead of spending hours cooped up in a stuffy room, about 30 kindergarten-through-12th grade science teachers will spend two weeks tromping through the grass and muck of wetlands on the southern High Plains of Texas. Their aim: to bring science to life and, in turn, make science more appealing and worthwhile to the students they will face when the fall term begins anew.

This science experience, scheduled June 17-27, is called the West Texas Environmental Project for Integrative Studies in Science and Mathematics, or WTETP for short. The focus of this excursion is the region's many playa lakes, the shallow catch basins that teem with an amazing abundance of life. These lakes play a pivotal role in the region's ecosystem, and provide students of science countless opportunities to better understand plant and animal life on the plains.

Dr. Richard Powell with Texas Tech University's College of Education, and Judy Kelly of West Texas A&M University, have developed the West Texas Environmental Project to meet two broad goals: to familiarize pre-college teachers with innovative trends in curriculum theory for pre-college instruction, and to apply these innovative trends to the areas of science and mathematics.

"By reaching these goals, teachers who participate in WTETP will have opportunities to become familiar with alternative teaching strategies and curriculum development

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Science Teachers Study High Plains Environment

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approaches for their classrooms,” Powell said.

The need for such a program arose from the realization that science literacy in the United States is declining. Education leaders have expressed the need for a different kind of curriculum in the areas of science and mathematics, and for alternative teaching strategies in these two areas and at all school levels, according to Powell.

The program is funded by the 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. The Center, based in Amarillo, conducts research into nuclear weapons materials and coordinates a large educational outreach program aimed at building academic excellence in science and mathematics.

The Center’s education program manager, Effie Harle, said supporting science and mathematics teachers is a big part of the Center’s mission.

“Teachers are life-long learners, but they often don’t have the resources or the time to seek out opportunities to increase their own knowledge,” Harle said. “Programs such as the West Texas Environmental Project are perfectly geared for their needs and their timeframes.”

During their two-week field trip, the science teachers will examine environmental problems that have local and global implications. This will engage the teachers in first-hand exploration of environmental issues and help them to develop classroom curriculum materials that focus on specific dimensions of environmental issues. Along the way, the teachers will be exposed to the scientific fields of waste management, agriculture, geology, hydrology, and related careers. They also will learn more about related mathematical careers. This experience will enable the teachers to better encourage their own students to

-more-

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pursue careers in these fields.

To learn more about this and related programs sponsored by the Amarillo National Resource Center for Plutonium, contact the Center at (806) 376-5533, or e-mail the Center at center@pu.org. The Center's web site is <http://www.pu.org>. Educational materials also are located in the Electronic Resource Library, an interactive library of searchable information on plutonium accessible from the Center's home page, or at <http://plutonium-erl.actx.edu>

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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 sub-projects.

In the area of coordination and technical support, Drs. David Boyle and Paul Nelson represented the Nuclear Group at three Center Governing Board meetings and participated in a day-long strategic planning session in Amarillo. Dr. Igor Carron was also involved in numerous project coordination efforts this quarter, including:

- Organization with Dr. T. A. Parish of the NATO Advanced Research Workshop on "Safety issues Associated with Plutonium Involvement in Nuclear Fuel Cycles" to be held near Moscow, Russia September 2-6, 1997. These efforts included, but were not limited to, contacting participants, making logistical arrangements, corresponding with NATO, and working up the budget.
- Participation in preparing the final financial statement for the NATO Advanced Research Workshop on "Nuclear Materials Safety Management" held in Amarillo, March 13-17, 1997.
- Coordination with Oak Ridge National Laboratory (ORNL) on water reactors group deliverables to ORNL for integration of the Center's work into an ORNL technical report.
- Coordination activities with Dr. K. L. Peddicord and French educational institution for their possible involvement in educational activities at the Moscow Engineering Physics Institute on subjects related to plutonium disposition and nuclear materials safety management education.
- Coordination of some activities related to the possible involvement of the water reactors group faculties with the Nuclear Energy Agency's work on plutonium studies.

Activities related to information support included expansion of the Nuclear Group Internal Technical Working Documents series by three reports and three updates of the Calendar of Conferences located at <http://trinity.tamu.edu/~igor/hi.html> (May 24, June 10, and July 11). This quarter also saw a redesign of the Nuclear Group home page to enhance its appearance, readability, and ease of use. Several new links were added.

Sub-project participants also began an overhaul and update of a database for tracking Nuclear Group deliverables. Dr. Carron accepted leadership for this task, with direction from Dr. Nelson and organizational support from Ms. Alexander and Mrs. Payton.

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

- Coordinating with the Electronic Resource Library (ERL) and the Center on documents to be added to the ERL electronic database.
- Updating different people involved in Center and the Nuclear Group activities of news and information relevant to their activities.
- Providing technical explanations and assistance to Ms. Alexander in the editing and production of Nuclear Group Internal Technical Working Documents.

Ms. Alexander assumed primary responsibility for coordinating, compiling, and editing the proceedings of the NATO Advanced Research Workshop on "Nuclear Materials Safety Management" and for editing and arranging the publication of the Moscow Engineering Physics Institute FY 1996 final report. Both documents are expected to be published next quarter.

INTERNATIONAL STUDIES

Support of Russian Activities

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

During this quarter, Dr. Marvin Adams continued to fulfill his duties as a member of the US/RF joint study team for the water reactor option for disposition of weapons Plutonium. In this capacity, he participated in meetings in Moscow May 12-14 as a member of the US delegation. In addition, Drs. Abdurrahman, Adams, Carron, Parish, and Yavuz (as well as their students) continued to support the US/RF joint study team by benchmarking various reactor-analysis codes. A draft report including this group's results was issued by ORNL on May 2 ("Neutronics Benchmarks for the Utilization of Mixed Oxide Fuel – Updated Progress Report for Fiscal Year 1997, Volumes I-IV, May 2, 1997). The final report on these benchmark studies is expected to be issued in August, and the Center's team continues to provide input for that.

