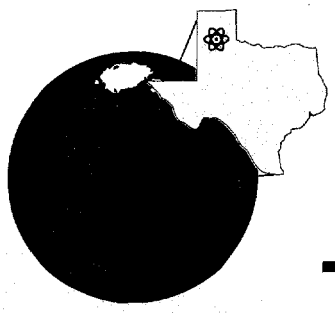

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The Amarillo National Resource Center for Plutonium

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

Quarterly Progress Detailed Report

1 November 1996 through 31 January 1997

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CENTER PROGRAMS

PLUTONIUM INFORMATION RESOURCE

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PLUTONIUM INFORMATION RESOURCE

ELECTRONIC RESOURCE LIBRARY

Electronic Resource Library

Co-PI: Mr. George Huffman, Amarillo College
Co-PI: Dale Cluff, Ph.D., Texas Tech University
Karen Ruddy, Ph.D., Researcher and Information Scientist, Amarillo College

The Plutonium Information Resource task is known as the Electronic Resource Library (ERL), which is managed within Communication, Education, and Training. Refer to the appended section for the ERL to see the project management checklist.

The ERL was established as a World Wide Web entity on January 2, 1997 at http://plutonium-erl.actx.edu. The ERL is a state-of-the-art electronic library and information retrieval system that serves as the Center's resource for further development of the national archive of historical, policy, and technical information on plutonium.

Amarillo College (AC) provided an electronic on-line system that facilitates document selection and retrieval and is available to users through the Internet and Z39.50 compatible research library networks. Progress was made toward establishing the World Wide Web presence of the ERL across the networks with over 100 links to other Internet and Telnet locations containing information about plutonium. Hypertext links make the exponentially expanding information-base on plutonium available via the Internet readily and easily retrievable by the users of the ERL.

The Document Exchange Laboratory at AC Lynn Library is in full operation with two shifts per day providing over 100 hours per week of document exchange from paper form to digital form with progress toward complete electronic exchange of documents throughout the DOE complex by the year 2000. This is in congruence with the electronic exchange initiative of the Office of Scientific and Technical Information.

Progress was made toward establishing the second Document Exchange Laboratory at Texas Tech University (TTU) Library with the TTU site moving forward on three tasks:

1. Continuation of the bibliographic project to identify, document, and compile all materials on plutonium published in the Government Research Annual Index (GRAI) from 1988 back to 1986.
2. Completion of training on the use of the National Technical Information Service (NTIS) database that is available through the Electronic Reserve Room on the ERL server hosted on the AC campus. This new resource will allow the bibliography to be finished back to 1983 quickly.
3. Resolution of network installation problems and investigation of local usage of Adobe software.

AC successfully coordinated planning and implementation of the ERL with federal agencies and the national laboratories, meeting the goal of achieving the access requirements set forth in March of 1994 by the National Coordinating Committee on Technology in Education and Training. AC made progress toward establishing an electronic document exchange federation at DOE laboratories, DOE headquarters, and other federal agencies that are engaged in digitizing materials in order to track full text/image documents across the Internet with the goal of sharing records and saving labor and other costs associated with duplicate scanning efforts

AC successfully implemented a functional and efficient Portable Document Format (PDF) conversion and presentation system with 100 full text/image documents available through the ERL web pages. AC made progress toward obtaining rights and permissions for delivering electronic versions of copyright and intellectual property materials to the ERL users.

AC successfully initiated the development of core literature for specific sub-disciplines by compiling the MOXBIB (mixed-oxide fuel bibliography), and FWRBIB (fast water reactor bibliography) and making them accessible through the Electronic Reserve Room of the ERL. AC made progress toward collaborating with Texas A&M University and The University of Texas researchers on the establishment of the core literature.

AC successfully established the ERL as a subscriber to the following indexing and abstracting services: Nuclear Science Abstracts 1948 to 1976, NTIS 1964 to present, International Nuclear Information System (INIS) 1976 to the present; as well as the following document delivery services: Canada Institute for Scientific and Technical Information (CISTI), the Genuine Article (full text access to the Institute for Scientific Information, Inc., or ISI), The British Library Document Supply Centre (BLD) and University Microfilm Inc. (UMI).

AC successfully contracted with the AMIGOS Bibliographic Council, regional office of On-line Computer Library Center (OCLC) for access to library resources from DIALOG (Knight-Ridder), Silver Platter Information, Inc., and host of CD-ROM, bibliographic, document delivery, on-line database services; thus establishing the ERL as a subject-specific service provider/interface for users.

The Z39.50 gateway through the Harrington Library Consortia Web On-line Catalog of the DOE Reading Room Collection was implemented.

ADVISORY FUNCTION

DOE SUPPORT

Senior Technical Review Group (STRG)

Bill Harris, Director, Amarillo National Resource Center for Plutonium

We finished and distributed the STRG report on Business Arrangements for implementing MOX title "Recommendations for Government/Industry Cooperation to Disable Weapons Plutonium in Nuclear Power Plants".

The following is a complete list of reports:

- "Screening Process to Determine Reasonable Alternatives for Storage and Disposition of Weapons-Usable Fissile materials"; March 1995.
- "Long-Range Research and Development Plan Fissile Materials Disposition Program"; July 1995.
- "A Methodology for the Analysis and Selection of Alternatives for the Disposition of Surplus Plutonium"; September 1995.
- "The Overall Fissile materials Disposition Program; Plutonium Immobilization Alternatives; Join US/Russian Work; and Deep Borehole Disposition"; February 1996.
- "Comments and Recommendations Based on the PEIS Briefings and Reactor-Based Plutonium Disposition Options"; March 1996.
- "Review of the Office of Fissile Materials Disposition Technical Summary Report for Surplus Weapons-Usable Plutonium Disposition", July 1996.
- "Comments on the Predecisional Draft of the Joint US/Russian Study of Plutonium Disposition Options Steering Committee Summary Report"; August 1996.
- "Recommendations for Government/Industry cooperation to Disable Weapons Plutonium in Nuclear Power Plants"; September 1996.

Multiattribute Utility Analysis Team (MAUA)

Co-PIs: James S. Dyer, Ph.D., and John C. Butler, Ph.D. The University of Texas at Austin

Progress was made on the report "Analysis and Selection of Alternatives for the Disposition of Surplus Plutonium". Final data requirements were received from OFMD and a preliminary analysis was completed. This first draft has been reviewed by Howard Canter and his comments will be incorporated before Feb. 20. The report is viewed as favorable to OFMD and does support the Record of Decision (ROD). In particular, we analyzed the use of "hybrid" alternatives where R&D and licensing efforts are pursued for two technologies in parallel. This analysis demonstrates that the use of such a hybrid is optimal for certain probabilities that Russian policy will require the degradation of weapons-grade plutonium. In addition, the report supports the ROD by demonstrating that the recommended technologies consistently outperform other alternatives under a wide variety of measure weights and assumptions.

The report should be ready for release by March 1, 1997. We have also been working on the Methodology Report which will be co-released with the results on March 1, 1997.

We plan to continue working with Department of Energy (DOE) on several other issues: business relationships with MOX fabricators and utilities, alternative site selection, and additional analyses as needed to support DOE/OFMD's recommendation.

STATE SUPPORT

Pantex Economic Impact (Perryman)

Bill Harris, Director, Amarillo National Resource Center for Plutonium

The Perryman report was widely distributed, and planning on Perryman briefings has begun.

ENVIRONMENTAL, PUBLIC HEALTH AND SAFETY

CURRENT ENVIRONMENTAL, HEALTH AND SAFETY

Aquifer Testing, Tracer Tests, And Produced Water Treatment

PI: Randall Charbeneau, Ph.D., P.E., The University of Texas at Austin
Co-PI: Joseph F. Malina, Jr., Ph.D., The University of Texas at Austin

During the past quarter, researchers at the University of Texas at Austin (UT) were involved in two major subtasks in this project area. The first sub-task involves the perched aquifer tracer test performed at the Zone 12 Treatability System. The second sub-task involves evaluation of disposal of produced water through the Pantex Plant treatment system.

The perched aquifer tracer test, originally proposed for commencement on June 1, 1996, officially began on July 15, 1996, and continued into this quarter, terminating on September 19. Treatment system effluent (free of dissolved High Explosives-HE) was dosed with potassium bromide which serves as a conservative tracer, and injected into well PV-4 in the Center of the treatability system well pattern. Water was produced from the three extraction wells, EW-1, 2, and 3, and concentrations of bromide and HE were monitored. The results from the tracer test will be interpreted to characterize solute transport within the perched aquifer and provide evidence of HE displacement and recovery using groundwater recirculation. The field test and chemical analyses were carried out by researchers at Texas Tech University, while the data analysis, interpretation and modeling are being performed by researchers at UT. Efforts during the last quarter have concentrated on calibration of flow and transport models (MODFLOW and MT3D). Calibration of groundwater hydraulics is nearly complete, and solute transport calibration is ongoing. This work should be finalized soon after the remaining data are received, and a final report will be submitted during the present quarter.

The purpose of the evaluation of the Pantex Plant wastewater treatment system was to determine its capacity to treat additional wastewater and still operate with a no-discharge permit. This provides an early-warning analysis in case an alternative treatment system becomes necessary to treat the produced water from the groundwater remediation program. This sub-task was completed, and a final report submitted.

Aquifer Testing, Tracer Tests, And Produced Water Treatment

PI: Ken Rainwater, Ph.D., P.E., Texas Tech University
Co-PIs: Heyward Ramsey, Ph.D., David Thompson, Ph.D., Lloyd Urban, Ph.D., Tony Mollhagen Ph.D., and Rick Zartman, Ph.D., Texas Tech University

During the past quarter, researchers at Texas Tech University were involved in two major subtasks in this project area. The first sub-task involves the perched aquifer tracer test performed at the Zone 12 Treatability System (ZTTS). The second sub-task includes field and modeling efforts for investigation of potential wetlands enhancement by discharging future treated effluent from the perched aquifer recovery systems to the ditch and playa system at the Pantex Plant. The third sub-task consisted of equilibrium isotherm tests for sorption of HMX and RDX on core materials from the perched aquifer and its aquitard. Progress for the first two subtasks is reported in the following paragraphs.

The perched aquifer tracer test, originally proposed for commencement on June 1, 1996, officially began on July 15, 1996, and continued into this quarter.

The ZTTS as modified ran continuously for 53 days, then was interrupted by several temporary power failures beginning on September 6, and the test was finally terminated on September 19. Complete raw data packages of the measured concentrations and water levels have been provided as they became available to the researchers at UT-Austin for related modeling. A complete report of the collected tracer test data was provided in January, 1997.

The investigation of potential wetlands enhancement through the discharge of treated perched aquifer effluent into the ditch and playa system will allow evaluation of this concept as an alternative to direction injection through wells. This effort has three major components. First, during July, 1996, double-ring infiltrometer tests were performed at selected sites in Playas 2, 3, 4, and 5, and in the ditches that lead to all five playas on the Plant. The data from those tests were evaluated and interpreted for application in hydrologic modeling. Second, the hydrologic modeling to simulate the increase in inundated area in each playa that might be caused by introduction of up to 400 gpm in the ditch system leading to each playa is currently on-going. Those simulations were completed in this quarter. Those results will be used in the next quarter to evaluate the potential ecological modifications that would result from the increased flows to each playa. The report summarizing these findings will be produced by May 1, 1997. The work continues as a no-cost extension.

Combined Oxidation And Bioremediation Of High Explosives

Aydin Akgerman, Ph.D., P.E., Texas A&M University

Groundwater investigations have shown that the perched aquifer beneath Zones 11 and 12 is contaminated with high explosives (HE) such as RDX, HMX, TNT, AND TNB. Studies on bioremediation of HE have shown that the first step in ring cleavage in bioremediation is the slowest step and as the molecules get smaller, the bioremediation rate increases significantly. This work explores the possibility of combining catalytic (or UV/ozone or UV/H_2O_2/ozone) oxidation with bioremediation. Other studies have shown that the first ring cleavage step is the fastest in catalytic oxidation whereas the reaction slows down for oxidation of the smallest molecules. Hence, a combined reaction scheme of catalytic oxidation/bioremediation might be the optimum solution for destruction of HE.

During this period we have studied catalytic oxidation of TNT and RDX in solution over the Pt/TiO_2 catalyst at different temperatures and at different catalyst amounts. The reaction is studied using both total organic carbon and HPLC analysis. A detailed report is included.

Biodegradation Of High Explosives

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

The first quarter of the 1997 fiscal year of funding was initiated with the primary objectives of rejuvenating the RDX acclimated microbial population and performing initial exposure studies to assess chromium toxicity. The first task was to determine an appropriate concentration of hexavalent chromium (Cr[VI]) to be used in acclimation reactors and to observe the inhibitory effects of Cr(VI) on culture growth and RDX degradation. The Alderson Playa culture previously used in kinetic studies by others was exposed to duplicate reactors with varying levels of Cr(VI) in Oxoid Nutrient Broth #2 (Oxoid Ltd., London, England) with 5 mg/l of RDX present. Chromium was added as potassium dichromate ($K_2Cr_2O_7$) from a stock solution of 300 mg/l in water. Na_2EDTA was added as a complexation agent on an equimolar basis with Cr(VI) to insure that all of the Cr(VI) remained in solution. Biomass was added from Oxoid reactors that had been spiked with the Alderson Playa culture and undergone two weeks of recent enrichment in Oxoid with 5 mg/l RDX and 1 mg/L HMX. To measure growth, two 0.5 ml samples were taken from each reactor, diluted 1:10 in phosphate buffer (pH = 7.0) and analyzed in duplicate for optical density at 600 nm via spectrophotometer. Culture growth was monitored as a function of time to assess Cr(VI) inhibition. The results support preliminary experiments that demonstrated an inhibition in growth at Cr(VI) levels above 2.0 mg/l. After nearly 4 days, the growth in the reactors containing 1.0 mg/l Cr(VI) were the same as those containing no Cr(VI). The reactors containing 5 mg/l had nearly the same level of growth, but a level of inhibition was clear. While the reactors with 10 mg/l and 20 mg/l Cr(VI) demonstrated growth at nearly every sampling stage, a strong level of inhibition was evident. Samples from the present experiment have been taken for future HPLC analysis to determine the effect of Cr(VI) on RDX degradation. These have yet to be run. However, preliminary experiments revealed that removal rates of RDX in Oxoid after several days were insignificantly different for Cr(VI) concentrations lower than 2.5 mg/l; whereas higher concentrations of Cr(VI) severely limited RDX degradation. From the work done so far with Cr(VI), it appears that Cr(VI) is inhibitory. This inhi-

bition is observed as reduced growth rates and suppressed RDX degradation by the Alderson Playa culture in Oxoid at Cr(VI) levels greater than 2.0 mg/l. Consequently, the Cr(VI) concentration for acclimation reactors will be in the range of 1.0-1.5 mg/l, below the inhibition level.

Identification Of High Explosives Degrading Microorganisms

PI: Caryl E. Heintz, Ph.D., Texas Tech University
Co-PIs: Tony Mollhagen, Ph.D., and Ken Rainwater, Ph.D., P.E., Texas Tech University

The goal of this sub-task was to characterize, and identify if possible, bacterial isolates capable of degrading HMX and/or RDX submitted to us at Texas Tech University (TTU) by Dr. Robin Autenrieth at Texas A&M University (TAMU). In addition, the carbon and nitrogen sources these organisms were capable of metabolizing and the optimum ratios of carbon to nitrogen for growth were to be determined by TTU. The purpose was to provide information to Dr. Autenrieth who would design a culture medium which would support the growth of the organisms in a biofilm. Establishment of the biofilm on granular activated carbon and evaluation of its ability to degrade high explosives was to be accomplished by Dr. Gerry Speitel at University of Texas (UT).

During this quarter, no organisms were received from TAMU. Therefore, to advance toward the goal of funding and identifying aerobic bacteria capable of degrading RDX and/or HMX, we felt our time and resources would best be invested by developing a procedure that could be used for screening large numbers of contaminated soil samples for the presence of High Explosives (HE)-degrading bacteria. This report presents progress to date.

Our screening method was based on the premise that the presence of nitramine explosives in soils or water provides an opportunity for growth of bacteria which are able to use these compounds as an energy source or as a carbon and/or nitrogen source for growth. Since the pendant groups attached to the rings of both RDX and HMX are nitrites, the best HE-degrading organisms in HE-contaminated samples should be able to use nitrites as a nutrient.

Using standard bacteriological techniques, we examined soil collected in October 1995 from the burning ground at the Pantex site for the presence of nitrite-utilizing chemolithotrophic bacteria. Few heterotrophic organisms can grow using inorganic nitrogen sources only. Using a chemolithotrophic culture medium containing potassium nitrite as the sole source of nitrogen, we isolated 10 strains of nitrite-utilizing bacteria from the burning ground and maintained them in culture in the laboratory for performing the following tests:

a) the ability to be maintained on subculture on chemolithotrophic and chemoheterotrophic media
b) the ability to grow on a culture medium containing 10 ppm RDX
c) the ability to utilize RDX at an initial concentration of 10 ppm.

All isolates grew under the first two conditions. Authentic samples of RDX were first received in December of 1996, and experiments are in progress to determine the ability of these isolates to degrade RDX. These tests are to be completed by May 1997, at which time the funding terminates.

Development Of Biofilm Treatment For High Explosives

Co-PIs: Tony Mollhagen, Ph.D., and Caryl Heintz, Ph.D., Texas Tech University

It is assumed that microbial degraders will be present where any non-toxic, metabolizable substance is present because microbes will adapt to exploit available energy or nutrient resources. In the context of the Pantex Plant, it follows that sites with long-term contamination by High Explosives (HE) will potentially have microbes that have developed the capacity to degrade HE for nutrients or energy. Thus one might expect the highest potential of these kinds of microbes at historical burning grounds, landfills, ditches, sludge basins, and Playas 1, 3 and 4.

This sub-task was to begin to evaluate the potential of organisms occurring in soils or sediments at historical burning grounds, landfills, ditches, sludge basins, and Playas 1, 3 and 4. However, funding for the project arrived so late that only a few candidate soils were examined under very limited conditions. Soil samples were obtained only from the burning grounds, the ditch leaving Zone 12, and all three of the playas.

There were only four experiments. Replicated sequencing batch reactors, were respectively seeded with soil from the ditch leaving Zone 12 and from Playas 2, 3, and 4. They were maintained under aggressive aeration, at 30C, for more than 90 days. All received a single, initial feeding of 6 mg/L HMX. Sucrose was supplied as a carbon source at a minimalist C:N ration of 20:1. Replicated controls (with HMX, without seed) and blanks (without HMX, with seed) were maintained with the treatments.

As funds were received too late to complete the work, and its continuation was not funded by the Center in the present year, there are few meaningful results.

Under the conditions of all the experiments, HMX was degraded from 6 to 4.5 mg/L in a little more than 70 days. HMX levels in the controls also declined but not to the same extent. The difference, however, was not significant for the period of study.

It is clear that the study conditions do not offer much potential for developing either an in situ soil treatment strategy or an above-ground pump-and-treat technology for contaminated groundwater.

Chemical Models And Redox Chemistry Of Chromium

PI: Bill Batchelor, Ph.D., P.E., Texas A&M University
Co-PIs: Elizabeth Carraway, Ph.D., Mark Schlautman, Ph.D., Bruce Herbert, Ph.D., Texas A&M University

A series of solution experiments were conducted to investigate the effects of natural organic matter (NOM) on the reduction of hexavalent chromium by ferrous iron. The results show that Cr(VI) reduction by Fe(II) in the presence of oxygen and humic acid was strongly dependent on pH. In the absence of humic acid, the reaction rate for Cr(VI) reduction increased with increasing pH. In the presence of humic acid, however, the rate of Cr(VI) reduction decreased with increasing pH. Cr(VI) reduction by Fe(II) at pH 4 and 5 appears to have been enhanced by humic acid at shorter time periods, but may be adversely affected at longer time periods. At pH 6, Cr(VI) reduction by Fe(II) was always adversely affected by the presence of humic acid. In general, higher humic acid concentrations at lower pH values had the largest effect on the overall reduction of Cr(VI) by Fe(II). These results were presented at the 1996 Fall meeting of the American Geophysical Union.

The experiment to test the reoxidation potential of chromium in Pantex soils has been continued during this quarter. Samples from the reactors were collected; however, due to problems with the ICP-MS chromium analysis has not been possible. Once the ICP-MS has been fixed, the collected samples will be analyzed and data reported. Because of our sampling/analysis methodology, no deleterious effects are expected with the longer than normal sample storage.

A milestone report on zero valent metal (ZVM) remediation of chromium, chlorinated organics and high explosives was submitted during this quarter (January, 1997). A series of reduction experiments was conducted with trichloroethene (TCE) at low initial concentrations (~ 20 ppm) and two ZVMs – iron (Fe^0) and palladized iron (Pd/Fe^0). The low initial concentration of TCE was selected in order to more closely match the concentrations found at the Pantex site. The first-order kinetic analysis of these reduction experiments shows that the half-life of TCE decreases substantially with decreasing TCE-to-ZVM ratios. The rate constants predict half-lives of 88 hours for iron (Fe^0) and 8 hours for palladized iron (Pd/Fe^0). These values are almost fourteen and twenty five times faster than those obtained at 540 ppm TCE for iron (Fe^0) and palladized iron (Pd/Fe^0), respectively. Results from experiments containing both TCE (20 ppm and 540 ppm) and Cr(VI) (2000 ppb) indicate no competition for reduction sites between the target contaminants. Overall, our results to date indicate that the use of ZVMs, particularly palladized iron, could result in rapid (time scale of 8 hours or less) simultaneous removal of both TCE and Cr(VI). Analysis of the reduc-

tion of a model explosive, dinitrotoluene (2,4-DNT), by ZVMs could not be completed because of instrumentation problems.

Soil Vapor Extraction Model Development

PI: Ken Rainwater, Ph.D., P.E., Texas Tech University

In this task area, the TTU research team is responsible for the development of a two-dimensional computer model to allow simulation of the soil-vapor extraction process, allowing for placement of extraction and passive vent wells in an unsaturated porous medium with a known initial distribution of residual liquid volatile organic contaminants (VOCs). The Pantex Plant includes several sites with known or potential residual VOCs from fuel or solvent losses. This project builds on previous experience at TTU in large-scale experiments and radial-flow modeling of soil-vapor extraction. The finite difference modeling approach taken in this research is somewhat unique in that the model accounts for the changes in air permeability over time as the VOC liquids are evaporated and removed.

During this quarter, the coupled model for a single VOC component was completed. A detailed report on the mathematical development of the model with demonstration of its application to a single component in a small scale solution domain was submitted to the Center. Work in the last quarter has focused on upgrading the model for multi-component VOC mixtures and modifying the solution procedure to allow increases in the spatial and temporal step sizes for application to larger scale problems. Work in the next quarter will include development of the graphical user interface to facilitate general use.

Sorption Of Volatile Organic Compounds At Pantex

Aydin Akgerman, Ph.D., P.E., Texas A&M University

Ongoing work has shown that the most important parameters that control the soil vapor extraction of volatile organic compounds (VOCs) from soil are the adsorption isotherm parameters for adsorption of VOCs on soil, the interaction of VOCs with each other during desorption, and the effect of water (present as soil moisture) on the VOCs' desorption from soil. This research investigates each of these factors as it applies to VOCs existing in Pantex soils.

During this quarter we continued our studies on binary mixture adsorption using a well defined adsorbent, and started the experiments for isotherm measurements in presence of water. The experiment on the effects of water on VOC adsorption are temporary put on hold due to equipment problems. A detailed report is included.

Chromium Sorption On Pantex Soils

PI: Ken Rainwater, Ph.D., P.E., Texas Tech University
Co-PIs: Heyward Ramsey, Ph.D., and Tony Mollhagen, Ph.D., Texas Tech University

Chromium contamination at levels of a few mg/L have long been noted, primarily in and near Zone 12, at the Pantex Plant. Work by TTU researchers in the previous quarters included a report on potential Cr-waste-waters discharged by the former cooling tower in Zone 12 and equilibrium isotherm tests of Cr sorption on core materials from the perched aquifer and its aquitard. In this quarter, one-dimensional column tests were performed to observe Cr sorption under flow conditions.

One-dimensional column tests for Cr sorption under flow conditions were originally planned under this sub-task. These tests were delayed by the request from Dr. Randy Charbeneau to proceed with the HE sorption isotherms immediately after the Cr isotherms. During this quarter, 1-D column tests were performed using columns 25 cm long and 2.5 cm in diameter. The column tests were performed in the same manner as similar tests done previously by TTU researchers with core material from well BEG-PTX-02. A low-flow, high-pressure pump was used to drive a flow of a few mL/min. through the packed columns. The injected solution was Pantex groundwater with added Br and Cr concentrations at 10 mg/L each. The ef-

fluent concentrations of Br and Cr were measured and used to calculate dispersion and retardation coefficients.

In the previous progress report, it was planned to complete both the tests and the report of results by January 15, 1997. However, unexpected difficulties with the pump and the packed columns delayed the experiment completion. Great care was necessary to prevent clogging of the flow apparatus by transport of fine-grained particles over the duration of a test. Some tests had to be suspended and repeated to get proper continuous flow conditions. The tests were completed, and the report of these tests will be submitted by February 28, 1997.

FUTURE ENVIRONMENTAL, HEALTH AND SAFETY

Phytoaccumulation Of Selected Heavy Metals, Uranium, And Plutonium In Plants

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

Research is continuing in the field, greenhouse, and laboratory to identify plants that will accumulate/exclude Cr and the actinide elements. The mechanisms involved in accumulation/exclusion and transport of Cr were the focus of research activities during this period.

A field experiment to determine Cr tolerance of common field crops in the High Plains of Texas has been initiated at Lubbock using a number of cool season species including wheat, rye, bromegrass, alfalfa, clover, and canola. Severely cold weather during late December has caused some winter kill in some species. The extent of the damage will not be known until growth resumes in the spring. The 100 mg CrIII/kg soil treatment reduced growth rates of nearly all species in two different soil textures under field conditions. A second series of greenhouse experiments was initiated using canola and wheat as cool season species. The tissue samples from the first series of greenhouse experiments evaluating sorghum and sunflower as accumulators are being analyzed.

Plant species have been tested in nutrient culture for their tolerance to CrIII and CrVI. Chromium VI was the most toxic Cr source to plants but there are measured differences between Cr translocation from the roots to shoots among Cr sources. All species tested continued to grow in 0.04 mM CrVI or CrIII. None of the species grew in 1.0 mM Cr VI. Only two species (soybean and canola) continued to grow in 0.2 mM CrVI and 1.0 mM CrIII. Thus these two concentrations are being used for future screenings of Cr-tolerant species. Loblolly pine appears to tolerate I mM CrIII, but its overall growth, even with the controls, is very low. In summarizing in vivo and in vito experiments it is apparent that soybean is more tolerant of Cr than is sunflower, We hypothesize that either sunflower accumulates more Cr than does soybean or that soybean can sequester its Cr, and therefore can tolerate higher levels. We are in the process of testing this hypothesis by measuring the Cr content in the organs of each species. We are comparing the amount of Cr in each organ with each species as well as between species. From these data, we are assessing and comparing the capability of these two species to absorb and translocate Cr. Furthermore, by comparing their growth and accumulation performance, we will then be able to determine the cellular and physiological bases of accumulation. For sunflower, the highest concentration was 20,240 mg/kg in roots with 1.0 mM CrIII and was 6,285 mg/kg in shoots with 1.0 mM CrVI. For soybean the highest concentration was 11,900 mg/kg in roots with 1.0 mM CrIII, and 1,400 mg/kg in shoots with 1.0 mM CrVI. Sunflower Cr accumulation appears to be greater than that of soybean.

Previous experiments showed that Cucumis sativum (cv. lemon cucumber) avoids uptake and translocation of CrIII by an unknown mechanism. Recent experiments have shown that this remains the case when CrIII is complexed with the fungal siderophore (a natural Fe chelating agent) ferrichrome. Roots of plants exposed to chromic ferrichrome (CrFe) did absorb Cr, especially in the plants that were supplied with Fe as well. Little transport to the shoots occurred, with a maximum of 2.1 µg/g Cr detected in the shoots of the -Fe/+CrFe plants. However, this results in a phytoextraction coefficient (ratio of final concentration in the shoots, to the initial concentration in the growth medium) of about 20. The rhizofiltration coefficient (similar to phytoextraction coefficient but considered the amount of metal absorbed by the roots) was a respectable 2,340. However, cucumber roots had also exhibited good rhizofiltration behavior in a previ-

ous experiment using CrIII with ferrichrome. Ferric chelate reductase (FCR) assays were performed on the roots of freshly harvested plants. Interestingly, the FCR activity of Fe-stressed plants was inhibited (<0.5 µmol/g fresh weight/hour) in plants that were lacking both Fe and CrFe.

Plants have been collected from a serpentinaceous deposit (Coal Creek Serpentinite, Gillespie County) and some have been screened for Cr accumulation. The soil from this site does not seem to contain high levels of Cr (31.5 mg/g) despite the presence of serpentine. Opuntia sp., Yucca sp. and agarita from this site do not contain notable Cr concentrations.

POLLUTION PREVENTION AND AVOIDANCE

Alternative Uses For High Explosives

C.G. Willson (PI), The University of Texas at Austin
Co-PIs: M.A. Hale, D.T. Clausi, The University of Texas at Austin; B. Combs, K. Kuhrts, Pantex Division of the Mason & Hanger Corp.; J. Hashemi and D. James, Department of Mechanical Engineering, Texas Tech University; Geoffrey Lindsay, Rich Hollins, Naval Air Warfare Center Weapons Division (NAWCWD), China Lake, CA

Progress continued on the development of a three dimensional compression design intended to use waste explosives recovered from dismantled nuclear weapons to compress C60 with the goal of transforming the fullerenes into diamond. This is a collaborative effort involving modeling work at TTU and Pantex, machining at Pantex and UT, and materials analysis at UT. A fourth compaction test was performed on November 8, 1996 and the work piece was recovered intact. This represents a significant accomplishment toward the ultimate goal of this project. We now have a working design which allows for the study of materials under extreme temperatures and pressures. Analysis of the sample material after detonation revealed only the presence of graphite. The C60 was completely converted but there was no evidence of the presence of diamond by either Raman spectroscopy or X-ray diffraction. We believe that this experiment produced diamond, but the pressure was reduced before there was sufficient cooling. The next tests will focus on quenching.

Work has continued on the development of a one dimensional compression design capable of achieving pressures needed for the destruction of C60 while maintaining the ability to recover the entire sample. Changes in the mass and standoff distance of the flyer have been investigated to increase the compression pulse. At the same time, impacting plates of varying thickness have been added to ensure full recovery of the sample. Once these studies have been completed, a matrix of experiments has been designed for one dimensional compressions. These compressions allow rapid and inexpensive investigation of sample additives and verification of sample characterization techniques.

Work has also progressed on the development of a pelletized fuel used as a means of recovering some of the energy contained within the waste explosive. The waste explosive will be ground to a size less than its critical diameter, mixed with unrecyclable polymer, and bound in the form of a pellet. Safe combustion of this pelletized fuel to generate heat that can be converted to electrical energy provides a means to turn this high energy explosive into a resource. Studies have been done at Pantex investigating the limits of the hydro-machining process to rubbleize various explosives to a safe and workable size. Numerous binder materials have been tested at UT and at the China Lake Naval Weapons Center based on binding ability, cost, combustibility, and environmental impact. Several appear as viable options.

COMMUNICATION, EDUCATION, AND TRAINING

PROGRAM IMPLEMENTATION

Program Management

Communication, Education, and Training (CET) is responsible for Task 1, Task 4, and training. The training program continues to evolve; no activity this quarter. 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 six plus one graduate assistant - no change over the previous quarter.

For the reporting period, graduate assistant Alcantar assisted the Center's Education Program Coordinator with the Center's exhibit program and worked with the Building Foundations for Mathematics and Science Success research project.

Program management has been engaged in the following:

- Guiding the Electronic Resource Library project which came on-line in January, 1997 (Refer to Task 1);
- Planning the NATO workshop on Nuclear Materials Safety Management that will be held in Amarillo in March;
- Guiding the co-development of the Agriculture Communication and Education Schedule with representatives from the Texas panhandle agriculture community which was delivered in January and is a documented effort to advance information exchange between elements of the Texas Panhandle agriculture community and the Center;
- Performing human resource needs analysis within CET in order to fill the positions of Information Resource Specialist, Training Program Coordinator, Science Information and Resource Center Project Coordinator, and Community Liaison;
- Strategic planning;
- Drafting the Center's publication policy; and
- Furthering education and outreach collaborations with the Pantex Plant Citizens Advisory Board and the DOE.

During this quarter, communication program personnel:

- Brought the Center's World Wide Web site on-line (see http://www.pu.org).
- Continued to develop the Center's Speakers Bureau and prepared fourteen speeches including the following:

11/20/96	Amarillo National Bank officers
11/20/96	Boatmen's First National Bank officers in Amarillo
12/04/96	Downtown Amarillo Kiwanis Club
12/05/96	Agriculture community of the Texas Panhandle
12/12/96	Pantex Neighbors
1/02/97	Kiwanis Club of the Texas High Plains
1/11/97	American Association of University Women in Amarillo
1/27/97	Carson County Commissioners
1/29/97	Amarillo Chamber of Commerce
1/30/97	Austin Rotary

- Revised the Center's information brochure (refer to the appended section for CET to see an example).
- Published Volume II issue IV of the Center's newsletter with a distribution of 4,500 which included 3,000 to Pantex personnel (refer to the appended section for CET to see the issue).

- Published three different guest editorials in November and December, one by Dr. Margaret Maxey in the Dallas Morning News, Plano Star Courier, El Paso Times, Bay City Daily Tribune, Victoria Advocate, and Corpus Christi Caller Times and two by Amarillo community leaders Zerm and Patterson in the Amarillo Globe News.
- Published two letters to the editor on November 17, one by Bill Harris and the other by Elda Zounar, both from the Center, in the Amarillo Globe News (refer to the appended section for CET to see the letters).

The communication program personnel continued to develop and implement the Communication Program Plan as follows:

- Met with the Editorial Board of the Amarillo Globe News (12/9/96) that lead to an Amarillo Globe News editorial.
- Prepared an interview with KGNC Radio in Amarillo (12/12/96) and local television networks for Bill Harris and Rick Hartley of the Center (1/28/97).
- Briefed the staff of Texas Senator Teel Bivins on issues related to the work of the Center (1/7/97).
- Generated a series of at least ten letters to the DOE and state political officials supporting the DOE decision on mixed-oxide fuel fabrication.
- Distributed a series of Dallas Morning News editorials (1/19/97 - 1/21/97) on the relationship between mixed-oxide fuel and the Center statewide to the various newspaper, radio, and television media; and to key political officials at the state and federal levels.
- Facilitated interviews with the Houston Chronicle and a Texas Tech University publication, The Agriculturist on 1/29/97 and 1/31/97 respectively.

During this quarter, K-16 education program personnel:

- Co-sponsored with Southwestern Bell the third annual Student Research Conference at West Texas A&M University in November. Thirty schools from Texas, New Mexico, and Kansas participated in this event which allowed graduate students to present their research projects to peers and panels of judges. Students of award winning research projects received cash prizes. (Refer to the appended section of CET for the Call for Papers and the November 17th editorial "Kudos to WTAMU" by Zounar.)
- Represented the Center at the National Association of Partners in Education (NAPE) conference in Washington, DC in November. The theme was Children at the Center: Partnerships Linking Education, Community & Economic Development. (Refer to the appended section of CET for a trip report to the conference.)
- Committed funds to support the Pantex Plant Regional Science Bowl in February and the Amarillo College High Plains Science Fair in March.
- Continued to work with Amarillo Independent School District (AISD) on the Caprock Cluster Tech Lab project.

The Technology Laboratory at Fannin Middle School is in the final stages of installation with implementation expected to begin by mid-February. The lab is designed to accommodate all seventh and eighth-grade science students in the school and will enable students to focus on the scientific method with opportunities for research to synthesize and support hypotheses. With the system's multi-faceted graphing and weather station, students will collect, analyze and graph weather data in Palo Duro Canyon. This station will enable users to project weather patterns for the distant future. Math programs and publishing software will broaden the possibilities for student learning. In addition, the lab features a dual platform with Macintosh and IBM, and will provide an Internet connection and a variety of reference software pieces.

At Caprock High School, the advanced technology laboratory opened with five twelfth-grade students who are focused on research in their career areas. Upon completion of their research projects, students will make formal presentations to an audience of community and school representatives, thus providing the assessment piece for their projects. Student projects include:

(a) medical research - three students are working with a physician at Harvard Medical School and local doctors; (b) investigation of life on Mars - one student is working with space-exploration scientists; and (c) use of plutonium in the Texas panhandle - one student will produce a brochure.

The 1997 Spring semester is the pilot period and these students will receive only high school credit for their work. Future students will receive credit for the Distinguished Achievement Program which will be applied toward graduation.

- Continued the Center's exhibit program by coordinating with Pantex personnel to plan, set-up, and staff an exhibit at the Amarillo Farm and Ranch Show (12/3 - 12/5/96). The exhibits were "Plutonium Past, Present, and Future" and mixed-oxide fuel research.