Dr. K. L. Peddicord followed up with the Institute of Nuclear Power Engineering (INPE) regarding the development of a directory of nuclear engineering faculty in Russia. He also participated in coordinating the visit to The University of Texas and Texas A&M University of Alexander Tsyboulia of the Institute of Physics and Power Engineering (IPPE).

Dr. David Boyle coordinated addition of a new task, funded by the Communication, Education, and Training division of the Center, which provides a "Special English" course for the MEPhI MS program in nuclear materials management.

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

A partial computational domain for phase III modeling has been completed for the Pantex facility. The domain includes eight AT-400A containers stacked vertically on each side of the walkspace for a total of sixteen containers.

Air velocity and temperature distributions have been predicted for the partial domain for two different inlet conditions. For the first case, cool air entered through the ceiling and exited through the walkspace on the floor. The air velocity accelerated as the flow reached the AT-400A containers closest to the ceiling. The flow around most of the AT-400A containers in the stack on each side of the walkspace was very small indicating that most of the air moves in between the stacks in the walkspace. The predicted air temperature distribution showed that the hottest location occurred around the third stack of AT-400A containers from the floor and not the containers actually closest to the floor. The second case simulated had cool air entering through the walkspace on the floor and exiting through the ceiling. The location of the hot spot of air within the stack of AT-400A containers changed to the containers located nearest to the floor. The maximum temperature decreased by three percent although the temperature distribution around most of the AT-400A containers increased when compared to the case of air entering through the ceiling and exiting through the floor.

We are currently extending the partial phase III domain to the full phase III domain. The full phase III computational domain will possibly be composed of twenty two of the partial domains, since one row at the Pantex facility will include nominally 22 stacks, giving a total of some 704 AT-400A containers to be included in the model. Current grid generation limitations might reduce the number of AT-400A containers; however, we have been looking into other grid generation packages so that grid limitations concerning the number of sub-domains that constitute the computational domain can be eliminated.

Milestone: Manageable computational grid for flow around cylinders for both facilities to be completed for a section of the full computational domain. Completed 7/97. Extension to full computational domain expected to be finished in late September to early October of 1997. Predicted completion date for full domain was 7/97.

Automation, Robotics, and Tele-Operation

Pls: 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-Pls: 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. It appears that most of the funds will be spent well before the year is out. Several (at least 4) students will be finishing or have finished by early fall 1997. Their thesis and resulting papers will be supplied to the Center in fulfillment of the deliverables.

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. 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 they 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 Inter Agent 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 3-D Teleoperational Task

- Literature Review (completed)

The initial phase of this study began with a review of the human engineering literature related to three-dimensional tele-operational task. Among various tele-operation sensing requirements, the television (depth perception) requirement was investigated in detail. The review included literature regarding: (1) various depth cues relevant to human depth perception; (2) psychological principles in display design; (3) display formats including 2-D planar, 3-D perspective, and stereoscopic displays; (4) operator hand control; and (5) measures of tele-operation performance.

- Formalization of the Experiment (completed)

Based on the literature, a laboratory experiment was proposed and formalized. The task to be used in the experiment will be picking up a virtual object and placing it into a storage rack in a simulated tele-operational task environment. The experiment will include as independent variables, visual display formats (such as 2-D planar, perspective, and stereoscopic displays), visual enhancement types, and task difficulty. The dependent measures will include time to completion, number of errors, subjective ratings of workload, and end effector motion. Five male and five female subjects will serve as participants in this study. They will be recruited from the student population at Texas Tech University.

- Development of the Computer Simulation (completed)

The equipment used for this experiment include a Silicon Graphics Indigo 2 (SGI Indigo 2) workstation, a six-degree-of freedom Spaceball 2003 and Crystal Eyes 2 eye wear with an emitter. The workstation is equipped with 4 GB hard disk, 192 MB RAM, a MIPS R 4400 processor with a frequency of 250 Mhz, and a 21" monitor with a resolution of 1280 × 1024. The experimental task was constructed using TELEGRIP (the software release No. 3.0) software running on the SGI Indigo2. Other computer tools were required for the development of the computer simulation. These included tools (external Motif and C language) for the development of appropriate interface displays to integrate with the simulation, and for development of algorithm to interface the Spaceball 2003.

- Preparation for the Experiment (in progress)

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 has been distributed to his dissertation committee, and a preliminary exam is being scheduled. In addition, a proposal to use human subjects has been submitted to the Institutional Review Board at Texas Tech University. Preparations for the experiment are almost complete and we anticipate beginning the experiment some time in September.

Safety and Reliability

The self-assessment of survival (reliability) project demonstration unit is in the programming stage, with both the system user interface and data modeling algorithms in progress. Efforts include programming in LabWindows and C++. A limited demonstration should be ready in the

September-October time frame. This demonstration will serve to establish proof of concept in a real-time environment, as well as to serve as the centerpiece for Mr. H. Lu's doctoral research and dissertation. One presentation was made this quarter regarding this project.

The prototype controller project is now complete. One presentation was made this quarter regarding the prototype controller project. A copy of Ms. S. Patro's doctoral dissertation has been forwarded to the nuclear group at Texas A&M.

The conclusion of Mr. H. Lu's doctoral research work (as described above), and description in his dissertation, will bring items this task to completion. Completion is expected in December 1997.

Presentations and Publications

H. Lu and W. Kolarik, "Time Series Modeling of System Self-Assessment of Survival," Proceedings of the 6th Annual Industrial Engineering Research Conference, pp. 1-6, 1997.

S. Patro and W. Kolarik, "Intelli-Control An Intelligent Process and Quality control Application Prototype," Proceedings of the 6th Annual Industrial Engineering Research Conference, pp. 95-100, 1997.