Implementation Of Grant Funded Projects

Proposals for the following projects (including the Electronic Resource Library in Task 1) were processed and projects were initiated for FY 97:

- Environmental Project for Integrative Studies in Science and Mathematics
- High School Computer-Based Physics Curriculum
- Middle School Science Resource Manual
- Building Foundations for Mathematics and Science Success
- Texas Prefreshman Engineering Program (TexPREP)
- Science Information and Resource Center

COMMUNICATION PROGRAM

Public Outreach

PI: Judy Oskam, Ed.D., Texas Tech University

Public outreach is the grant-funded correlate of the Center's communication program. During this time period, communications faculty and staff coordinated with the Center's staff to develop copy for television public service announcements (PSA). Production time is currently being scheduled with KACV-TV, Amarillo.

- PSA copy developed (10/96)
- PSA copy reviewed and approved by Center staff and Pantex (1/97)

Coordination is ongoing between Texas Tech University and KACV-TV to schedule production and editing.

Science Information And Resource Center

PI: Zane D. Curry, Ph. D., Texas Tech University
Co-PI: Marie Gentry, Ph. D., Texas Tech University

Progress continued on the design of the Science Information and Resource Center. Proposed site arrangement, building/furniture plan, and area isometrics were completed. Perspective drawings of the following spaces were completed: four administrative offices, conference room, multi-media classroom, lobby, lockers/seating area, food service area, public seating area, children and adult's exhibit areas, exterior facades. In the larger spaces, multiple perspectives and/or isometric drawings were needed to provide comprehensive information about the spaces. In addition, text descriptions of proposed functions, furniture, and finishes for each space are in progress. All final drawings have been CAD generated in order to produce photo real 3-dimensional drawings.

- A graduate research assistant was hired for the FY97 project.

- For FY97, project personnel will design and develop two exhibits that will inform and educate viewers on environmental and nuclear research of the Center. Exhibits will rotate through the Don Harrington Regional Discovery Center, an interactive educational science center for children and adults in Amarillo. Preliminary information gathering for the exhibit designs began. A teacher advisory committee was established for the purpose of capitalizing on their expertise for the development of the exhibits.
- Project 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 schedule was:

Amarillo Airport	October - December
Amarillo Farm and Ranch Show	December 3 - 5
Don Harrington Discovery Center	December - April, 1997

Staging at the Discovery Center will be delayed due to the popularity of the exhibit at the Amarillo airport.

EDUCATION PROGRAM

Continuation Of K-16 Science And Mathematics Education

PI: Judy Kelley, West Texas A&M University

The Third Annual Panhandle Area Mathematics and Science Conference was held Saturday, September 28, at West Texas A&M University. Approximately 730 teachers, speakers, students, and exhibitors registered for the day-long event. In addition to the keynote session which addressed appropriate use of technology in mathematics and science classes, there were almost 150 presentations. Four of the speakers were participants and leaders in Department of Energy funded projects in Nevada. Two speakers were Presidential Award Winning Teachers. K-12 teachers from approximately 70 school districts in the Panhandle and South Plains attended. Students in teacher preparation programs at West Texas A&M University, Texas Tech University, Lubbock Christian University, and Wayland Baptist University also participated. Exhibitors included the Pantex Plant and the Amarillo National Resource Center for Plutonium. Evaluations from the conference were very positive.

Sessions that related specifically to the Amarillo National Resource Center for Plutonium were:

- Computer Activities For The Physics Classroom: a presentation by participants in the physics teacher project funded by the Center.
- Digging Into A Mountain Of Science: a presentation of experience-based learning activities in the areas of geology, energy, and environmental sciences.
- Critical Thinking: a presentation of critical thinking exercises that enhance the understanding of waste management issues.
- Teaching With Natural Analogs: a presentation focusing on the use of natural analogs in a nuclear science unit.
- Natural Analogues--What Are They? How Do We Instill Their Importance To Our Students?: a presentation that featured nature as the teacher teaching us how to store radioactive material.
- Performance-Based Activities For Teaching Natural Energy In The Environment: a presentation based on the manual of activities developed in the Center's middle school science project.
- Chemistry Road Show: chemistry demonstrations that entertain, excite and educate students.

Participants came from the following public schools, private schools, colleges, and universities; Alamo Catholic--Amarillo, All Saints Episcopal--Amarillo, Amarillo ISD, Amarillo Montessori Academy, Amarillo College, Booker ISD, Borger ISD, Bovina ISD, Boys Ranch ISD, Brownfield ISD, Bushland ISD, Canadian ISD, Canyon ISD, Channing ISD, Clarendon ISD, Claude ISD, Dalhart ISD, Dimmitt ISD, Diocese of Amarillo, Dumas ISD, Farwell ISD, Floydada ISD, Frenship ISD, Friona ISD, Greenwood ISD, Gruver ISD, Hale Center ISD, Happy ISD, Hart ISD, Hedley ISD, Hereford ISD, Highland Park ISD, Kress ISD, Lakeview ISD,

Littlefield ISD, Lorenzo ISD, Lubbock ISD, Lubbock Christian University, Meadow ISD, Memphis ISD, Miami ISD, Muleshoe ISD, Nazareth ISD, Nazarene Christian Academy--Hereford, New Deal ISD, Paducah ISD, Perryton ISD, Plainview ISD, Patton Springs ISD, Pringle-Morse ISD, Plemons-Stinnett-Phillips ISD, Ralls ISD, River Road ISD, San Jacinto Christian Academy--Amarillo, Sanford ISD, Shallowater ISD, Shamrock ISD, Silverton ISD, Slaton ISD, Smyer ISD, Spearman ISD, St. Vincent de Paul--Pampa. St. Andrew's--Amarillo, Texas Tech University, Trinity Fellowship--Amarillo, Tulia ISD, Wayland Baptist University, West Texas A&M University, Wheeler ISD, White Deer ISD, and Whiteface ISD.

Speakers at the Panhandle Area Mathematics and Science Conference represented the following locations/organizations in Texas; Amarillo, Amarillo College, Amarillo Garden Center, Borger, Canyon, Cedar Hill, Dalhart, Dallas, Georgetown, Greenwood, Happy, Hereford, Lockney, Lubbock, Lubbock Christian University, Miami, Olton, Pampa, Plainview, Region XI ESC, Region XVI ESC, Region XVII ESCShallowater, Slaton, Springlake-Earth, Stratford, Texas Agriculture Extension Service, Texas Tech University, Texas A&M University, University of Houston--Clearlake, and Wilson.

Speakers from outside Texas came from Reno and Las Vegas, Nevada; Santa Monica, California; and Arvada, Colorado.

Technology training for grades K-12 science and mathematics teachers was conducted on December 3, 4, 5, 17, and 18. Region XVI Education Service Center provided the computer labs for the training, and the Panhandle Information Network assisted with recruitment of participants. The training provided hands-on opportunities for each participant to learn how to access science and mathematics resources available on the Internet, to practice finding and retrieving those resources, and to learn strategies for using those resources in science and mathematics classes. Participants also learned about the Amarillo National Resource Center for Plutonium, its mission, and its education program. Seventy teachers from 28 different school districts participated in the training. Before the training, 35 participants indicated they had never used the Internet, 22 had used it occasionally, and 12 had used it regularly. After the training, 55 participants indicated they would like to use the Internet regularly and 13 would like to use it occasionally. As part of the evaluation, participants were asked to rate statements on a scale of 1 to 5 with 5 indicating strongly agree and 1 indicating strongly disagree. Fifty-six participants indicated they strongly agreed with the statement: "The goals of the training were accomplished." Fifty-eight participants indicated they strongly agreed with the statement: "I would recommend this training to other teachers."

Teachers from the following school districts participated in the technology training:

Borger
Bushland
Canadian
Canyon
Childress
Clarendon
Claude
Darrouzett
Dimmitt
Farwell
Follett
Friona
Ft. Elliot
Gruver
Hart
Hartley
Hereford
Kress
Memphis
Miami
Pringle-Morse
Plemons-Stinnett-Phillips
Silverton
Spearman
Spring Creek
Sunray
Valley
Wellington

Environmental Project For Integrative Studies In Science And Mathematics

PI: Richard Powell, Ph. D., Texas Tech University
Co-PI: Judy Kelley, West Texas A&M University

This project was initiated on January 15, 1997 through five primary activities:

- Project director and two educational consultants (one high school and one middle school science teacher) met in Floydada, Texas on January 11 for five hours to discuss the project and project management.
- Project director recruited two elementary teachers, four middle school mathematics and science teachers, and three high school mathematics and science teachers for the advisory panel. Three of these people will serve as integrative curriculum specialists since they are from Carver Academy in Waco, Texas and Brown Barge Middle School in Pensacola, Florida - all integrative learning schools.
- Three-hour meeting on February 1 in Rawls, Texas was conducted between the project director and educational consultants to discuss readings to be used in the project.
- With Center staff, advisory panel met on February 4 in Plainview, Texas for three hours in order to stimulate the dialogue about the curricular nature of the project.
- Announcements were developed and distributed in order to recruit teachers for the summer institute. Additional announcements have been sent to selected teachers throughout the state of Texas since these teachers have been recommended by school district curriculum specialists, university faculty, and members of the Texas Education Agency. (Refer to the appended section of CET to see the announcement.)

High School Computer-Based Physics Curriculum

PI: Jan P. Spears, West Texas A&M University
Co-PI: Terence C. Ahern, Ph.D., Texas Tech University

Area high school physics teachers who participated in the summer workshop developed simulations and accompanying lessons in their classrooms during the Fall 1996 semester. These include simulations of systems to study/demonstrate frames of reference, planetary gravity, Colulomb's Law, Newton's third law and the difference between velocity and acceleration. Ms. Spears developed additional simulations and associated activities for the study of forces in one and two dimensions, conservation of momentum and inclined plane systems.

Dr. Ahern, Ms. Spears and the teachers met on January 25, 1997 to plan compilation of the first version of the Resource Manual. Each teacher adopted specific parts of the manual framework to develop further. Problems with implementation of project objectives were discussed and adjustments were made to time schedules based on the teachers requests. In addition, all teachers expressed interest in including computer-based laboratory exercises in the manual. Teachers were provided with a HyperCard problem stack template developed by Ms. Spears into which they can enter physics problems suitable to their own students. The resulting problem sets will provide students with additional practice involving physics problems. Teachers were also introduced to the concept of computer-supported, peer instruction.

Physics Teachers Network (PTN) web page has been mounted on the Experimental College of education web server (http://memo.edu.ttu.edu/ptn/PTN.html) in the College of Education at Texas Tech University. Information on the Center, the principle investigators and the teachers participating in this project will be available at this site. The site will include information on instructional design and links to other web sites relevant to the project. PTN will function as an instructional resource area for secondary physics teachers. Once the Resource Manual is completed, it will be available through the PTN.

One of the goals of PTN is to create a virtual community of teachers who can meet on-line to discuss important curricular and management issues. Dr. Ahern had previously designed and developed the Idea Web (1991) and is currently testing the feasibility of using it in the project for collaborative computer conferencing. The Idea Web incorporates a visual interface that facilitates computer mediated small group

collaboration. Once feasibility has been determined the teachers will be able to interact with Dr. Ahern, Ms. Spears and each other via the Internet. Teachers were provided with a HyperCard problem stack template developed by Ms. Spears for use in their classrooms. Teachers can enter physics problems suitable to their own students into the template. The resulting problem set will provide students with additional practice in solving physics problems. Teachers will test the program in their classrooms during the spring 1997 semester.

Middle School Science Resource Manual

Co-PIs: Gerald Skoog, Texas Tech University; Treasure Brasher, West Texas A & M University

During the reporting period, two workshops were conducted at the Conference for the Advancement of Science Teaching in Austin on Friday, November 1, 1996. The workshops introduced the manual *Activities for Teaching Fundamental Concepts of Nuclear Energy and Related Topics* that was developed during the summer phase of this project. The workshops were attended by 70 teachers who received copies of the manual. The workshops were conducted by Treasure Brasher and Margaret Williams, a teacher at Pampa Independent School District who helped develop the manual. The manual received positive feedback from the teachers.

Recruitment plans are being made for the one-week summer workshop where the manual will be introduced and used by science teachers in the Amarillo area.

Building Foundations For Mathematics And Science Success

PI: George Mann, Ph.D., West Texas A&M University
Co-PI: Richard Powell, Ph.D., Texas Tech University

This project was initiated on January 15, 1997 with the purposes of: improving elementary students' mathematical and scientific literacy, (2) improving future teachers' knowledge and understanding of instructional planning and delivery of mathematics and science content, (3) promoting elementary students' interest in pursuing a career in a field related to mathematics and science. To accomplish the objectives of the project, the following activities have been accomplished:

- Needs and interests of target students have provided project personnel with information needed to identify appropriate Super Saturday classes which are scheduled to begin in five elementary schools on February 1, 1997.
- Personnel have been identified to conduct the Super Saturday component to the project. Instructional materials which were needed have been secured. The component has been advertised and has an expected enrollment of 430 student participants.
- Interns have been selected and are receiving training for Intercession Camp instructional responsibilities.
- Site directors have been provided copies of evaluation plans.
- Work will continue to complete and report on the milestones for the project as specified in the proposal. These include:
    a) Needs Assessment Report
    b) Personnel Report
    c) Class Offering Report
    d) Assessment Plan Report
    e) Student Participation Report
    f) component Evaluation Report
    g) Report of Progress of Presentation and publication Preparation

The completion date of this project will be January, 1998.

Texas Prefreshman Engineering Program (TexPREP)

Co-PIs: Charles N. Kellogg, Texas Tech University; Therese Jones, Amarillo College

The reporting period is the time of the year for planning, organizing and preparing activities and materials to be used during the summer program.

Major activities included:

- Prepared and sent requests for contributions. These were sent to businesses and industries in November. Requests to individuals were mailed February 1. Efforts will be continued so that sufficient funding is generated to provide the number of teachers needed. Student numbers are expected to increase this summer.
- Updated and duplicated all the materials for student recruitment and application. Two thousand application packets have been printed and collated for distribution to area schools. Sets of information sheets and between five and twenty-five application packets (depending on size of school) are being assembled. These will be delivered or mailed to math and science teachers and counselors at 60 schools in 23 towns and cities of the Texas Panhandle during the week of February 10, 1997. Letters of invitation to previous first- and second-year participants to apply for second- and third-year slots are being prepared and will be sent with an application packet to qualified students at that time.

Recruitment and publicity activities included:

- Made Amarillo PREP presentation to local teachers at the Texas Association of Minority Engineers Meeting.
- Presented Amarillo PREP information at the PTA meeting at Sam Houston Middle School.
- Printed and distributed two thousand brochures to the various area school districts.

Activities and classes for the summer program are being planned. Prospective teachers and staff are being sought and interviewed. Classroom and activity sites have been reserved. Plans for field trips and recruitment of speakers have begun.

Needs Assessment And Roadmap

PI: William M. Marcy, Ph. D., Texas Tech University

All project milestones were previously accomplished. The prototype World Wide Web server is being maintained by Texas Tech University at aln.coe.ttu.edu. From this location, link to the distance education Masters of Engineering Program. For further information, contact Dean Fontenot or John Chandler at Texas Tech University at 806/742-3451.

NUCLEAR AND OTHER MATERIAL STUDIES

PROGRAM IMPLEMENTATION

Coordination and Technical Information Support For Nuclear Group Activities

PI: Paul Nelson, Ph.D., P.E., Texas A&M University
David Boyle, Ph.D., Gia Alexander, Igor Carron, Ph.D., and Donna Greer, Texas A&M University

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

In the area of technical support, Dr. Paul Nelson attended three meetings of the Center Governing Board, as well as an internal coordination meeting, to provide technical support and input to the Center staff. Dr. Igor Carron also provided technical support to the Center staff, and was designated as the Texas A&M University point of contact for coordinating video conferences.

Drs. Boyle, Carron, and Nelson participated in the Nonproliferation and Arms Control Public Hearing in Amarillo on 4 November. Drs. Boyle and Nelson also attended the Center-sponsored Media Training Class in Amarillo on 5 November and the Nuclear Group Quarterly Meeting on 20/21 November.

Dr. David Boyle coordinated Center storage activities with the DOE's John Kirby and Mason-Hanger employees at Pantex. This coordination activity clarified inconsistencies regarding: (a) official DOE estimates for the maximum number of pits for eventual storage at Pantex, and (b) the specific buildings within Pantex Area 12 to be upgraded for storing strategic reserve and surplus pits. He also composed questions and comments addressing DOE's Nonproliferation and Arms Control Assessment that were formally submitted by the Center to DOE. Finally, Dr. Boyle authored a storage white paper that was used by the Center to provide information to State and community officials about DOE's announced preferred alternative for the interim storage of surplus pits at Pantex.

Activities related to information support included expansion of the Nuclear Group Internal Technical Working Documents series by eight reports, publication of a Nuclear Group Newsletter, and dissemination of the newly updated Nuclear Group Calendar of Conferences. Participants in this effort also distributed information from the Center and other sources to appropriate investigators within the Nuclear Group. Dr. Carron also located and provided technical documents to the water reactor group in the preparation of benchmarking problems for the assessment of computer models designed to simulate the behavior of MOX fuel in traditionally uranium-burning reactors.

To enhance the working relationships between DOE/DP (Pantex) and the Universities, all subproject participants assisted with coordination of the visit on 16 January of three representatives from the Pantex Plant to Texas A&M University.

INTERNATIONAL STUDIES

Support Of US And Russian Joint Study Activities

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

As a member of the US/Russian Joint Studies Team on Water Reactors, Dr. M. L. Adams participated in meetings at the Kurchatov and Bochvar Institutes in Moscow November 10-13. At these meetings the US/Russia team agreed upon specific deliverables and deadlines for their benchmarking effort.

The first deadline was that draft results, computed with several different code systems, of US and Russian computational benchmark problems (defined at the November meetings), were to be exchanged by February 3, 1997. ORNL and the Center divided the US-side work roughly in half, and the Center successfully accomplished its portion and delivered a large body of results to ORNL by January 28.

Dr. K. L. Peddicord traveled to Russia from January 12-19, and took part in meetings involving the Center-related activities. These included discussions with Dr. Victor Bolyatko and Professor V. V. Khromov of the Moscow Engineering Physics Institute (MEPhI) concerning ongoing projects with the Amarillo Center, and plans for activities during 1997. A meeting took place with Dr. Alexandre Dmitriev and Ms. Olga Romenkova of the RF Gosatomnadzor concerning Dr. Dmitriev's trip to Texas in April and May to present a series of lectures on regulatory issues related to plutonium disposition. Meetings were held with Dr. Victor Gubanov of Minatom and Professor Leonard Lazarev and Dr. Mikhail Moshkov of the Khlopin Radium Institute in St. Petersburg concerning the NATO Advanced Research Workshop to be held in Amarillo on March 17-21, 1997. Finally, meetings took place at the Obninsk Institute for Nuclear Power Engineering (OINPE) concerning joint educational and research programs between OINPE and the Center.

From December 6-19, Natela Ostrovskaya of the Obninsk Institute for Nuclear Power Engineering traveled to Texas to develop a home page on the World Wide Web for her university. Also, Dr. Igor Carron has completed the manuscript of a detailed trip report regarding his October visit to MEPhI.

Concerning other activities with the Moscow Engineering Physics Institute, we received Dr. Khromov's FY 1996 report on his effort to establish at MEPhI an MS degree program on Materials Protection, Control, and Accountability (MPC&A). This document is currently planned to appear as part of a Nuclear Group Internal Technical Working Document in the next quarter. Professor Khromov has made good progress, adjusting early drafts of the curriculum in response to our e-mailed comments and specifying general course content in preparation for detailed development of individual courses.

Professor Khromov has been successful in obtaining DOE/NN support for his MS Program, in addition to the assistance provided by us. However, DOE/NN is strictly limiting its support to that part of Khromov's program which is directly MPC&A related (MPC&A courses and their associated laboratory equipment). We have agreed informally with the DOE/NN project leader for this activity to split the effort of supporting Professor Khromov's program. Under this arrangement, DOE/NN will help Khromov develop a consistent and comprehensive set of graduate-level MPC&A courses and will provide the related laboratory equipment and computers. This MPC&A element constitutes the backbone of the unique MS program that Khromov has conceived. However, good MPC&A courses by themselves don't constitute a full, stand-alone MS degree program. A complete MS program requires additional elements as well: non-MPC&A courses, student arrangements, visiting lecturers, cooperative work opportunities, academic links, avenues for research funding, etc. Texas A&M University support will be used to assist Professor Khromov in these areas.

Dr. David Boyle has continued his efforts to coordinate the Center support of Khromov's activity with that being provided separately by DOE/NN. He attended a meeting with the DOE/NN project team at Sandia on 6-7 January. Some concerns regarding this coordination effort are emerging, primarily associated with DOE/NN's apparent desire to control all US communications (and possibly all US funding) going to Khromov on this topic. We will continue to work with DOE/NN where possible. However, it may be advisable to have Professor Khromov accomplish the integration of DOE/NN and Texas A&M University activities supporting him, rather than to achieve that integration here in the US.

Final payment was made to MEPhI on its FY 1995 subcontract with the Center. Initial payment was made to INPE on their subcontract to provide the Center a source book of institutions of higher education in the former Soviet Union that have a program in nuclear engineering or a field closely allied to nuclear engineering.

STORAGE: FACILITY DESIGNS

Feasibility Study for Plutonium Pits Storage In A Warehouse Facilities

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

Phase II modeling for the FD-LANL and Pantex facilities will be completed on time in March. Phase II modeling of the flow field in both facilities includes buoyancy forces; phase I modeling did not. The computational domain used in phase I and phase II consists of the walk space between two rows or racks with the additional space between the top of each rack and the ceiling.

Prior to predicting the temperature distribution, the velocity profile, and the pressure profile for the computational domain used in phase II, checks are being performed for a simpler geometry, duct flow. The computational domain consists of a straight duct of length 4 m and width 0.5 m. The walls of the duct were assumed to have a constant temperature of 100 degrees C. Buoyancy forces were included (the ratio of the Grashoff to Reynolds squared equaled three) and the resulting velocity profile and temperature distribution as predicted by the code were deemed correct.

Next, the phase II computational domain was used in the simulation. The constant surface heat flux boundary condition was replaced by a constant wall temperature boundary condition in order to have significant buoyancy forces. For an inlet flow of 0.1 m/s through the floor and exiting through the ceiling, the program would not converge. The reason for this is that the height of the computational domain used in phases I and II for forced flow is not sufficient for the case when the flow is due to buoyancy forces. A recirculation region exists that is caused by the sudden expansion in the computational domain as the flow reaches the top of the racks. The height of the computational domain is not sufficient to capture this recirculation region and therefore the code does not converge. In order to make the code converge the computational domain must be extended by approximately 4 m in the vertical direction. Another way to make the code converge is to prohibit flow from exiting through the ceiling (worst case scenario).

Another case was run with the phase II computational domain but with the following boundary conditions. The flow entered uniformly through the ceiling at a rate of 1 m/s and exited through the floor (flow in the direction of the gravity vector). A constant wall temperature of 100 degrees C was again used giving the ratio of the Grashoff to Reynolds number squared a value of three. The resulting velocity field and temperature distribution looked very similar to the results obtained in phase I when no buoyancy forces were included; the convective terms dominated the buoyancy terms.

Robotics, Automation, And Tele-Operation Program

PIs: Alan Barhorst, Ph.D., Texas Tech University; Dick Volz, Ph.D., Texas A&M University; George Kondraske, Ph.D., The University of Texas at Arlington/
Co-PIs: Jose Macedo, Ph.D., Mica Ensley, Ph.D., William Kolarkik, Ph.D., Micheal Parten, Ph.D., Hua Li, Ph.D., and Jeff Wolstad, Ph.D., Texas Tech University; Jeff Trinkle, Ph.D.; Louis Everett, Ph.D., and John Poston, Ph.D., Texas A&M University; V. Sreenivasan, Ph.D., The University of Texas at Arlington

This is the last progress report for the project under its current title. For 1997 the project is re-titled to reflect the use of robotics in DOE DP and MD, it is called "A Research Program in Automation, Robotics, and Tele-Operation." The following is a brief report on progress to date. The size of the project precludes the inclusion of reports in this format. We use the Nuclear Group, technical working document series as the avenue for major reports. In general, the progress has been close to what was described as deliverable dates. Some projects are ahead of schedule and some are behind, and some have not been started due to shortages of willing student help. The projects that are behind have been bolstered by concentrating resources in these areas. Some of the projects that have not been started will be attempted again in FY 1997 using the FY 1996 funds carried over, if they relate to the work we are continuing. Areas not started in 1996 that are not continued into 1997 have been absorbed into the functional projects. The funding of this project supports nearly 20 students and partially supports the investigators listed. Even though some of what we proposed is not being completed due to lack of student help, other areas are getting more results than expected or proposed.

This report will proceed by institution.

Texas A&M University (TAMU)

The work on reviewing all existing and proposed storage facilities is on hold until a student is found. The parallel work on domain analysis (radiation exposure, etc.) has also been postponed until a Nuclear Engineering student can be found.

Work on a stability tool for a generic manipulator/gripper continues. This project involves embedding high fidelity grasp stability models in to the commercial Robot animation package TELEGRIP. Work is on schedule to slightly ahead of schedule.

Work on an animation tool capable of animating the dynamic motions of a generic manipulator/gripper continues. This tool is used to model contact interaction beyond the imbedded tools in TELEGRIP. Work is on schedule.

The Integration of TELEGRIP with Inter-Agent and the installation of QUEST and the incorporation of the existing Storage facility models has been completed.

The design of a Modularized Simulation Construction set has been reorganized due to the change of DOE storage plans. This effort is now geared at integrating TELEGRIP into the tele-operation testbed. Previously we used non-standard code for the robot simulations. Now we use the DOE standard TELEGRIP for the simulations. This will expedite the acceptance of these research results into the DOE complex, and will allow us to quickly get back into storage scenario simulation when the need arises. This work is progressing well.

The TAMU side of the bi-directional link between TTU and TAMU is completed.

The work on integrating Virtual Reality based inspection into the simulation testbed is progressing well. The transition to the tasks for 1997 has commenced. This work is on schedule. This capability can be used for training and actual inspection. This work will be demonstrated again at a future meeting.

Texas Tech University

In the machine to human interface, the work is well ahead of schedule, and the results are good. One Ph.D. thesis (partially funded by the Center) has been completed and one MS thesis is being written at this time. The work is ahead of schedule for FY 1997 at this time. A literature review for another thesis has been completed and will be submitted to the Nuclear Group document series mentioned above. The PhD thesis completed is currently available in the Nuclear Group document series.

Progress in the safety and reliability task has been good. A PhD thesis will be defended in March 1997. These results will be published in the literature and in the Nuclear group documents.

The self-assessment of reliability model has made good progress. A PhD proposal has been defended and the work is on schedule.

The bi-directional link between TTU and TAMU robotics test-beds is behind schedule. Difficulties with the initial plan of attack have been removed via the change of plans to use TELEGRIP as the virtual video link. Other problems have occurred with bugs in the proprietary robot control software. Solutions have been devised. The project should be back on schedule by late February.

Work on the high-fidelity manipulator modeling tool is progressing well. Three more papers since last quarter have been submitted for journal review. Progress on the implementation of the models into TELEGRIP has been delayed until the bi-directional testbed is fully functional. Two MS thesis proposal have been accepted and these theses are scheduled for completion summer 1997. One PhD thesis has been completed (mostly funded from related sources) and one other is well under way (again mostly funded from other sources). This project is on schedule.

Work on mobile platforms is generally on time. This work is being completed via undergraduate Senior design project teams and uses only minor amounts of funding from the Center.

The University of Texas at Arlington

At UT Arlington, work continues toward performance modeling and measurement. This task is slightly behind schedule but should be completed as specified in 1997.

The University of Texas at Austin

The module modeling of wheeled vehicles is progressing as planned. The dynamics models are complete. Fine tuning of numerical algorithms is still progressing. Reports have been and will be submitted to the Nuclear Group document series.

Development Of Nondestructive Assay Methods For Weapons Plutonium And Mixed Oxide Fuel Safeguards

PI: Naeem M. Abdurrahman, Ph.D., The University Of Texas At Austin
Co-PI: Bernard W. Wehring, Ph.D. The University Of Texas At Austin

Our activities during this quarter covered both computational and experimental related work. We continued our computational effort focusing on the neutronics of a new nondestructive assay concept that uses graphite slowing down time spectrometry. We have developed a computational model of a cylindrical graphite slowing down time spectrometer, and performed a number of assay simulations using a detailed BWR fuel assembly model. In addition, we investigated the isotopic resolving power and self shielding effect in the fuel assembly for the graphite spectrometer.

On the experimentally related part, we have successfully transferred the pulsed neutron generator, described in our previous progress report, from The University of Michigan to The University of Texas at Austin. The neutron generator is now being set up at the Nuclear Engineering Teaching Laboratory of The University of Texas. We have completed the design and have started the fabrication of the generator support structure which consists of several steel bases. We have also completed the assessment of the vacuum requirements of the new generator and are now in the process of ordering the required pumps and controllers for the new system.

Two papers have been submitted to the American Nuclear Society Annual Meeting to be held in Orlando, Florida in June 1997. One paper presents our preliminary investigations of the graphite slowing down time spectrometer, the other is a review of new generation of neutron sources some of which would be suitable for slowing down time spectrometry and other active neutron interrogation methods for fissile assay applications.

STORAGE: FACILITY ANALYSIS

Aircraft Accident Forecasting For An Integrated Plutonium Storage Facility

Co-PIs: James C. Rock, Ph.D., P.E., CIH, Texas A&M University; Michael T. McNerney, Ph.D., The University of Texas

The Pantex Site Wide Environmental Impact Assessment (SWEIS) was published in Nov. 1996, based on the July 1996 Draft DOE Standard 3014-96: "Accident Analysis for Aircraft Crash into Hazardous Facilities." The SWEIS used very conservative assumptions about aircraft accident probabilities and about the consequences of an accident, should it occur. Most are listed in section 4.15.7 of the SWEIS. There is room for improvement. From page S-11 of the SWEIS Summary: "The dominant accident in terms of the risk from radioactive material releases to the public involves the crash of an aircraft into a weapons storage magazine, nuclear explosive bay, or a special purpose building that results in the detonation of the conventional explosives in the weapons." A related comment is found in Volume I, page 4-312, section 4.15.6: "It is estimated that ... the offset localizer, relocation of the VORTAC, and 65% use of the GPS would result in an 82% cumulative risk reduction. This risk reduction was estimated using the Solomon Model." The DOE Standard 3014-96 says the Solomon Model is inappropriate for accident analysis.

To ensure appropriate mitigation measures of the dominant accident, we are reducing the conservatisms in aircraft accident modeling and consequence analyses. To that end, Dr. McNerney continues to improve the top tier of the hierarchy of conservatisms used in aircraft accident modeling. Known accident rates for aircraft models that dominate Amarillo traffic are lower than those assigned to generic classes of aircraft. Dr. Rock's skid distance model of intermediate conservatism is nearly ready to be submitted to a peer-reviewed journal.

Tom Golder of Lamb Associates is facilitating our collaboration with members of the Sandia Labs. In January, Dr. Rock met with Dr. Jaime Moya's group from Sandia to start collaboration on two projects: the rocket sled test to crash an old jet engine into a simulated weapons storage bunker, and aircraft fuel pool-fires in a simulated weapons bay. Dr. McNerney is working with Dr. Y.T. Lin's group. RAMS data for Jan 97 shows fewer overflights of zone 4 than occurred in Jan 96 due to the newly offset localizer. Such data will support a new route-based accident model required to recompute the benefits of the initiatives of the Amarillo Overflight Working Group air traffic control initiatives.

Post Explosion Transport (Pet) Study

PI: Dale Klein, Ph.D., The University of Texas at Austin
Co-PI: Steven Manson, The University of Texas at Austin

This research has been undertaken to augment the computational models currently used to perform safety analyses of the PANTEX cell facilities. In the event of a contained chemical explosive transient during disassembly activities, there is some concern that a release of 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 verification and validation of the completed Post Explosion Transport (PET) code. This code is capable of solving transient thermal hydraulics problems in geometries sufficiently representative of the PANTEX cell rooms. The main tasks completed in the past quarter involved demonstrating the convergence of the PET code. This verification effort began in December, and revealed errors in the centerline boundary condition implementation. A linearized initial condition was also implemented to minimize errors attributed to thermal shocks. Finally, as a result of this work, the vorticity boundary condition was reformulated in order to influence the convergence properties of the code. The next step is to incorporate the PET code into the MELCOR package, so that a full two-dimensional simulation of a cell room explosion transient can be calculated. This task is currently scheduled for completion in March, 1997.

A Basic demonstration of a typical transient solution of a PET code problem (compressible flow, low heat load, Cartesian geometry) is viewable on the world wide web at:

http://uts.cc.utexas.edu/~boyce/tanim.html.

STORAGE: STORAGE/SHIPPING CONTAINERS

Radiation Damage And Microstructural Changes Of Stainless Steel Due To Long-Term Irradiation By Alpha Particles From Plutonium

Co-PIs: Ron R. Hart, Ph.D., Texas A&M University; Kenan Ünlü, Ph.D., The University of Texas at Austin

Progress continued on understanding material problems in stainless steel that may be caused by high fluence irradiations of alpha particles from Pu. Emphasis this quarter was on Rutherford backscattering and channeling analyses of single crystal iron following implantations of alpha particles.

The iron crystal was first electropolished to remove surface oxide and then quickly placed in the target chamber of the 160 KV accelerator at Texas A&M. After alignment of the <100> axis of the crystal with an incident beam of 140 keV protons it was found that the random to aligned backscattered yield of 140 keV protons near the surface of the iron was 20:1. This result is characteristic of an undamaged single crystal. The iron was then implanted with 40 keV alpha particles to fluences of 1E15, 1E16, and 1E17/cm^2. These fluences correspond to irradiations of alphas from Pu for 1, 10, and 100 years, respectively. Backscattered energy spectra of 140 keV protons incident along the <100> axis were measured after each He irradiation. It was found that the aligned backscattered yield increased only slightly after the 1E15/cm^2 implant but showed a marked increase at all backscattered energies (or analysis depths) after the 1E16/cm^2 implant. Only a small additional increase was seen after the 1E17/cm^2 implant. Although these results are preliminary they suggest that the lowest fluence produces only small lattice disorder or strain. However, the marked increase of the aligned yield after the 1E16/cm^2 implant suggests the formation of He bubbles and a correspondingly large increase in lattice disorder or strain. The little additional increase in aligned yield after the 1E17/cm^2 implant suggests significant He release or indiffusion. This work will be continued next quarter. However, instead of iron a single crystal of stainless steel 316 (presently on order) will be used as the target.

Test samples of stainless steel 316 were prepared for transmission electron microscopy (TEM). Initial TEM measurements using the test samples were performed.

A Contributed paper entitled "Effect of Long Term Alpha Radiation on Stainless Steel Used in Pu Encapsulation" was submitted and accepted for publication at the American Nuclear Society annual meeting, Orlando FL, June 1-5, 1997.

Dr. Ünlü attended the MRS fall meeting, Boston, MA. Possible collaboration for TEM measurements was discussed with Dale Alexander, Argon National Laboratory, Materials Science Division.

There were several discussions of a collabrative nature with Dr. Bill Moddeman, Applied Technology Division, Pantex. It is anticipated that Dr. Moddeman's expertise in surface science will be of great value to this project in the coming year.

Air Monitoring For Detecting Releases Of Plutonium In A Future Integrated Storage Facility

PI: H.M. Liljestrand, The University of Texas at Austin

Co-PIs: A.R. McFarland, Ph.D., and W.H. Marlow, Texas A&M University; P.K. Dasgupta, Ph.D., and S. Liu, Ph.D., Texas Tech University

This research effort is to develop an optimized system for detecting plutonium releases in the Integrated Storage Facility. The system will ultimately provide meaningful data for alarm purposes, for determining the exact source of leakage, and a quantitative basis for indoor and outdoor exposure to such releases. The research program is divided into four subprojects, which include (principal investigator(s) from each institution are noted in parentheses) development of a method for detecting the occurrence and isolating the location of leakage from storage (H.M. Liljestrand and R.L. Corsi, The University of Texas at Austin), (2) development of a method for predicting the best sampling and monitoring locations (A. McFarland, Texas A&M University), (3) development of a methods for accurate detection of plutonium aerosols (P.K. Dasgupta, Texas Tech University) and (4) plutonium leak detection by conductivity methods and optical de-

tection of plutonium aerosols (W. Marlow, Texas A&M University). This research activity was not selected for continued, additional funding by the Center in FY 97, and an extension through 8/31/97 has been granted to complete work.

SUBPROJECT 1—Development of a Tracer-Based Fingerprinting System to Identify and Locate Plutonium (Pu) Storage Container Leakage
H.M. Liljestrand and R.L. Corsi, The University of Texas at Austin

The premise behind a tracer-based fingerprinting system is that small quantities of other inert tracers, e.g., perfluorocarbons, could be added to helium in a container headspace. The use of multiple tracers at varying concentrations would allow for container-specific fingerprints. For example, if three tracers were all detected simultaneously in a specific ratio it would be possible to immediately identify the specific container from which they were released. It would then be possible to rapidly isolate and remediate the specific failure on the target container. This primary task consists of six major sub-tasks. These include (a) the identification of a list of potential tracers, (b) a rigorous literature review on the effects of alpha radiation on each of the tracers listed in (a) (future experiments will confirm this task), (c) selection of final "target" tracers, (d) design of a fingerprinting scheme, e.g., specific tracers, tracer combinations, and concentration variations to allow for container-specific identification, (e) selection and potential design of an appropriate on-line monitoring system to allow detection of target tracers with required sensitivity, (f) development of fingerprint feedback software to facilitate leakage notification and container identification, and (g) development and testing of a prototype detection/fingerprint system.