S. Patro, "Neural Networks and Evolutionary Computation For Real-Time Quality Control," Ph.D. Dissertation, Department of Industrial Engineering, Texas Tech University, May, 1997.

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

The theory that will be used to add contact/impact with flexibility into the simulation testbed is being verified via experimental work being completed by two graduate students. As reported last time, the planar manipulator testbed will be used to verify the flexible body contact/impact model used. This testbed will be ready for data acquisition in late August or early September. The simulation models for the contact/impact are complete. In another project the theory used to model closed loop flexible machines, where the loop closure constraint is interior to the domain of the flexible components. The simulation models are nearing completion and an experimental configuration will be completed in mid to late August. In work related to the contact aspects of gripping objects, another master thesis is nearing completion, with satisfactory simulation results. No experimental investigation was planned for this work. Several papers have resulted from work supported totally or partially by the Center. An updated list of accepted papers is provided, and other papers in review will be included in subsequent reports.

Presentations and Publications

Barhorst, A. A. (1997). Symbolic Equation Processing Utilizing Vector/Dyad Notation. *Journal of Sound and Vibration*, accepted for publication.

Ortiz, J. L. and Barhorst A. A. (1997). Closed-Form Modeling of Fluid-Structure Interaction Problems with Nonlinear Sloshing--Potential Flow. *AIAA Journal*, 35(9):1510--1517.

Ortiz, J. L. and Barhorst A. A. (1997). Large-Displacement Nonlinear Sloshing in 2-D Circular Rigid Containers--Prescribed Motion of the Container. *International Journal of Numerical Methods in Engineering*, accepted for publication.

Barhorst, A. A and Volz, R. A. and Kondraske, G. V. (1997). Robotics, Automation, and Tele-Operation Program for Safe Handling and Long-Term Storage of Nuclear Components. *In Proceedings of The ANS 7th Topical Meeting on Robotics & Remote Systems*. April 27--May 1, 1997, Augusta, GA.

The University of Texas-Austin

Mobile Platforms

We are continuing our development of the modular simulator for wheeled mobile robots. We have developed motion planning, system-level control, and dynamic simulation algorithms that are all compatible with the modularity of simulator. This work has also led to some new perspectives on kinematic synthesis of mobile robots. We have written one article and are in the process of writing two more articles this summer. We will submit these articles to the center in the near future.

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

Progress continued on the development of the slowing down time spectrometer with the main focus during this quarter being on the setup and testing of the neutron generator that will drive the slowing down time spectrometer. Several design issues were addressed and completed:

- We have succeeded in achieving a minimum vacuum level in our system of $3.0\text{E-}6$ Torr ($1\text{ atm.}=760\text{ Torr}$). This was done using the turbo/roughing pump system that we currently have. We anticipate that by the end of 8/97 we will install an ion pump that will improve on this number and help achieve a $1.0\text{E-}6$ Torr (or better) level on routine basis.
- We have conducted tritium release calculations to insure compliance with NRC and Texas regulations during the testing and operations of the generator. The calculations will be part of a comprehensive document that will be presented as part of the licensing of the generator as a radiation producing machine. The licensing procedure is expected to be completed by the end of 9/97.
- We have designed the radiation monitoring procedures for the neutron generator laboratory. This involved acquiring neutron and gamma-ray monitors and computing the maximum doses expected from our system. We are currently working on interlocking the monitors with the generator to insure proper compliance with regulatory limits.
- The cooling system for the generator has been designed and its parts have been ordered. The system is based on a circulating cooler that will provide water to cool the bending magnet, the beam catcher, the target holder and the turbo pump. The water lines to perform this task are currently in place and we expect to test the cooling system by the end of 8/97.

The design of the graphite structure that will be used for the spectrometer has been completed. The graphite pile will be a rectangle that is 100 cm. x 100 cm x 120 cm. The neutron source will penetrate the 100 cm x 100 cm surface and be placed at the center of this rectangle. The sample will be placed off center at around 33 cm. from the surfaces. Neutron detectors will surround the sample. This construction will be finished by the end of 8/97.

Computationally, we are continuing our MCNP work to model, realistically, a graphite slowing down time spectrometer (see previous quarterly reports). Our efforts are currently focused on two tasks. The first task is to establish, using our previously constructed models, the ability to extract the masses of the fissile materials from measurements made in a graphite assay device. The second task is to model our experimental setup and use the results as a benchmark to guide our laboratory work. Both efforts are expected to end by 11/97.

Presentations and Publications

Several papers have either been presented and published or accepted for presentation at the American Nuclear Society meetings as follows:

M. A. Elsayi, N. M. Abdurrahman, A. I. Hawari, and B. W. Wehring, "The Use of Graphite for Slowing Down Time Spectrometry," was presented at the 1997 Annual Meeting of the American Nuclear Society and published in *Trans. Am. Nucl. Soc.*, 76, 139 (1997).

A. I. Hawari, N. M. Abdurrahman, and B. W. Wehring, "Neutron Sources for Nondestructive Assay of Nuclear Materials Using Slowing Down Time Spectrometry," was presented at the 1997 Annual Meeting of the American Nuclear Society and published in Trans. Am. Nucl. Soc., 76, 143 (1997).

N. M. Abdurrahman, M. A. Elsayi, D. R. Harris, "Resolution Function in Slowing Down Time Assay Devices," has been submitted and accepted for presentation at the 1997 Winter Meeting of the American Nuclear Society

STORAGE: FACILITY ANALYSIS

Aircraft Overflight

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

Accident Probability and Consequence Analyses

The State of Texas recommended in the Pantex Site-Wide EIS that there is a continuing need for monitoring the radar tracks of aircraft flying in and around Amarillo Airport and the Pantex Plant. The intent is to assure information necessary to properly evaluate the evolving risk of an aircraft accident into plutonium storage facilities at the Plant. At the request of the Department of Energy, Dr. McNerney and Dr. Rock evaluated the requirements of radar monitoring and submitted recommendations to the Department of Energy. It was recommended that a commercially available radar monitoring and flight tracking product with a widely installed base at airports be provided at the Amarillo Airport. Currently, there are three vendors that supply such system to US airports: TRACOR, HMMH, and the Flood Group. The TRACOR system was endorsed by the research team.

As of August 3, 1997, B.K. Cooper of Tracor reported that he has not yet submitted a written proposal. We encouraged him to do so. Analysis has been completed on the air traffic data provided by Tom Golder of Lamb Associates. Unfortunately, the data was not sufficient to allow the research team to further assess aircraft accident risks at the site because it does not allow one to identify the type of aircraft associated with the flight track. It will be necessary during the next quarter to obtain more detailed traffic data for the Amarillo airport in order to make further progress. If DOE does not install an automated system for collecting air traffic data, this data will have to be obtained from Amarillo Airport and possibly from the US Air Force for the military air traffic.

Dr. Rock and his research assistant Jacqueline Kiffe are making great progress in preparing reports on the intellectual efforts dedicated to improving accident algorithms for the highest level of screening analysis. Below, under Milestones and Deliverables we list the manuscripts in preparation with projected delivery dates.

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

Post Explosion Transport (PET) Study

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 plutonium 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 a new package of codes which will provide a framework for running the now complete PET code. This package, now essentially finished, will fulfill the role that was originally intended to be played by the MELCOR library. This will allow more expedient solutions of the complete post-explosion transient simulation, with consistent and more accurate time-stepping and less computational overhead. The new package also enables full two-dimensional modeling of conduction through the cell walls, unlike MELCOR, which was limited to a one-dimensional approximation. Furthermore, the new package will allow researchers to make changes to the solution procedure with considerably greater ease.

The final stage of this research effort is now underway. 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 by December, 1997.

STORAGE: STORAGE/SHIPPING CONTAINERS

Radiation Degradation

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

Microstructural and Surface Studies of Stainless Steel

The study on understanding material problems in stainless steel that may be caused by high fluence irradiation of alpha particles from Pu progressed this quarter with emphasis on electron microscopy. The primary accomplishments were: improvements of the TEM and SEM sample handling/preparation procedures, observations of implanted and unimplanted initial samples using SEM and TEM, and analyses of initial implanted samples using neutron depth profiling.

Several samples were prepared for SEM analysis and implanted with He-3 ions with fluences between $1 \times 10^{16}/\text{cm}^2$ and $1 \times 10^{17}/\text{cm}^2$. Micrographs were taken at different magnifications and compared to unimplanted samples. The surface structures of high implant and low implant samples show distinct differences, but, at this stage, it is not clear whether these differences can be attributed to the sample handling procedure or the helium implantation. More samples will be analyzed in order to have a correct assessment of this behavior. The same samples were analyzed using neutron depth profiling, and the results were compared to the TRIM-90 code. As was expected, good agreement with NDP and TRIM-90 was found. To improve the performance of NDP even further higher resolution detectors will be employed for future NDP studies.

The preparation of samples suitable for TEM initially caused difficulties due to the fact that both the electrolyte used and the operating parameters needed to be optimized for stainless steel. After improving the procedure, satisfactory TEM samples were obtained and analyzed. The initial results show that for doses of $1 \times 10^{16}/\text{cm}^2$ and $3 \times 10^{16}/\text{cm}^2$ only minimal effects on the microstructure are visible as compared to unimplanted samples. At these low fluences no helium bubbles were observed. More samples will be prepared and implanted with higher He-3 doses as the study progresses.

Air Monitoring

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

Texas Tech University

During the previous reporting quarter, we had conducted the Ce (III) aerosol collection and analysis. The current quarter was earmarked for fabrication of combined aerosol collection and spectroscopic analysis system. We have successfully fabricated the combined system by resolving all the interfacing problems.

In order to minimize interfacing problems, liquid flow rates to and from the particle collection system have to be controlled and balanced with that for spectroscopic analysis system. Lower sample injection rates through the analytical system than that of particle collection system liquid effluent flow rates will lead to loss of sample and thus underestimation of the analyte. The reverse situation, i.e. higher sample injection rate to the analytical system, on the other hand, will cause air loading to the concentrator columns leading to noisy response. Increased flow rate through particle collection system is beneficial in quantitative collection of particles from larger volume air sample. Where as, increased sample flow rates through the analytical system will cause flow restriction. Liquid flow rates were adjusted to get best signal to noise conditions. We had also modified the means of liquid pumping and aspiration from the particle collection system, in order to eliminate potential interference from an unknown substance leaching out from the peristaltic pump tubing. In the current configuration, a HPLC pump and a syringe pump are utilized for liquid transfer to and from particle collection system, respectively. Other minor interfacing problems also have been solved. The combined collection analysis system was used to analyze lab generated test Ce(III) aerosol. Early results indicates that the system can reliably measure Ce(III) in the levels of lower double digit ng Ce(III) per cubic meter of aerosol.

With this, we have successfully completed the fabrication of combined aerosol collection analysis system.

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

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

Sandia has loaned Texas A&M University a surplus tritium transportation container for use as the laboratory experimental chamber for this project. It was delivered in late March and a new cap for the container has been fabricated to facilitate the measurements of conductivity with argon gas back fill as well as with room air. A Ludlum electrometer board has been delivered for use in the conductivity measurements where it serves as the primary amplifier to drive the signal-recording instrumentation. As of the time of submission of this report, electronics development is in progress with the expectation that the program of measurements will begin during August, 1997. This marks a delay of at least a month due to unforeseen difficulties in detection circuitry.

The basic computational model for gas conductivity due to isolated radioactive decays has been completed. A calculated example showed distinct differences between the electron and ion pulses due to alpha decay in argon gas. In both cases, the amplitudes of the pulses in a weak electric field due to electrodes separated by 20 cm. are easily within the measurable range and their temporal characteristic are sufficiently different to be readily measurable. The preliminary report of this work has been pub-

lished as *Technical Summary: Feasibility Study of Conductivity Monitoring for Leak Detection in Double-Walled Plutonium Containers*, ANRCP-NG-ITWD-97-05.