Under sub-task (e), elution curves have been developed for time varying releases, specifically source terms with exponential decay, step input and ramped increased releases, under four circulation/mixing conditions, completely mixed, partially mixed, completely mixed in series and plug flow. Under sub-task (f), a combination continuous monitor and sample collection system has been selected for testing.

For the period 1/16/97-1/31/97, a graduate research assistant has been appointed. Standard mathematical techniques to address sub-task (f) development of fingerprint feedback software are being reviewed.

SUBPROJECT 2—Development of Improved Sampling Systems for the Collection of Plutonium Aerosols
A.R. McFarland, Texas A&M University

Two categories of studies on the sampling of simulated Pu aerosols have been conducted. First, there are basic data that are lacking in the technology of air sampling system design, including characteristics of acceptable bends in transport lines. Studies are currently underway to develop such design criteria. Second, the trend in continuous emission monitoring (CEM) in the nuclear industry is to use single point sampling in accordance with the Alternate Reference Methodology (ARM) that was approved by EPA in November, 1994 for use at all DOE facilities. To comply with the requirements of the ARM, samples for CEM must be withdrawn from a location in the stack or duct where the flow is well mixed. Although mixing criteria are specified in the ARM, there is no a priori means for determining if a sampling location is suitable. During the current year, numerical modeling of flows in ducts has been improved via Large Eddy Simulation (LES) techniques using sub-grid modeling

With respect to research into aerosol transport components, the effects of curvature ratio and tube flattening on losses in bends are being investigating . The methodology for design of air sampling systems for the nuclear industry is provided by ANSI N13.1-1969, "Guide to Sampling Airborne Radioactive Material in Nuclear Facilities." In that standard, it states the curvature ratio of bends shall be at least five, where the curvature ratio is the radius of curvature of the bend divided by the tube diameter. There does not appear to be a well-founded basis for this criterion, so tests have been conducted to either verify the criterion, or to offer a new value. It would be helpful to designers if value were less than five. Currently, there are no criteria for acceptable flattening of tube cross-section in bends.

All work to be performed on this sub-project during the period 11/1/96 to 1/15/97 was completed earlier. See ANRCP-NG-ITWD-96-10, November 27,1996 for a summary of numerical predictions and experimental results for aerosol deposition in bends.

Numerical Simulations of Tracer Gas Concentration in Mixing Elbow and Straight Pipe

H. Gong, A. Langari and A.R. McFarland, Texas A&M University

Progress has been made on numerical simulation of tracer gas mixing (sulfur hexafluoride SF_6) in an elbow and a straight pipe. Two different approaches were used in numerical computations. One was to treat air and SF_6 as a two-species gas. The mixing and transport of SF_6 was simulated by solving the momentum and mass conservation equations that describe the turbulent convection and diffusion for SF_6. A commercial code, FLUENT, was used to solve the governing equations and the tracer gas concentration COV was calculated from the mass fraction of SF_6 obtained from FLUENT. The other numerical approach was based on the Lagrangian method. It was assumed that the SF_6 gas was comprised of inertial-less points, which followed the flow perfectly and which had negligible thermal diffusion. Individual SF_6 particle trajectories were calculated and the SF_6 concentration COV was obtained by tracking a large number of SF_6 particles released into the flow field at the same location where the tracer gas was introduced in physical experiments. Numerical results were compared to experimental measurements. The particle tracking code and the FLUENT two-species gas model both correctly predict the trend of mixing as exhibited by the experiments, however prediction by the particle tracking code more closely approximate the experimental results.

SUBPROJECT 3—Collection of Plutonium Aerosol Particles Through an Electrical Means Followed by an Automated IC Measurement

P.K. Dasgupta, Texas Tech University

Aerosol particles are naturally charged or can be deliberately made to be highly charged. When introduced to an electric field, these charged particles will deposit onto the oppositely charged electrode. The composition of the aerosol particles can be obtained through chemical or radiochemical analysis. To date, an automated annular tubular aerosol collection system using an electrical means has been developed and its performance has been found to be in excellent agreement with that experimentally predicted.

An experimental system has been developed consisting of three major parts; an aerosol generation system, and aerosol collection interface, and an ion chromatographic measurement system. Experimental results for 0.8-2.1 micrometer particles have shown high collection efficiency (about 90%). Research is progressing on schedule.

SUBPROJECT 4—Plutonium (Pu) Leak Detection by Conductivity Methods and Optical Detection of Pu Aerosols

William H. Marlow, Texas A&M University

Calculations of the electric current pulse due to the passage of a single alpha particle through either air or a noble gas in a weak electric field are in progress with initial results having been obtained. The purpose of this study is to provide the design basis for initial experimental work to develop a practical system for monitoring pit leakage in double-walled containers under study in the AL-2100 Program of DOE/DP at Sandia, Los Alamos, and Lawrence Livermore National Laboratories. Laboratory studies are being conducted of the fractional removal of aerosol particles from air streams flowing through reticulated vitreous carbon foam. These studies are intended to determine if modern low density microporous materials can be used as aerosol capture media which will provide size-related spacial separations of 0.5 to 10 micrometer plutonium particles arising from leakage or other dispersal processes. If successful, these materials may in the future be used to provide samples for ultraviolet fluorescence detection of ultra-small quantities of airborne plutonium.

The conductivity monitoring project will be directly funded under its own account, rather than as a subproject beginning next quarter, because of direct support from DOE and Sandia. The graduate student performing laboratory studies is having some minor experimental problems, and his final report will be delayed.

DISPOSITION: WATER REACTOR OPTIONS

MOX Fuel Fabrication: Gallium Removal, Gallium Cladding Interactions

Co-PIs: N. Abdurrahman, The University of Texas at Austin, and M. Adams, Texas A&M University
Other Investigators: D. Anistratov, F. Best, I. Carron, R. Hart, Y. Hassan, S. O'Kelly, T. Parish, C. Philips, W. Pitt, W. D. Reece, and J. Rennie, TAMU; M. Roundhill, Texas Tech University; K. Unlu, and M. Yavuz, The University of Texas at Austin

Drs. W. Wilson Pitt, Fred R. Best, and Ron R. Hart participated in the OFMD Water-Reactor Programmatic R&D Integration Meetings in Albuquerque and Los Alamos Dec. 10-11. The program confirmed that the Center is making significant contributions with its experimental investigations into gallium removal and gallium-cladding interactions. No changes to the Center efforts were suggested. It was recognized the temperature-driven gallium-cladding experiment has yet to be finally defined, and that ORNL, LANL, and the Center should finalize this soon.

Progress continued on research and development of practical dry methods for removal of gallium from weapons plutonium, a collaborative effort with researchers at LANL, LLNL, and PNNL. Further experiments have verified last quarter's report that gallium trioxide can be volatilized from a matrix of cerium oxide (a surrogate for plutonium oxide) by reduction to the suboxide, with the gallium then collected on copper wire or mesh. A preliminary report is in preparation, as is a disclosure of invention for filing. A new furnace was ordered and installed to replace one whose temperature controller had failed. An FTIR instrument is being modified for is in gas-phase measurement of gallium in the quartz-tube reactor off-gas.

Progress continued on beam-driven studies of the interaction of gallium with fuel cladding. Ga was implanted at room temperature into zircalloy-4 at an energy of 100 keV to fluences of 10^{15}, 10^{16}, 10^{17}, and 10^{18} per cm^2. The highest fluence corresponds to total release of about 30 ppm by weight of Ga from a MOX pellet. Scanning electron microscopy (SEM) showed that the surface of the zircalloy-4 remained smooth up to the highest Ga fluence of $10^{18}/cm^2$, in contrast to the surface roughening observed last quarter after implantation of 100 keV Ga at room temperature into stainless steel 316 to a fluence of $2\times10^{17}/cm^2$. A target-heating arrangement was then tested and 100 keV Ga was implanted into zircalloy-4 at fluences of 10^{16}, 10^{17}, and $10^{18}/cm^2$ while maintaining the target at typical cladding temperature (375 °C). For the higher-fluence implants SEM indicated significant surface texture. Grain boundaries were clearly delineated. Analyses will continue next quarter.

The location of the temperature-driven gallium-cladding interaction experiment was modified to incorporate fireproof walls and a larger entrance to accommodate handling of materials. Vendors have been contacted regarding the design and manufacturability of the internal fuel pin heaters. A project design has been completed but awaits final parameters from ORNL.

The previous paragraphs contain some important research progress this quarter. What follows is a very brief but more detailed list of activities.

- Drs. Best, Hart, and Pitt participated in DOE OFMD Experimental Program Integration Meetings in Albuquerque and Los Alamos, Dec. 10-11. Dr. Pitt presented gallium-removal results.
- Dr. Pitt presented gallium-removal results to the Center Nuclear Group quarterly meeting in Amarillo in November.
- Dr. Pitt presented gallium-removal results to the Center Board of Governors in Amarillo in January.
- Dr. Best and S. O'Kelly collaborated closely with ORNL to finalize the design of the temperature-driven Ga-clad experiment. Dr. Best and students calculated the heat-transfer characteristics of many design variants as part of this effort.
- Drs. Reece and O'Kelly continued efforts to refurbish a laboratory in preparation for the temperature-driven Ga-clad experiment.
- Drs. Pitt and Philips continued experimental demonstrations of gallium removal, replaced a furnace, and began modifying an FTIR instrument.

- Drs. Hart, Rennie, and students implanted gallium ions at several different fluences into different zircalloy-4 samples, some at room temperature and some at prototypic clad temperatures.
- Dr. Unlu used SEM to examine the surfaces of many Ga-implanted samples.

MOX Use In Reactors: Water-Reactor Options For Disposition Of Weapons-Grade Plutonium

Co-PIs: N. Abdurrahman, The University of Texas at Austin, and M. Adams, Texas A&M University
Other Investigators: D. Anistratov, F. Best, I. Carron, R. Hart, Y. Hassan, S. O'Kelly, T. Parish, C. Philips, W. Pitt, W. D. Reece, and J. Rennie, TAMU; M. Roundhill, Texas Tech University; K. Unlu, and M. Yavuz, The University of Texas at Austin

Benchmarking efforts in support of the US/RF joint study on water reactors were very intense this quarter, and a great deal was accomplished. A large body of results, the content of which we had agreed upon via discussions with ORNL, was delivered to ORNL in January for inclusion in the Feb. 1 report that was sent to Russia. These results included: *evaluations* (documentation and interpretation) of three sets of experimental benchmarks ("PNL", "Saxton-65", and part of "Saxton-67"); MCNP results of all possible variants of one of the RF VVER-style computational benchmarks; and CASMO results of the entire set of US PWR-style computational benchmarks. Also, MCNP criticality calculations of many of the Saxton-65 experiments were completed early in the quarter, and a draft report was delivered to ORNL in November. Work began on meeting the next set of deadlines (in March).

Progress continued on the Mixed Oxide Data Repository (MOXDAR). The server was upgraded to Windows NT 4.0 and a Variety search engine was installed. More documents were scanned, indexed, and placed on the MOXDAR Virtual Library.

Progress continued toward a capability to model the VVER-1000 power plant. A model of the unique features of the horizontal steam generators of VVER 1000 is being developed for the French code CATHARE. Communication with ANL Laboratory has been established to obtain input information for other components of the VVER 1000.

The special session on Methods for Analysis of Reactors with MOX Fuel remained on track. The paper review was conducted over the Internet, with six papers accepted for the special session. The session, with Drs. Abdurrahman and Adams as co-chairs, is scheduled for Tuesday morning, June 3, at the ANS meeting in Orlando.

The previous paragraphs contain some important research progress this quarter. What follows is a very brief but more detailed list of activities.

- Dr. Adams conducted numerous negotiations with ORNL to determine which benchmark tasks would be performed by the Center and which by ORNL.
- Drs. Abdurrahman and Yavuz completed evaluations of two sets of MOX critical experiments performed at PNL in the 1970s, and transmitted results to ORNL.
- Dr. Carron assisted Dr. Abdurrahman and his student E. Reott in evaluating roughly one third of the "Saxton-67" critical experiments; this was transmitted to ORNL.
- Dr. Carron, Dr. Abdurrahman, and his student G. Radulescu evaluated the "Saxton-65" critical experiments and transmitted evaluations to ORNL. Some inconsistencies regarding fuel and critical core specifications were identified and resolved by using data from other documents such as blue prints of the fuel rods.
- Drs. Abdurrahman and Yavuz submitted a summary, "Analysis of Critical Experiments Performed at PNL Using Rectangular Parallelepipeds Containing MOX Fuels," to the summer ANS meeting.
- Dr. Abdurrahman and his student G. Radulescu performed MCNP calculations of many of the Saxton-65 configurations. For the single-region experiments, where different lattice pitches were used, a positive correlation between calculated k_{eff} and the moderator/fuel volume ratio was obtained.

- Dr. Abdurrahman and G. Radulescu delivered a draft report of MCNP results to ORNL in November.
- Dr. Abdurrahman and G. Radulescu submitted a summary, "MCNP Criticality Benchmark Calculations of the SAXTON Plutonium Program Experiments," to the summer ANS meeting.
- Dr. Abdurrahman and G. Radulescu used MCNP to calculate several variants of the RF computational benchmark, a VVER-style lattice with MOX fuel, and delivered results to ORNL.
- Dr. Abdurrahman and students transferred the MOXDAR database from a UNIX platform to a Windows NT 4.0 platform, which allows use of the powerful Verity Search Engine.
- Dr. Abdurrahman and students updated MOXDAR's PDF archives, which now contain 43 PDF documents.
- Dr. Abdurrahman and co-workers tested the SCALE-4.3 code system on a sample PWR case from an ORNL report.
- Dr. Parish and his student G. Cuevas-Vivas used CASMO-3 to calculate all variants of the US computational benchmark, and transmitted results to ORNL. Dr. Parish also discovered an error in the ORNL specification of the problem.
- Dr. Parish and his student G. Alonso-Vargas submitted a summary to the ANS summer meeting. It was accepted.
- Dr. Parish and his student B. Rearden made progress toward a new WIMS-D4m model of a VVER-style lattice.
- Dr. Adams participated in the paper review, in January, for the upcoming ANS meeting to be held in Orlando in June.

MOX Use In Reactors: MOX Fuel Evaluation Project

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

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 to verify the efficacy of fuel designs under power reactor conditions. The work this past quarter has been to lay the ground work for the development of thermal models for fuel behavior at high burnups typical of current LWR's. These models will be used for the subsequent thermal and mechanical analysis.

The technical exchanges with Belgonucleaire (BN) have proceeded towards this goal. The COMETHE code by BN embodies the state-of-the-art modeling which will be used for this project. The work of this Quarter was to reach agreement with BN regarding the technical scope of the project and complete a Memorandum of Agreement between BN and the Texas Engineering Experiment Station (TEES) under which the collaboration will be performed.

On December 14, 1997, a meeting was held in Brussels between John Alvis, a graduate student in the Department of Nuclear Engineering at A&M, and Marc Lippens, Project Manager at Belgonucleaire. The purpose of the meeting was to review technical requirements, thermal performance data which can be used for model development, and terms of the Memorandum of Agreement. Based on that meeting, the final MOA has been agreed upon and signed. The date of completion of the MOA for transmittal to BN was January 31, 1997. This was a milestone originally anticipated for March, 1997, which has been completed early.

DISPOSITION: NON-PROLIFERATION/TRANSPORTATION

Transportation Analysis Of Mixed Oxide Fuels

PI: Hani 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 issued 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 effect 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 sought to compliment 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.

Modeling for Safe Routing

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

Documentation was produced summarizing routing criteria and models applicable to highway transportation of defense-owed fissile materials. This documentation builds on previous research identifying both formal and informal Department of Energy routing practices and is used to ensure models under development capture both formal (or regulated) and informal (or practical) DOE routing objectives. The synthesis of literature review relating to hazardous materials transport and related multi-objective path problems in near completion.

Internal documentation reinforces prior conclusions about two key parameters that are not adequately modeled by a single DOE declassified routing model. In particular, routing risk has been found to be very sensitive to the varying spatial and temporal properties of population and travel time parameters. As a result of this finding, work has begun to develop a Geographic Information Systems interfaced with a time-dependent routing algorithm in order to determine if current DOE declassified routing models adequately capture this variance. To date, a sample area was used to examine the impact that different levels of data aggregation has on population density estimates. Specifically, population density estimates for counties and block groups were loaded into the GIS and the corresponding population densities within different buffer zones of an Interstate Highway were calculated. The level of data aggregation used was found to have a significant impact on population density estimates, especially for small bandwidths. Work on the GIS program is being expanded to include a multi-state network.

The research effort continues towards the development of an integrated framework and procedures for a priori routing strategies that recognize the time-varying, stochastic nature of risk and travel characteristics, both of which are inherent to this problem. Specifically, we have completed implementation of code for extending algorithms for determining the minimum time paths in stochastic, time-varying networks to algorithms for determining minimum cost/risk paths and best paths with respect to multiple objectives in such

networks. Work continues on the extension of algorithms for determining least time, least cost as well multi-objective path problems of time paths in stochastic, time-varying networks in such networks to include time-dependent shortest -path algorithms with curfews.

To test these procedures, we have initiated the set-up of an example network of Texas using 1992 population statistics from the U.S. Bureau of the Census and actual distances to show results of the algorithms with respect to minimum time paths, minimum population paths and paths that are pareto-optimal with respect to both objectives. Analysis of results for shipments from Austin to Amarillo is currently underway. Extensive testing of algorithms on randomly generated networks to calculate performance and to compare characteristics of solutions continues.

A technical paper titled "Least Expected Time-Paths in Stochastic, Time-Varying Networks," by Miller-Hooks and Mahmassani is currently waiting review for submission.

Dr. Hani S. Mahmassani attended the Nuclear Group Quarterly Meeting in Amarillo, Texas on November 20, 1996 and gave presentation titled "Transportation and Routing Strategies for Nuclear Shipments."

Ms. Elise Miller-Hooks, UT-Austin doctoral student and research assistant, attended session titled "Cross Cutting Issues on the Disposition of Surplus Weapons Plutonium" for the Third Annual Student Research Conference at West Texas A&M (sponsored by Southwestern Bell Telephone Foundation and Amarillo National Resource Center for Plutonium) held on November 1, 1996 and gave presentation titled "Multi-objective Hazardous Substance Transport in Stochastic, Time-Varying Networks." In a Seminar on Doctoral Student Research in Transportation Modeling at the January 1997 Transportation Research Board Meeting held in Washington, DC Ms. Miller-Hooks also gave a presentation titled "Optimal Routing in Time-Varying Stochastic Networks."

A report documenting routing criteria and applicable models is in the final stage of editing.

SUBPROJECT 1— Modeling for Safe Routing
Paul Nelson, Ph.D., P.E.. Texas A&M University

The A&M Transportation Group has finalized input regarding both non radiological and radiological risk assessments of transporting plutonium pits and mixed oxide fuel. The risk assessments will be performed using the computer code RADTRAN available from Sandia National Laboratories. Preliminary results have been obtained and a first draft of the report/thesis has been completed. Most parameters critical to the risk assessment were obtained from the Storage and Disposition of Weapons-Usable Fissile Materials Final EIS. Two hypothetical campaigns were considered. The first scenario was the case in which a MOX fuel fabrication facility was built at the Savannah River Site. This scenario involved transporting pits from Pantex to SRS and then MOX fuel to the hypothetical commercial power plant, the Palo Verde Generating Station. The second scenario included the MOX fuel fabrication facility at Pantex; this case would involve the shipment of MOX fuel from Pantex to Palo Verde. Risk assessment results will be provided for incident-free and accident cases for both the general public and workers in units of person-rem.

SUBPROJECT 2—Development of Source Term Components for Formulation and Initial Release of Plutonium-Containing Aerosol for Conditions and Effects Not Treated by Existing Models for Transportation Incidents
Co-PIs: Yassin A. Hassan, Ph.D., and William H. Marlow, Ph.D., Texas A&M University

The three dimensional computer program of fluid flow is complete. This program is validated with comparison with several test cases. Good agreement between the program predictions and available data is obtained. The state-of-the-art large eddy simulation (LES) algorithm is implemented. The assessment of this new technique is started. This approach resolves the turbulence large scales and the sub-grid scales are modeled with eddy viscosity model. The coupling between the particles and the fluid phase is complete.

SUBPROJECT 3—Investigation of Neural and Fuzzy Logic Analysis Techniques for Surety Issues in Transportation of Nuclear Materials

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

Progress continued on research and development of a methodology for assessing the risk associated with the transportation process of nuclear materials. We are using fuzzy risk assessment to overcome the difficulties faced when using probabilistic analysis, due to the vague nature and lack of information characterizing the problem.

We use a fuzzy fault tree that describes the sequence/combination of events that may lead to a failure during the transportation process. Such events may be due to human errors, weather problems, intelligence leaks, or other hypothetical problems. The top event of the tree is catastrophic system failure, such as the material loss or environmental containment. Each event in the fault tree has its own membership function in which the fuzzy variable is the probability that this event may occur, the so called fuzzy probability of occurrence. The membership grade is the degree of belief experts have that this probability may take on a certain value.

A literature study revealed some points of weakness in the theory developed to deal with independent fuzzy probabilities, specially when recalculating the probabilities of intersection and union of the events of a given set after adding a new event to the set. A new method has been used to overcome these points of weakness.

In collaboration with the responsible personnel at Sandia National Laboratories, we continued using the software PHASER (Probabilistic Hybrid Analytical Systems Evaluation Routine), which is used to calculate the membership function of the tree's top event. We have also developed algorithms that could be used along with PHASER for the calculation of fuzzy membership functions of repetitive events during a transportation process.

- Presentation at the Third Annual Student Research Conference at West Texas A&M University
  a) Planned Completion Date - November 1, 1996
  b) Actual Completion Date - November 1, 1996
- Paper submitted to ICNN97
  a) Planned Completion Date- November 15, 1996
  b) Actual Completion Date - November 15, 1996

SUBPROJECT 4—Application of Existing Codes and Techniques

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

Progress continued on Transportation Analysis and development of an engineering modeling capability to establish safe transportation of MOX fuels and radioactive materials. The objective of the project is to achieve optimization of the transportation of mixed oxide fuels from a temporary storage site to a permanent location.

During this period, two undergraduate research assistants also conducted research by studying in detail and developing more familiarity in using and applying TRANSNET code. The analysis using the HIGHWAY program included calculation of several different types of routes by imposing one or more constraints during the routing calculations. Routes are determined by minimizing the total impedance between the origin and the destination. The purpose of the project is to develop and apply tools for the absolute and comparative analysis of risks during the transportation stage of various projected scenarios for the disposition of surplus weapons fissile material.

One of the special features of the HIGHWAY model is to calculate routes which will conform to the DOT regulations. State or local routing agencies may designate preferred routes as an alternative to Interstate highways through a series of state sub networks. In all cases, the estimated conservative population exposures to radiation from postulated transportation accidents might be a small fraction of the population radiation dose due to several routine-shipments. A major aspect of the current effort is to consider methods to identify procedures for selection of routes that avoid dense population areas and to keep potential

impact as low as practicable due to repeated radiation exposures to rural population along the selected routes.

DISPOSITION: GEOLOGIC DISPOSAL

Thermal/Mechanical Modeling Of The "Can-In-Canister" Plutonium Immobilization Process

PI: Kenneth S. Ball, Ph.D., The University of Texas at Austin
Eric M. Taleff, The University of Texas at Austin
Theodore L. Bergman, The University of Connecticut
Edward E. Anderson, Texas Tech University, Jaime F. Cardenas-Garcia, Texas Tech University. Javad Hashemi, Texas Tech University

Progress continued on the system-level analyses of the poured stream of molten high-level waste glass. Profiles of the glass jet diameter, axial velocity, and temperature were calculated. The semi-transparent thermal radiation model predicted a cooling rate of approximately six deg. C per foot under conditions specified for the DWPF facility. The opaque radiation model, based on a diffuse gray medium but using a modified value of emissivity, can be used to predict cooling rates, but does not provide as accurate predictions of the radial temperature distribution. A detailed report has been submitted for presentation at the 1997 National Heat Transfer Conference.

Progress continued on room temperature experiments using analogous fluids (corn syrup). The experimental apparatus was modified to facilitate refilling the hydraulic cylinder and to eliminate air-bubbles in the fluid. Experiments show the buckling and thickening of the jet at impact, and confirm the theory of thin-beam buckling (Euler instability) used in the analysis of viscous flow behavior. High-speed videos reveal that the oscillating frequency of the jet is significantly higher than first estimated, in excess of 100 Hz.

Progress continued on high temperature experiments using DWPF glass surrogates. A new molten glass pour onto a thick, unheated cast iron plate was performed at 1050 deg. C. This pour configuration allowed the glass to spread over a larger area than in previous pour experiments, simulating the large basal area of the full canister. The glass pool cools and hardens upon contact with the unheated plate, forming a mound that intermittently collapses. Visual inspection of the bottom surface of the glass casting revealed ridges that had formed where molten glass flowed over hardened glass, trapping air between the hardened glass and the iron plate.

Progress continued on the detailed finite-element analysis of the molten glass jet. The incorporation of heat transfer, to allow detailed predictions of the temperature distribution throughout the molten glass jet, has resulted in numerical stability problems using the commercial CFD code FIDAP. It has been determined that the instability is an inherent limitation of FIDAP. Other codes are being tested to determine their suitability for studying the thermal behavior of the molten glass jet.

The study of the DWPF and plutonium glass radiative properties has been completed. Results from spectrographic measurements have been analyzed, indicating that the internal radiative heat transfer can be modeled as a diffusion process using an effective thermal conductivity. Exceptions to this finding are associated with those components of the can-in-canister filling process whose physical size is small (order of 1 cm), including the pour stream and elements that are adjacent to the free surface of the molten glass pool. The final report has been drafted and is presently being finished.

Progress continued on the development of the 2D thermal stress model for the glass pour. Two models are being considered: (a) the pour stream is defined as instantaneously spreading over the top of the container at the fill level; (b) the pour stream is defined as only having an effect at the point of contact with the fill level. Preliminary results point to model (b) as being more realistic. These models include convection and radiation effects on the various surfaces.

A number of presentations, publications, and other activities occurred during the last quarter. These are listed below:

- Brian M. Powers organized and chaired the Special Session on Nuclear Energy Issues at the Third Annual Student Research Conference at West Texas A&M University, 1 November 1996. This session was entitled, "Engineering Technology and Radiation: Can-in-Canister Disposition of Surplus Weapons Plutonium"
- Student presentations at the Third Annual Student Research Conference at West Texas A&M University (Special Session on Nuclear Energy Issues), 1 November 1996, included:
  a) B. M. Powers, "Experimental Investigation of Instabilities in a Molten Glass Jet Flowing into a Canister."
  b) M. W. Silva, "Computational Study of Container Filling with Highly Viscous Fluid." This presentation was awarded first place in the Special Session on Nuclear Energy Issues.
  c) M. Gomon, "Experimental Study of the Flow Behavior of a Highly Viscous Fluid."
  d) Hu and J. Li, "Thermo-Mechanical Study of a Glass Pour."
- Mark W. Silva was awarded first place in the best presentation competition for the Special Session on Nuclear Energy Issues at the Third Annual Student Research Conference at West Texas A&M University, 1 November 1996, for his talk entitled, "Computational Study of Container Filling with Highly Viscous Fluid."
- A poster entitled, "Canister Filling with a Molten Glass Jet," was presented by K. S. Ball at the Heat Transfer Picture Gallery, 1996 International Mechanical Engineering Congress and Exposition, 18 November 1996, Atlanta, GA. This poster was selected in a competition to be featured in an upcoming volume of the ASME Journal of Heat Transfer. Co-authors were K. S. Ball, T. L. Bergman, E. M. Taleff, M. Song, M. Gomon, B. M. Powers, and M. W. Silva. A color photocopy of the winning entry to be published in the ASME Journal of Heat Transfer is attached.
- A presentation entitled, "Canister Filling with a Molten Glass Jet," was made by K. S. Ball at the 1996 Annual Meeting of the Division of Fluid Dynamics of the American Physical Society, 25 November 1996, Syracuse, NY.
- An abstract entitled, "Canister Filling with a Molten Glass Jet," was published in the Bulletin of the American Physical Society, Volume 41, p. 1749, 1996. Co-authors were K. S. Ball, M. Song, M. Gomon, M. W. Silva, E. M. Taleff, B. M. Powers, and T. L. Bergman.

Immobilization Of Plutonium Into Ceramic Media

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

Based upon earlier results we have settled on the following approach. A combined barium zirconate-zirconolite two phase system will be used to immobilize PuO_2 largely in the barium zirconate and in the uranium oxides in the zirconolite phase. In addition sufficient hafnium will be incorporated in both phases to prevent criticality.

During this past quarter we have produced highly crystalline Pu containing zirconolite. This was necessary to carry out a Rietveld X-ray analysis to determine the location of Pu in the zirconolite lattice. This analysis has already been done for barium zirconate. We also prepared $BaZrO_3$ with 30% substitution of Hf for Zr. We are also in the process of determining whether this hafnium containing phase will also fix high levels of CeO_2.

Preliminary plans were completed to prepare plutonium substituted barium zirconate under the direction of Leonard Gray at Lawrence Livermore National Laboratory.

DISTRIBUTION OF QUARTERLY REPORT

1 November 1996 through 31 January 1997

Signed original mailed to Juan Williams by Roger Mulder.

Required by the CA, 1 copy to: Juan Williams, DOE/AL; John Kirby, DOE/AAO; George Werkema, DOE/AL; Carol B. Patterson, Office of Scientific and Technical Information (OSTI); Patent Attorney, Office of the Chief Counsel.

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DETAILED REPORTS

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PLUTONIUM INFORMATION RESOURCE

ELECTRONIC RESOURCE LIBRARY

Project Management Timeline Checklist

Project Year One FY 1995

Staff Development
- X Hire Information Scientist, 7/95.

Collection Development
- X Determine size and location of collections, 10/95.
- X Determine document types, 10/95.
- X Determine which documents have no MARC catalog records, 1/96.
- X Collaborate with DOE Public Info. Office and researchers to determine documents to be digitized, 4/96.
- X Develop forms for recording document titles to be digitized and linked, 4/96.
- X Compile titles and annotations of documents that are candidates for scanning, 3/96 and ongoing.
- X Compile UR.'s for linking sites, 3/96 and ongoing.
- X Contact remote sites for permission to link, 5/96.

User Assessment
- X Analyze scientific and researcher information interface /96.
- X Analyze k-16 information interface needs, 5/96.
- X Determine access needs of the ANRCP/DOE community, 9/95.
- X Determine access needs of general public, state and local governments, and elected officials, 5/96.

System Feasibility
- X Investigate/collaborate with current projects at Texas A&M (Nuclear group),7/95.
- X Investigate/collaborate with current projects at ORNL, 7/95.
- X Investigate/collaborate with current projects at DOE/OSTI, 7/95.
- X Investigate/collaborate with current projects at Los Alamos Laboratory,7/95.
- X Determine connectivity requirements to meet user need, 5/96.
- X Plan for establishing T-1 service to *Electronic Resource Library* Web Server, 5/96.
- X Determine user/interface/access methodology, 5/96.
- X Determine server/storage requirements, 5/96.
- X Confirm that Adobe Software will meet requirements, 5/96.
- X Resolve problems connected with scanning three categories of materials: (a) electronic, (b) print, and (c) film.
- X Specify special equipment needed to adapt reading room machines. 5/96.
- X Specify scanning technology to digitize historical archives, 5/96.
- X Specify software to import machine readable documents, 5/96.

System & Software Procurement
- X Produce preliminary report for consultant review, 1/96
- X Produce final report, 4/96.
- X Produce RFP for system and software, 5/96.

Cataloging and Classifying Documents
- X Create MARC bibliographic records for documents through OCLC, 8/95.
- X Transfer bibliographic records to the Harrington Library Consortium public access catalog, Ongoing.
- X Provide bibliographic records to DOE OSTI for documents not accessible through the Government Information Locator Service, Ongoing.

Project Year Two FY 1996

- X Produce electronic bibliography for DOE Reading Room Collection at Amarillo College, 1/96
- X Establish interim procedure for obtain full text of DOE Reading Room Collection at Amarillo College for researchers and scientist, 1/96.
- X Study scanning project contracted by Amarillo College Library and Pantex Plant for possible inclusion in final RFP for *Electronic Resource Library.1/96.*
- X Contact vendors to determine participation and cooperation for software, hardware, and networking possibilities. 2/96
- X Analyze *National Digital Library Federation* (NDLF), the joint venture of major research libraries and archives coordinated by the Commission on Preservation and Access to explore questions of transition from traditional library service to the new digital environment. 3/96.
- X Pursue establishment of *a DOE Digital Library Federation* (DDLF), a proposed joint venture of DOE laboratory and resource sites for creation of a coordinated distributed digital library of archives containing full text, indexed DOE documents unique to the site, recorded in a central bibliographic database scanned and produced for full text archive only at designated site, thus avoiding duplication of scanned titles and compatibility of technology. In progress.
- X Investigate/collaborate with current projects at Sandia Laboratory, 5/96.

System Procurement and Installation
- X Issue RFP to hardware and software vendors, 6/96.
- X Receive and install system, 9/96. (Installed first of August 96)

Establishing Connectivity
- X Install sufficient INTERNET bandwidth for information access, 9/96. (Done by end of August 96)
- X Obtain class C licence for LAN access to server, 6/96.(Done by end of August 96)

Staff Development
- X Hire quality control specialist and operators, 9/96. (Done by end of July, 96)
- X Train staff on server operating system, appl. software, and user interfaces, 9/96. (Scheduled for end of July)
- X Train scanning workstation operators, 9/96. (Done by end of July)
- X Establish quality control procedures, 9/96.
- X Contract for server management, 9/96.
- X Contract for Web site development, 9/96. (Done by end of August)
- X Contract with other sister sites for remote access and permission to link, 9/96. (In progress and ongoing)

System Testing/Production
- X Create test database of 100 documents or 10,000 pages, 11/96.
- X Test system indexing for full text access, 12/96.

User Training/Public Access Implementation
- X Contacting list of ERL users to establish IP (Internet Protocol) match for access to the Electronic Reserve Room of the ERL and to walk them through the services on the ERL. 12/96 and 1/97.

Collection Development
- _____ Investigate, purchase and install an Electronic Reserve Room software for "wrapping" the intellectual property materials so that the grants and permissions routines can be established and implemented with full cooperation from publishers and authors.

Project Year Three FY1997

Document Production/Utilization
_____Produce reports for document production, Quarterly.
_____Produce quarterly reports of system utilization, Quarterly

Document Procurement
_____Collaborate with ANRCP Center staff and DOE Info. office to add current scientific information, Ongoing.

Evaluate User Satisfaction
_____Conduct online survey of user needs/satisfaction, 10/97.
_____Interview public school teachers and students, 5/98.

Investigate Additional Information Types
_____Report on need for calendar information for Center Activities, 11/97.
_____Report on need for multi-media tour of Pantex Plant, 5/98.
_____Report on other needs of ANRCP for information, 5/98.

Project Year Four FY 1998

Document Production/Utilization
_____Produce reports for document production, Quarterly.
_____Produce quarterly reports of system utilization, Quarterly.Document Procurement
_____Collaborate with ANRCP Center staff and DOE Info. office to add current scientific information, Ongoing.
Evaluate User Satisfaction
_____Conduct online survey of user needs/satisfaction, 10/98.
_____Interview public school teachers and students, 5/99.
_____Investigate Additional Information Types

ENVIRONMENTAL, PUBLIC HEALTH AND SAFETY

PROGRESS REPORT

Perched Aquifer & Tracer Testing, Water Treatment

Combined Oxidation/Bioremediation of High Explosives

by

Aydin Akgerman, Chevron II Professor
Chemical Engineering Department
Texas A&M University
College Station, TX 77843-3122

December 1996

Summary

During this period we have studied catalytic oxidation of TNT and RDX in solution over the Pt/TiO_2 catalyst at different temperatures and at different catalyst amounts. The reaction extent is studied using both total organic carbon (TOC) and HPLC analysis.

We studied TNT oxidation at 180°C and 500 psig at catalyst concentrations of 0 - 2 g catalyst/liter solution. The initial reactor heat-up is performed at under an inert atmosphere (no oxygen) and takes about 2 h. It was observed that most TNT oxidation took place during this heat-up period, however the extent of oxidation was very much dependent on the amount of catalyst, indicating that catalytic oxidation is much faster than homogeneous wet oxidation.

Similarly with RDX (with a trace amount of HMX as impurity) we have observed complete oxidation at 180°C using 50 ppm RDX solution and 2 g catalyst/liter solution. In RDX oxidation we have not detected any intermediates, indicating that oxidation of primary products to mineralization is faster and no stable secondary products are formed.

Results and Discussion:

Initially we were using the HPLC in the Environmental Engineering Group at Professor Autenrieth's laboratories. Because of the logistics involved, we purchased a column and calibrated our HPLC for the same analysis. Figures 1 and 2 show our calibration of the HPLC response. Both for TNT and RDX the responses are linear, indicating the validity of HPLC analysis. Figure 3 shows the analysis of TNT and RDX standard solutions (feed solutions used). The impurity in the RDX analysis (peak 1) is HMX.

As explained in the previous report, the reactor is charged with the TNT or RDX solution and the catalyst, purged with nitrogen to remove any oxygen from the system in order to minimize the amount of reaction during the heat up period. When the reactor was brought to the operating temperature, air (oxidizing medium) was introduced. The reactor heat-up and temperature stabilization takes around 2 hours. It was assumed previously that not much reaction takes place during that period since the system was purged of oxygen. However, water itself is an oxidizing medium. Therefore we conducted a study where we varied the amount of catalyst in the system and sampled the reactor just before air is introduced.