DISPOSITION: WATER REACTOR OPTIONS

MOX Fuel Fabrication: Gallium Removal and Interactions with Zircalloy Cladding

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

Progress continued in our experimental studies of gallium removal processes. In a long term experiment, we showed that the gallium level could be reduced to below 20 PPM. In the 40 hour experiment, the 1%Ga₂O₃ in CeO₂ was reduced and removed by a flow of H₂ in a quartz reactor maintained at 900°C. A gas manifold has been added to the experimental system to allow experiments using Ar/H₂ and other mixed gases as the reducing gas. The reactor system has also been improved by replacing the Tygon tubing with Stainless steel tubing connected to the quartz reactor with special Swagelok fittings using Vespel/Graphite ferrules. A DRIFT(diffused reflectance) accessory has been installed on the FTIR instrument and is used for mid IR spectral measurements of oxide matrices. A Micromeritic ASAP2000 has been set up for BET surface area and pore size distribution determinations of the solid oxide matrices before and after the gallium removal tests.

The ICP gallium analytical method under development in the Department of Chemistry at Texas Tech has been used verify >90% removal of gallium from the cerium oxide matrices. The process for extraction of gallium oxide from cerium oxide before analysis needs to be improved to increase the sensitivity of the analysis and precision of the results. However, the only reason for the sensitivity limitation is that the surrogate cerium oxide has lines very close to those of gallium oxide. With plutonium oxide this should not be a problem, so the method should be useful as it stands in the "real" situation.

The project to study thermally-driven gallium-clad interactions at TAMU's Nuclear Science Center (NSC) continues to make progress. NSC staff, working in collaboration with ORNL and LANL, has completed the design specifications for the heaters that will be used to heat annular fuel pellets embedded with gallium. The heaters have been ordered and are expected to arrive in October. When fuel is available from LANL (expected November), the heaters will be fitted into the annular fuel and cladding and the experiment will begin. Meanwhile, the NSC staff has designed and built a prototype system that is approximately half the size of the future experiment. The prototype is being used to study coolant flow rates and temperatures, to verify the computer model of the experiment, and to test safety systems.

Progress continued on beam-driven studies of the interaction of Ga with fuel cladding. Transmission electron microscopy at 40,000x has been successfully performed on unimplanted samples of Zirc-IV. Although a Zr ion beam has been obtained, the lifetime of the ion source is presently too short to allow high fluence implantations. Redesigned source components have been fabricated to correct this problem. So that ion beam fluence may be better correlated with cladding damage in the reactor environment, computer modeling of fission-fragment-induced lattice displacements in Zircaloy is underway.

MOX Use In Reactors: Water Reactor Options for Disposition of Weapons Plutonium

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

Center researchers continued to collaborate with counterparts from Russia and from ORNL on benchmarking neutronics codes for calculations involving the use of MOX fuel from weapons-grade Pu. A substantial set of calculations was delivered to ORNL for inclusion in the final FY97 report of the US/Russia Joint Study Team on Water-Reactor Options. Our calculations included WIMS/DIF3D and WIMS/TWODANT modeling of the US LWR benchmark problem, WIMS/DIF3D modeling of the Russian VVER benchmark problem, WIMS/DIF3D modeling of 65 of the "Saxton" critical experiments, and

others. Several papers related to this work were submitted and presented; see the deliverables section below. As part of this effort, a software package is being developed to generate assembly-level burnup data using WIMS pin-cell depletions and DIF3D and/or TWODANT assembly calculations. In addition, MCNP has been used to generate two-group cross sections for MOX and uranium pin cells, for comparison against WIMS results. In other benchmarking work, final revisions were made of two evaluations and sample MCNP calculations for Battelle-Pacific Northwest Laboratory Split Table Critical experiments containing Mixed-Oxide Fuels. In addition, sample MCNP calculations with thermal treatment were performed on the evaluation "CS4-Low-Moderated Mixtures of Plutonium and Uranium Oxides with 8, 15, and 30 wt% Plutonium," and on the evaluations "CS3-Homogeneous PuO_2 -

Polystyrene at Low Hydrogen Content," pages 31-41 and 24-30, respectively, in ORNL Fissile Materials Disposition Program, May 2nd, 1997 Report. Finally, to facilitate the MCNP calculation of several benchmark problems, NJOY was used to create cross section libraries at several temperatures that are specified in the problems, and these libraries were tested.

Progress continued in our studies of the utilization of MOX fuel in domestic reactors. The study on burning MOX and producing tritium in the same reactor has been completed, as instructed by the Center, and a report summarizing this work is being generated. In addition, our work to quantify various MOX fuel-cycle strategies is now poised for rapid progress, for we now have reasonable confidence in the accuracy of our CASMO/SIMULATE model for MOX cores.

Drs. Abdurrahman and Adams attended the Annual Meeting of the American Nuclear Society and co-chaired the special session that they had organized: "Analysis Methods for Reactors with Mixed-Oxide Fuel."

Presentations and Publications

Edward James Reott, "Mixed Oxide Fuel Data Repository: MOXDAR," MS Thesis, The University of Texas at Austin, May 1997.

Georgeta Radulescu, "MCNP Critical Benchmarks for Mixed Oxide Lattices of the Saxton Plutonium Program," MS Thesis, The University of Texas at Austin, August 1997.

A paper entitled, "Gallium Interactions with Zircaloy Cladding," by Ron R. Hart, John Rennie, Kenan Unlu, and Carlos Rios-Martinez has been accepted for presentation at the Plutonium Future - The Science Conference, Santa Fe, New Mexico, August 25-27, 1997.