Figure 4 shows the results of TNT oxidation studies using different amounts of catalyst at 170°C - 180°C and 500 psig. In all studies the initial concentration of TNT in the solution was 30 ppm. The time scale from -5 to 0 are in hours indicating the heat-up period of the reactor under inert nitrogen atmosphere whereas the time scale for times > 0 are in minutes. As can be seen, significant oxidation is taking place during the heat-up period, but the rate is dependent on the amount of catalyst. The very top curve can be characterized as homogeneous wet oxidation with no catalyst. There the TOC reduction during the heat-up period (and there after) is minimum. On the other hand almost 80% TOC reduction is observed during the heat-up period for the case when 2 g catalyst/liter solution is used and the total TOC reduction is in excess of 90%.

Figure 5 presents HPLC analysis results for TNT oxidation at 175°C and 500 psig starting with 30 ppm solution and 0.5 g catalyst/liter solution. Figure a is at the end of heat-up period before introducing oxygen. As can be seen the concentration is already down to ~ 10 ppm. Figures b - e show reaction progression at 1, 7, 30, and 60 minutes reaction time showing the intermediates as well as TNT concentration. Figure 6 shows the same reaction at the same condition with 2 g

catalyst/l solution, all TNT is oxidized during the heat-up period. This shows the effect of the amount of catalyst. Although the TOC analysis does not come to 0 in Figure 4, HPLC analyses (which are more sensitive) indicate that no organic is left in the system, the TOC values are sensitive to the amount of dissolved carbon dioxide (reaction product) and hence are not very accurate at very low ppm level measurements.

The RDX standard solution was prepared by dissolving stock solution of RDX in methanol and adding that to hot water (~100°C) and allowing the methanol to evaporate. RDX concentration in water is 50.7 ppm and HMX is present as impurity. Figure 7 shows the results of a reaction at ~180°C and 500 psig using 2 g catalyst/liter solution. The top spectra is for the standard solution, the middle one is for the sample taken when the reactor heat-up is complete and time air is introduced, and the bottom one is at 1 min reaction time. The middle spectra indicate ~ 85% reduction in concentration during the heat up period and the bottom spectra show that the reaction is complete at 1 min. Compared to TNT, RDX oxidation is somewhat faster (compare to TOC reduction line for 2 g catalyst/liter solution in Figure 4), and the absence of other peaks indicates that the reaction intermediates are oxidized to complete mineralization much faster.

Work in Progress

In order to study the reaction kinetics we need to minimize the extent of oxidation during the heat-up period and maximize it thereafter. This means to heat up the system to the reaction temperature without a catalyst in the reactor (corresponding to heat-up with no catalyst, top curve in Figure 4) and introduce 1 - 2 g catalyst/liter solution after the heat up is completed. We are investigating two ways of introducing the catalyst to a high pressure system. The first way (which we currently use in another study) is to put the catalyst in a glass ampule and put the ampule in the reactor together with the solution. The reactor heat-up will then be completed without using the stirrer. When the reactor comes to the desired temperature, just before the oxidizing medium (air) is introduced, the stirrer is started which breaks the ampule and distributes the catalyst in the reactor. The second way is to slurry the catalyst in a loop and push it into the reactor with the oxidizing medium. Each method has advantages and disadvantages, but we will try both to determine which works better.

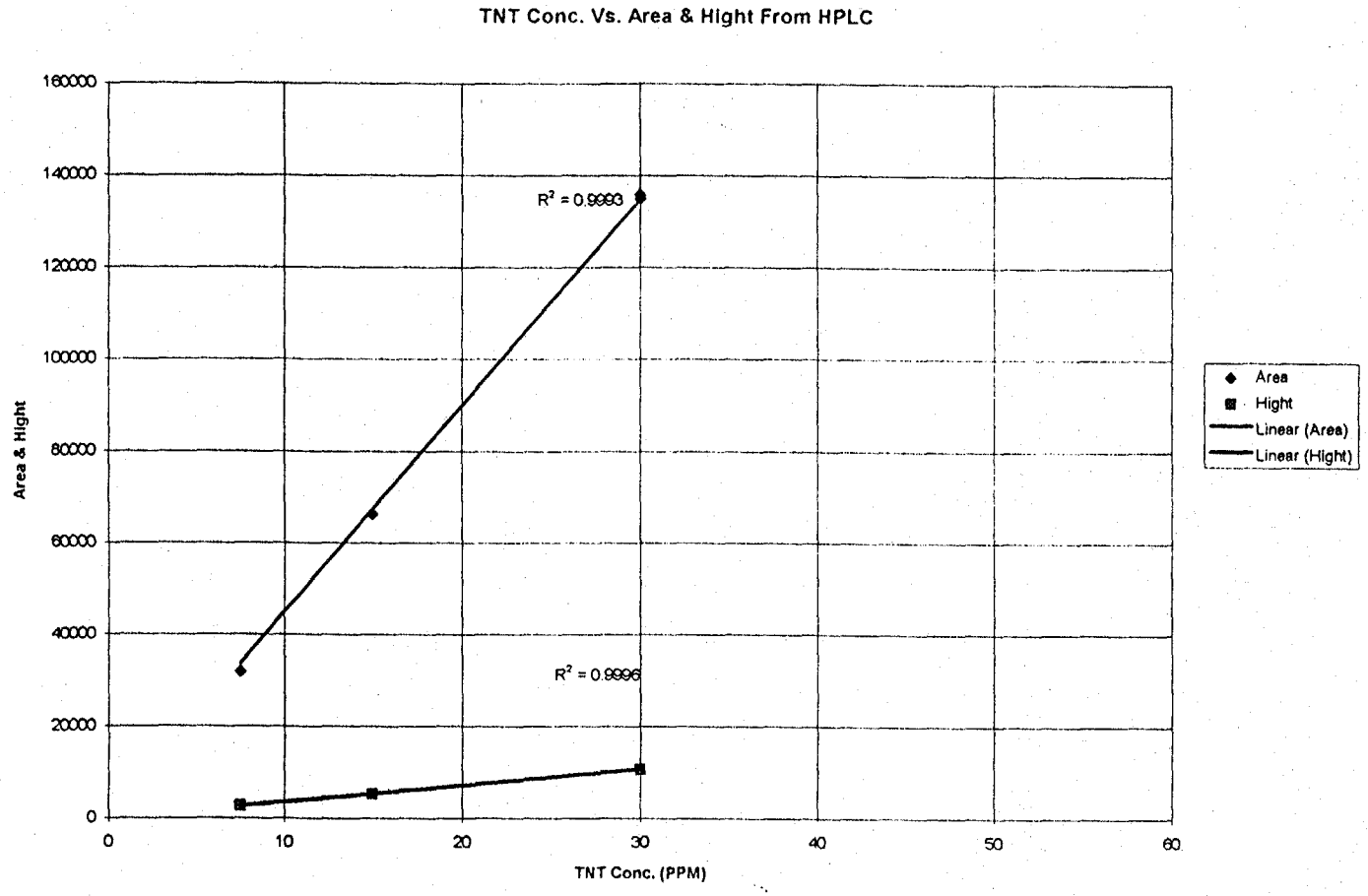

Figure 1. HPLC Calibration for TNT Analysis

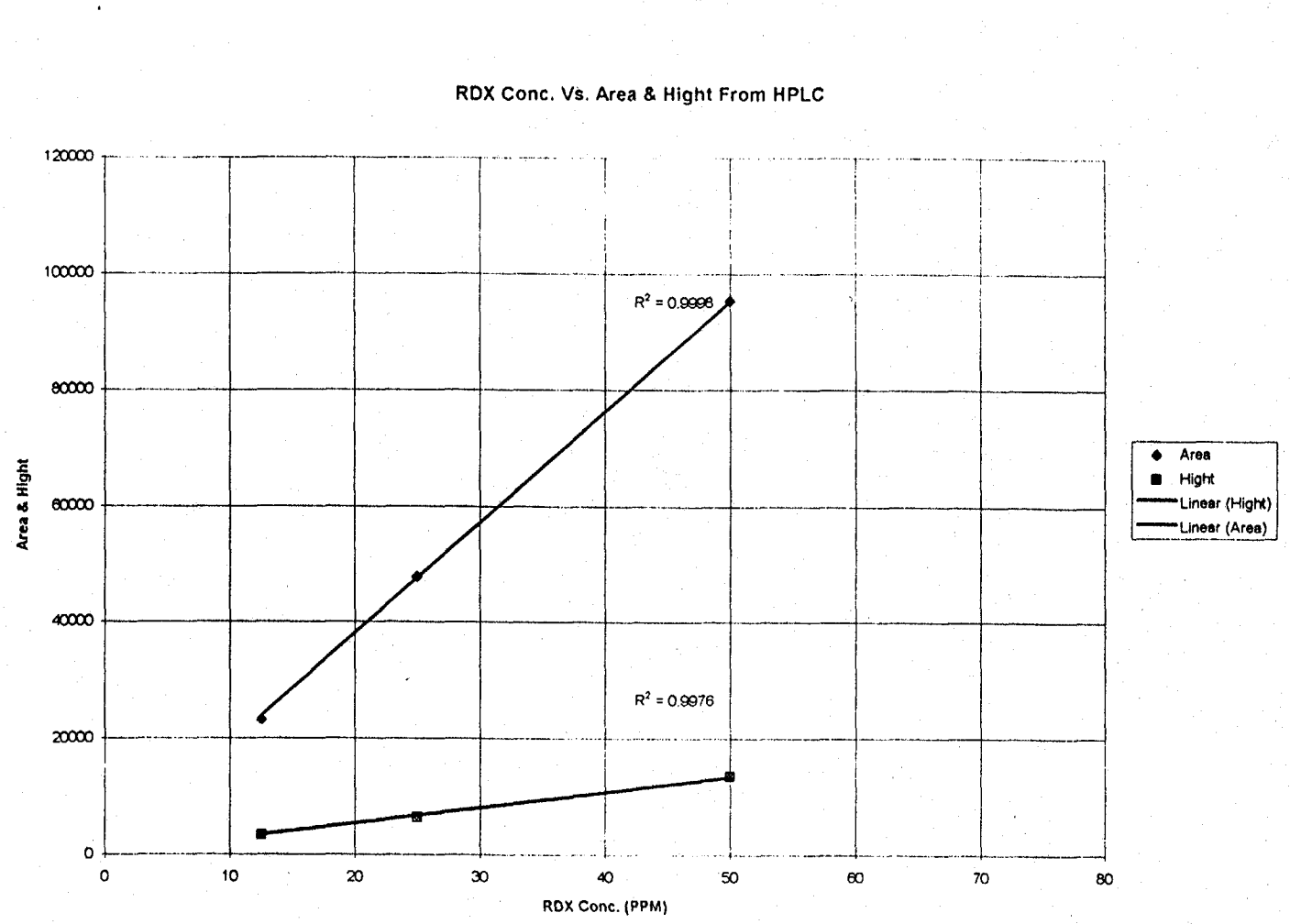

Figure 2. HPLC Calibration for RDX Analysis

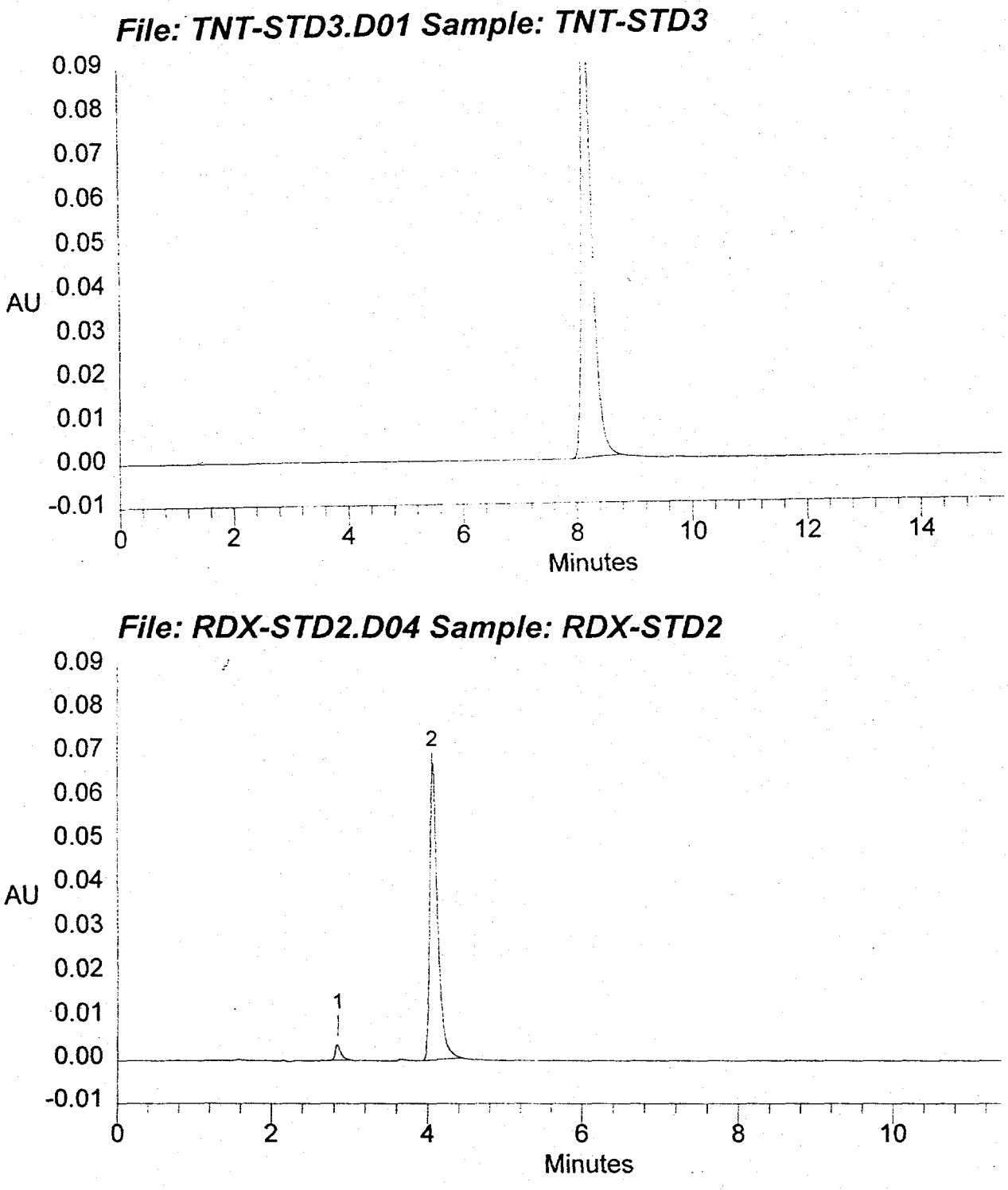

Figure 3. HPLC Analysis of TNT and RDX Standard Solutions

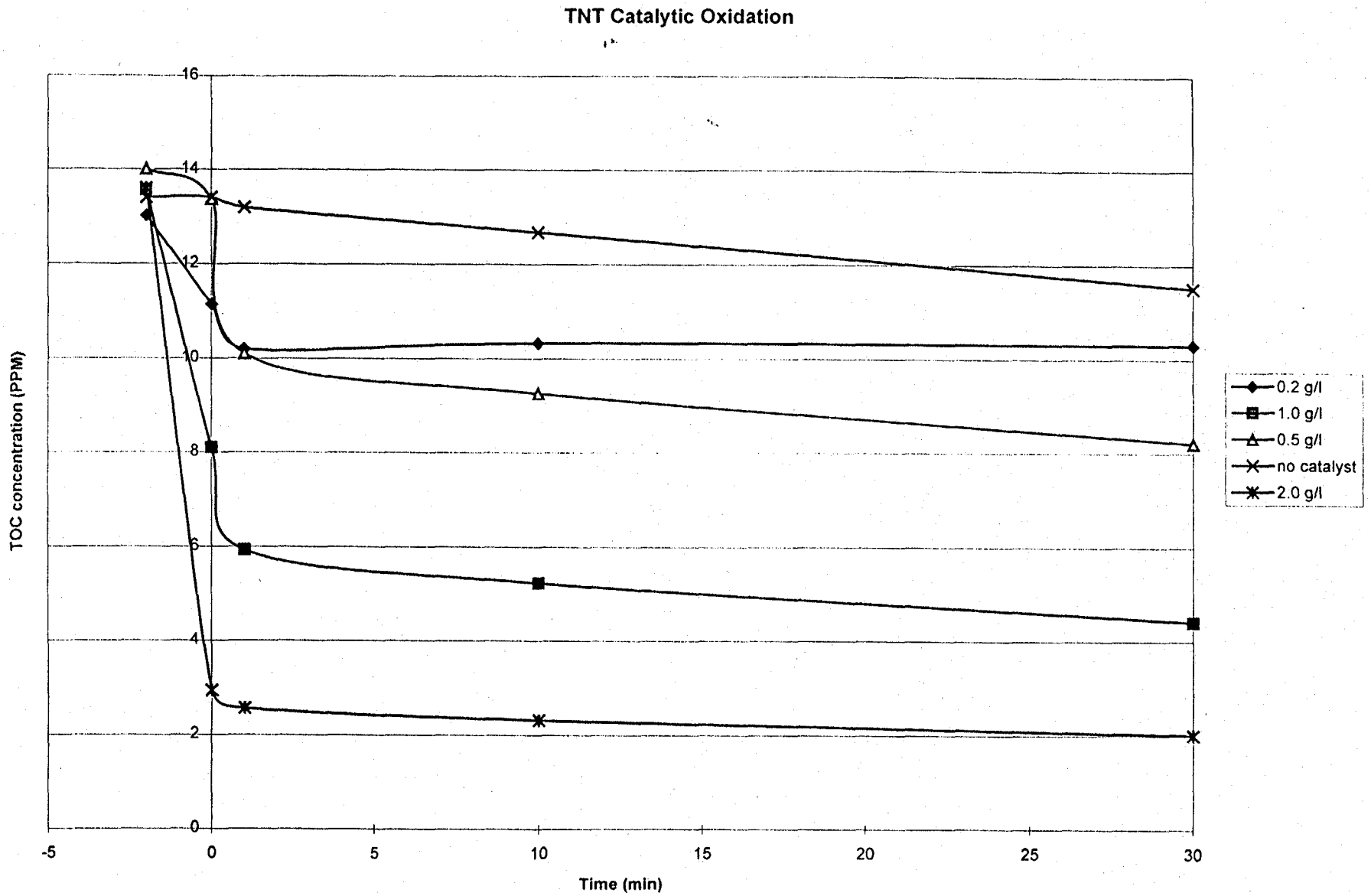

Figure 4. TNT Oxidation at 170°C-180°C and 500 psig with different amounts of catalyst