A paper has been drafted and submitted for presentation at the American Nuclear Society's 1997 Winter Meeting describing the use of MCNP to generate 2-group cross sections.

A paper entitled "Analysis of Enriched Uranium and Weapons Plutonium Reloads for PWRs Using BRACC" was presented at the 1997 Annual Meeting of the American Nuclear Society and published in the proceedings [Trans. Am. Nucl. Soc. Vol 76, pp 187-189 (1997)].

A paper entitled "Analysis of PNL Critical Experiments Performed Using Rectangular Parallelepipeds Containing MOX Fuels" was presented at the 1997 Annual Meeting of the American Nuclear Society and published in the proceedings [Trans. Am. Nucl. Soc. Vol 76, p. 247 (1997)].

A paper entitled "MCNP Criticality Benchmark Calculations of The Saxton Plutonium Program Experiments" was presented at the 1997 Annual Meeting of the ANS and published in the proceedings [Trans. Am. Nucl. Soc., 76, p. 231 (1997)].

A paper summarizing the TAMU Saxton Critical benchmarking work was submitted and accepted for presentation at the American Nuclear Society's 1997 Winter Meeting.

A paper entitled "MCNP Analysis of PNL Split Table Critical Experiments Containing Mixed-Oxide Fuels" was submitted and accepted for presentation at the ANS 1997 Winter Meeting.

A paper entitled "Criticality Benchmark Calculations Of Saxton-67 With MCNP" was submitted and accepted for presentation at the ANS 1997 Winter Meeting.

MOX Use in Reactors: Mixed Oxide Fuel Evaluation

PI: K. L. Peddicord, The Texas A&M University

The effort this quarter focused on evaluation of data to be used for the development of thermal modeling of oxide fuel at high burnups. These data have been obtained by Belgonucléaire through their international fuel irradiation programs as well through in-house experiments. A meeting was held on June 5 with Belgonucléaire to discuss these issues as well as other aspects of the Memorandum of Agreement between Belgonucléaire and the Texas Engineering Experiment Station. The other principal effort was the preparation and submission of the application by John Alvis to obtain a work permit from the Belgian federal authorities to enable him to spend a year at Belgonucléaire to develop the 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. It is anticipated that Mr. Alvis will go to Brussels in mid-August. Because of the delay in the issuing of the work permit, the milestone/deliverable list of the Task Plan have been revised accordingly. An additional deliverable was included involving the completion of an extensive bibliography of references for fuel performance modeling of MOX fuel. This will be published during the next quarter.

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 examine experimental data from international fuel irradiation programs. These data will serve as the basis for 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.

As part of this effort, K. L. Peddicord met with Marc Lippens and Didier Haas of Belgonucléaire (BN) on June 5, 1997. Discussions were held about the irradiation data which Belgonucléaire has obtained for oxide fuel over a number of years. BN has organized a number of international programs with participants from Europe, North America and Japan to carry out specialized irradiation experiments to examine various physical effects. In addition, BN has carried out in-house irradiation programs as well. The results represent a rich source of information on a number of phenomena.

Primary attention in the modeling will be given to the changes in the thermal response of oxide fuel as a function of burn up. Typically the exposures of fuel in light water reactor fuel cycles in Europe have not reached the same level as that used by utilities in the United States. As a result, there is a need to extend the modeling of thermal behavior, such as that incorporated into the COMETHE fuel performance code, to higher burn ups. COMETHE is one of the few fuel codes which has the capability to handle MOX fuel. This forms the basis of the Memorandum of Agreement concluded with Belgonucléaire. The advanced thermal models developed by John Alvis during his stay at Belgonucléaire will be incorporated into the COMETHE code. BN will then provide COMETHE for five years. The code will be used for the analysis of the thermal and mechanical behavior of mixed oxide fuel manufactured from weapons plutonium.

During this quarter, an additional deliverable was included. An extensive bibliography of references relating to the modeling of the performance of mixed oxide fuel was prepared and will be published. In addition, an abstract for paper was submitted to the NATO Advanced Research Workshop on "Safety Issues Associated with Plutonium Involvement in Nuclear Fuel Cycles". The paper will be presented at the Workshop which will held on September 1-5, 1997, in Moscow. The abstract was forwarded as well to the Amarillo Center. Finally, all paperwork has been submitted by John Alvis to the Belgian

federal authorities for the work permit which will be needed for his collaboration with Belgonucléaire. It is anticipated that this should be received shortly. Because of the delay, the milestone/deliverable list of the Task Plan has been adjusted to accommodate 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 plutonium. 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 plutonium. 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 rule-set 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: Dr. H. Mahmassani, The University of Texas at Austin

During the period of May 1 to July 31, 1997, work continued on developing an *a priority* routing algorithm for strategic nuclear materials that would enable more thorough risk assessment of potential highway routes. The model developed is a modification of a time-dependent least-cost path algorithm (TDLCP) originally developed for use in dynamic assignment problems for Intelligent Transportation Systems (ITS). Unlike the current routing model, 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 model 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 model is being tested for a real highway network extending from the Pantex Plant in Amarillo, Texas, to the Savannah River Site in Aiken, South Carolina. A Geographic Information System (GIS) was used to obtain the "cost" of traveling on a highway link. In this example network, cost was defined

as the residential population living within one mile of a highway link. Work has begun to propose a methodology that can be used to estimate a day-time population. Currently, data sources from the Department of Census such as the Census Transportation Planning Package, are being examined and State agencies who may prepare natural disaster evacuation plans which consider time-of-day variations in population densities are being contacted.

During the next period, the results from the example transportation network will be analyzed and a final report will be submitted.

A final report was submitted to the Center entitled "Review of Routing Criteria and Models for Radioactive Materials" by authors Laurie Bowler and Hani S. Mahmassani, June 1997.

A final report was submitted to the Center entitled "Optimal Routing of Spent Plutonium and other Hazardous Substances in Time-Varying, Stochastic Transportation Networks" by authors Elise Miller Hooks and Hani S. Mahmassani, July 1997.

Ms. Elise Miller-Hooks completed her doctoral dissertation titled "Optimal Routing In Time-Varying, Stochastic Networks: Algorithms and Implementations," June 1997."

Ms. Elise Miller-Hooks and Hani S. Mahmassani submitted for a paper for possible presentation at the 77th Annual Meeting of the Transportation Research Board, January 1998, Washington, D.C. and publication in *Transportation Research Record*., titled "Optimal Routing of Hazardous Materials in Stochastic, Time-Varying Transportation Networks," July 1997.

Modeling for Safe Routing

Dr. P. Nelson, TX A&M University

Task 2 of sub-project 2 (Modeling for Safe Routing and Transport of Surplus Weapons Fissile Material) was to "demonstrate the capability to apply the TRANSNET software, especially its radiological hazard assessment component (RADTRAN-4) by in fact applying it to hypothetical scenarios of interest." The associated milestone was to "complete one or more studies of comparative risks associated with different options conceivably arising under hypothetical scenarios of interest." This milestone was in fact reached, and the associated deliverable was the technical report authored by Ms. Amy Baker Caldwell, entitled "Risk Analysis of Shipping Plutonium Pits and Mixed Oxide Fuel," which was completed and published in the Nuclear Group Internal Technical Working Documents Series, July 3, 1997, Document No. ANRCP-NG-ITWD-97-07.

The following technical report has been completed and published in the Nuclear Group Internal Technical Working Documents Series: "Risk Analysis of Shipping Plutonium Pits and Mixed-Oxide Fuels," A. B. Caldwell, Texas A&M University, July 3, 1997. Document No. ANRCP-NG-ITWD-97-07

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

Dr. William Marlow and Dr. Yassin A. Hassan, , TX A&M University

A test case has been developed to validate the particle pattern behavior. This test case can be applied to plutonium as well as other particles. Due to the unavailability of exact solutions for most of the actual applications, a comparison between the program predictions and a simple test case having a known solution was conducted. Efforts are now being concentrated to obtain a reasonable description of the statistical behavior of the flow.

Application of Existing Codes and Techniques

Dr. R. Radha and Dr. Z. Huque, Prairie View A&M University

Progress continued on Transportation Analysis and application of codes and techniques. During this period, Mr. R. Santhappan, a graduate student in Civil Engineering, has developed expertise in the use and application of the TRANSNET program and especially the Highway Program. A method was identified to estimate the population along the selected route. The population will be computed by considering a corridor width along the route, density of population from census bureau, and using Geographical Information Systems Program. Efforts continue toward development of techniques to determine population exposure. This will enable avoiding dense population areas and keeping potential impact on the population as low as possible due to transportation of plutonium pits and mixed oxide fuels along the selected routes.

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

Dr. Don C. Wunsch II, Texas Tech University

No new information to report for this quarter. Completion of a publication report is currently underway and will be reported next quarter.

DISPOSITION: GEOLOGIC DISPOSAL

Immobilization: "Can-In-Canister" Option

PI: K.S. Ball, Ph.D., The University of Texas at Austin

Co-PIs: E.M. Talef, Ph.D., The University of Texas at Austin; T.L. Bergman, Ph.D., The University of Connecticut; E.E. Anderson, Ph.D., J.F. Cardenas-Garcia, Ph.D., and J Hashemi, Ph.D., Texas Tech University

Progress continued on room temperature experiments using analogous fluid (corn syrup) over a range of mass-flow rates and viscosities. By controlling temperature of the analogous fluid during each experiment viscosity was controlled at specific values typical of the molten glass during pouring. Results of the void fraction measurements at low mass flow rates are inconclusive because of scatter in the data. A clear trend has been observed at the highest mass flow rate (310 lb/hr), where the measured void fraction of the pour was inversely proportional to viscosity. This result is contrary to initial observations using a more limited set of data.

Progress continued in developing a detailed 2-D computational model of the glass pour which includes heat transfer and previous difficulties concerning software capabilities have been overcome. The computational fluid dynamics and heat transfer software FLOW-3D (Flow Science, Inc.) was purchased to replace the FIDAP (Fluent, Inc.) software, which was previously found not to handle heat transfer adequately in the desired problems. Preliminary results obtained from several 2-D simulations, both with and without heat transfer, indicate that FLOW-3D is capable of adequately handling both fluid flow and heat transfer.

Progress continued on high-temperature experiments. Initial flow visualization experiments were conducted, and preliminary visual data have been obtained for air flow about the falling jet of molten DWPF glass. The furnace was refurbished to correct wear from the high temperature experiments. A brief report detailing temperature profiles in the canister during filling experiments has been prepared for LLNL.

The 2-D Finite Element model of a glass pour using the can-in-canister configuration was finished and a Master of Science thesis and an Center Report are being finalized. The effect of different boundary conditions on the residual stress levels in the glass pour structure were examined. Additionally, the maximum principal stress criterion was used to assess the stress state and; determine crack formation

and direction of crack extension. Progress continues on the 3-D finite element modeling of the glass pour structure. The renewal of a grant from the Pittsburgh Supercomputing Center has allowed the resumption of work in this area after temporary delays.

Ceramic Materials for Immobilization of Plutonium

PI: A. Clearfield, Texas A&M University

Progress continues on the incorporation of materials into the perovskite phase BaZrO_3 . Cerium (IV) (our model for plutonium) was incorporated to a maximum of forty-eight mole percent in barium zirconate. Studies are now in progress to determine the maximum loading of uranium (VI) and the incorporation of both cerium and uranium simultaneously in the same phase. Initially, both UO_2 and UO_3 were used as starting materials. However, the products resulting from reaction at 1300°C in air were identical indicating the uranium (IV) oxidized to uranium (VI) during reaction. Problems previously noted in the incorporation of hafnium as a neutron sorber are under investigation. It has been suggested that barium hafnate (BaHfO_3) may form as a kinetic product in the mixtures, altering reaction conditions by leaving composition. We are continuing to study the solid solution ranges of uranium and hafnium in barium zirconate and cerium and uranium in barium hafnate. The presence of barium uranate (BaUO_4) has been noted as an impurity phase in the uranium loaded materials. This compound has been synthesized in pure form and structural analysis is in progress to determine exact atom positions so that two-phase Rietveld refinement of the uranium loaded compounds may be performed. Work is continuing on exploring the solid solution limits of the zirconolite phase.

Disposal: Disposition in Deep Boreholes

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 further development of a well testing code to interpret sequential hydraulic tests in low-permeability fractured media. A paper - Interpretation of Sequential Hydraulic Tests in Low-Transmissivity Fractured Media was submitted to *Water Resources Research*. This paper presents a new analytical solution for the interpretation of such tests and demonstrates the use of the solution on real test data from a hydraulic test in Switzerland. A second paper - Effect of Pre-Test Pressures and Temperature on Drill Stem Test Interpretation - was accepted and will be presented this fall at the Society of Petroleum Engineers (SPE) conference.

Geosphere Characterization

Considerable effort has been applied to the characterization of low-permeability heterogeneous formations. A primary reason for the increased activity is the importance of estimating formation properties for use in safety assessments at proposed nuclear-waste disposal sites, such as those in Switzerland, Germany, Sweden, and the USA. Methods for determining formation properties (e.g. transmissivity, static head, storativity, flow boundaries) are varied, but hydraulic testing is commonly used.

Hydraulic tests in low-permeability media typically consist of a sequence of multiple test events such as slug, constant pressure, and pulse tests. Each single test event can significantly affect the measured pressure response of subsequent test events. The pressure response can also be affected by borehole mud pressures that occur prior to testing (i.e. pre-test pressures) and other factors such as wellbore storage, wellbore skin, and wellbore temperature.

A new analytical solution has been developed that accounts for all of the above mentioned complexities. The solution technique treats a sequence of pre-test pressures and multiple test events (slugs, pulses, and shut-ins) as one test sequence, thereby accounting for the influence of one test event upon another. The solution is derived so that only a kernel function, the constant-rate pumping test solution, is required for new flow models. Furthermore, the solution is presented for any flow dimension allowing for interpretation in fractured formations where linear, radial, and fractional flow may exist. The solution is used to characterize the geosphere by inverse modeling to estimate the flow model and parameters.

Future Work

Future work on geosphere characterization is based on the remaining funds from the previous year's budget. Work planned is to examine the effect of nonlinear terms on the pressure response in low-permeability fractured formations. These nonlinear terms are normally neglected in the pressure continuity equation and could impact the interpretation of hydraulic tests in low-permeability media. Subsequent work will focus on the inclusion of constant-rate and pressure tests in the sequential analytical solution already developed.

ACRONYMS

2-D	2 Dimensional
3-D	3 Dimensional
AC	Amarillo College
ANRCP	Amarillo National Resource Center for Plutonium
ANS	American Nuclear Society
CET	Communication, Education, and Training
Cr	Chromium
DEL	Document Exchange Laboratory
DNA	Deoxyribonucleic Acid
DOD	US Department of Defense
DOE	US Department of Energy
DRIFT	Diffused Reflectance
DTIC	Defense Technical Information Center
EIS	Environmental Impact Statement
EPA	Environmental Protection Agency
ER	Environmental Restoration
ERL	Electronic Resource Library
FCR	Ferric Chelate Reductase
Fe	Iron
FFA	Future Farmers of America
FIDAP	Fluent, Inc.
FLOW-3D	Flow Science, Inc.
FTP	File Transfer Protocol
FY	Fiscal Year
Ga	Gallium
GAC	Granular Activated Carbon
GIS	Geographic Information System
HE	High Explosives
HMX	octahydro-1,3,5,7-tetranitro-1,3,5,7-tetraazocine
HPLC	High Performance Liquid Chromatography
INIS	International Nuclear Information System
INPE	Institute of Nuclear Power Engineering
IPPE	Institute of Physics and Power Engineering

ITWD	Internal Technical Working Document
LANL	Los Alamos National Laboratory
LLNL	Lawrence Livermore National Laboratory
MAUA	Multi-attribute Utility Analysis
MePhI	Moscow Engineering Physics Institute
MOX	Mixed Oxide Fuel
MOXDAR	Mixed Oxide Fuel Data Repository
NATO	North Atlantic Treaty Organization
NDP	Neutron Depth Profiling
NG	Nuclear Group
NSC	Nuclear Science Center
NTIS	National Technical Information Service
OCLC	On-Line Computer Library Center
ORNL	Oak Ridge National Laboratory
OSTI	Office of Scientific and Technical Information
P	Phosphorus
PDF	Portable Document Format
PET	Post Explosion Transport
RADP	Randomly Amplified Polymorphic DNA
RDX	hexahydro-1,3,5-trinitro-1,3,5-triazine
RSSCTs	Rapid Small-Scale Column Tests
SPE	Society of Petroleum Engineers
SRC	Soil Reduction Capacity
SRS	Savannah River Site
SSCS	Storage System Construction Set
STATSGO	Soil Sample Database
TAMU	Texas A&M University
TELEGRIP	Software that simulates the motions of robotic devices in virtual reality
TexPREP	Texas Pre-Freshman Engineering Program
TIF	Tagged Information File
TNRCC	Texas Natural Resource Conservation Commission
TTU	Texas Tech University
USA	United States of America
UT	The University of Texas at Austin
UT-Arl	The University of Texas at Arlington
UT-Austin	The University of Texas at Austin

UTCHEM	Three dimensional chemical flood simulator
VR	Virtual Reality
VR4	Virtual Reality 4
WTEP	West Texas Environmental Project