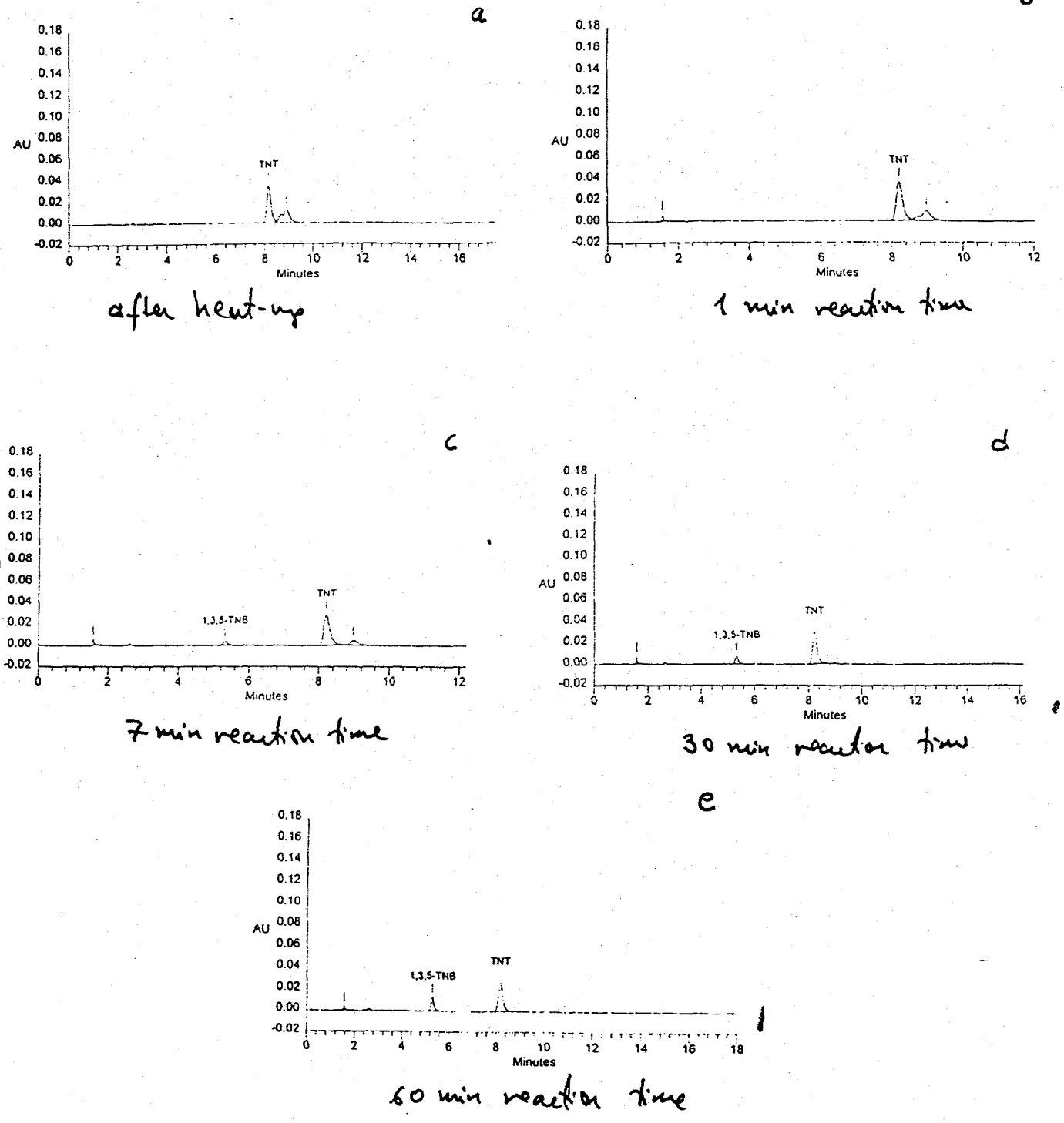

Figure 5. TNT Oxidation at 170°C-180°C and 500 psig with 0.5 g catalyst/liter solution

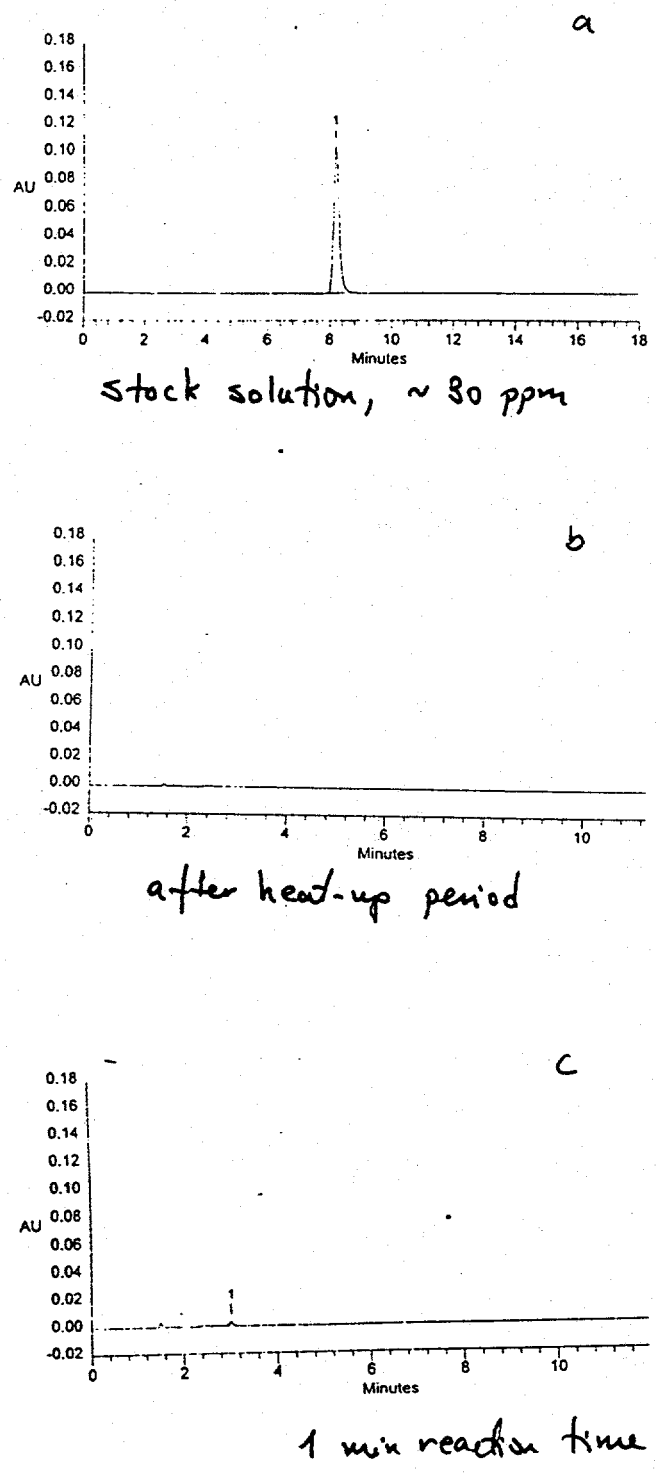

Figure 6. TNT Oxidation at 170°C-180°C and 500 psig with 2 g catalyst/liter solution

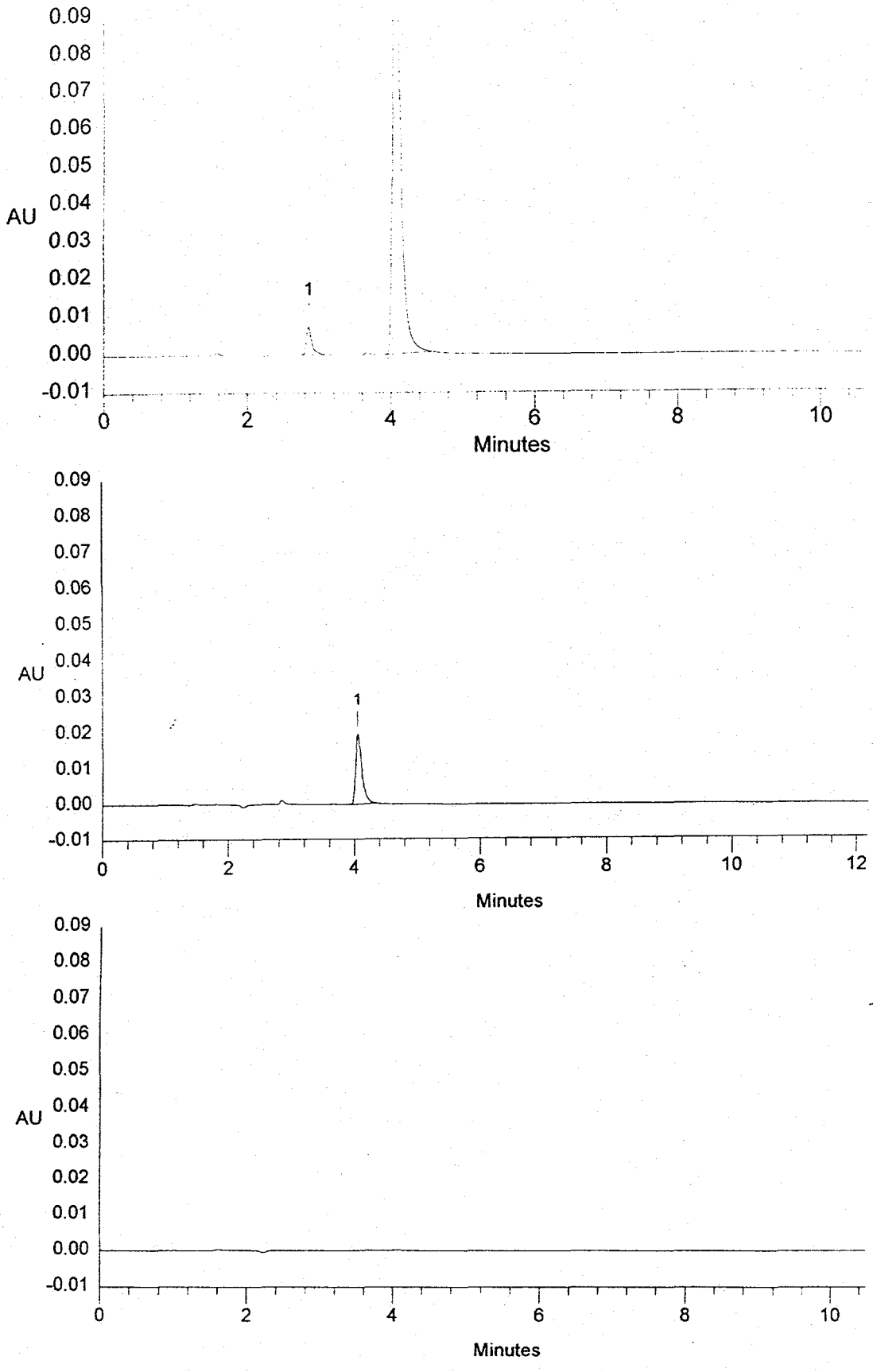

Figure 7. RDX Oxidation at 170°C-180°C and 500 psig with 2 g catalyst/liter solution

Detailed Quarterly Progress Report
November 1, 1996 to January 31, 1997
for
Chemical Models and Redox Chemistry of Chromium

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College Station, Texas 77843-3136

Redox Chemistry of Chromium

Chromium reduction experiments conducted during previous quarters appeared to show that aquifer solids consume some of the reducing capacity of ferrous iron and make the overall reduction kinetics slower. To further test this observation, a series of solution experiments was conducted to investigate the effects of natural organic matter (NOM) on the reduction of hexavalent chromium by ferrous iron. All experiments were performed under atmospheric conditions at ambient temperatures (22±2°C) in 1.0-L glass flasks wrapped with aluminum foil. The initial concentrations of Cr(VI) and Fe(II) were 20μM and 50μM, respectively. Background solution electrolytes were 0.050 M Na^+, 0.025 M Cl^-, and 0.025 M NO_3^-. Three different experiments were conducted: 1) Cr(VI) reduction by Fe(II) at pH 4, 5, and 6; 2) Cr(VI) reduction by humic acid (HA concentrations of 20 and 40 mg/L as Dissolved Organic Carbon) at pH 4, 5, and 6; and 3) Cr(VI) reduction by Fe(II) in the presence of humic acid (20 and 40 mg/L as DOC) at pH 4, 5, and 6. For the reduction experiments with Fe(II) in the presence of humic acid, solutions containing both Fe(II) and humic acid were stirred for at least 24 hours at each pH before Cr(VI) was spiked. Duplicate samples were taken and filtered through 0.45μ membrane before being analyzed for Cr(VI) and Fe(II). Standard method 3500-Cr D using diphenylcarbazide as a chelating agent was modified for the colorimetric measurement of hexavalent chromium. The method detection limit was 0.02 mg/L. Ferrous iron was measured colorimetrically by a modified Ferrozine method. The method detection limit was 0.05 mg/L.

Figures 1, 2, and 3 show the results from the experiments conducted at pH 4, 5, and 6, respectively. In these figures, the normalized (and background subtracted) hexavalent chromium concentrations remaining in solution are plotted versus logarithmic time. The results show that Cr(VI) reduction by Fe(II) in the presence of oxygen and humic acid was strongly dependent on pH. In the case of the reduction of Cr(VI) by Fe(II) alone, the reaction rate increased with increasing pH, whereas the rate decreased with increasing pH in the experiments of Cr(VI) reduction by Fe(II) in the presence of humic acid. It is seen in Figures 1 and 2 that Cr(VI) reduction by Fe(II) at pH 4 and 5 appears to have been enhanced by humic acid at shorter time periods, but that the opposite effect appears to occur at longer time periods. Cr(VI) reduction by Fe(II) at pH 6 was always adversely affected by humic acid. In general, higher humic acid concentrations at lower pH values had the largest effect on the overall reduction of Cr(VI) by Fe(II). These results were presented at the 1996 Fall meeting of the American Geophysical Union.

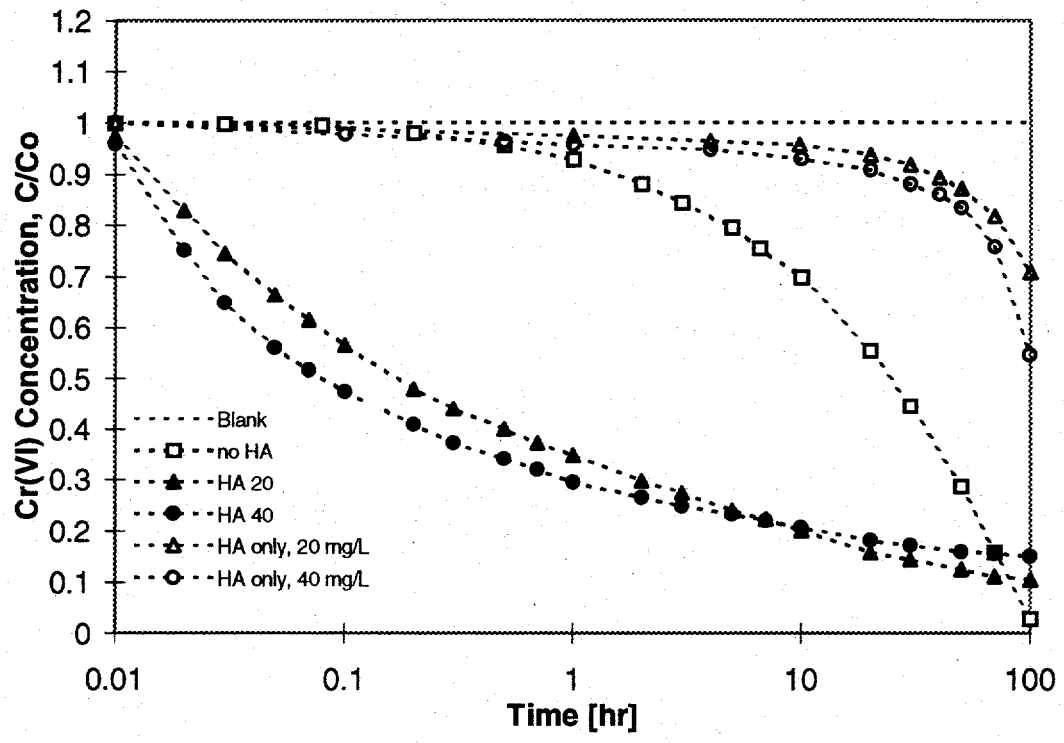

Figure 1. Cr(VI) Reduction by Humic Acid and/or by Fe(II) in the Presence and Absence of Humic Acid at pH 4.

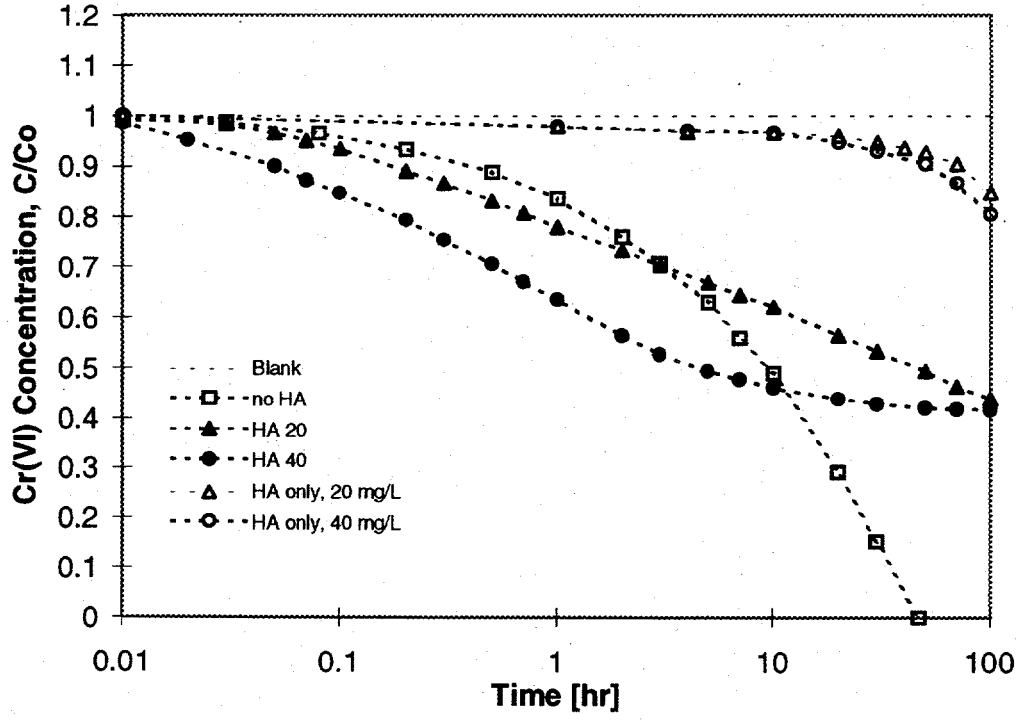

Figure 2. Cr(VI) Reduction by Humic Acid and/or by Fe(II) in the Presence and Absence of Humic Acid at pH 5.

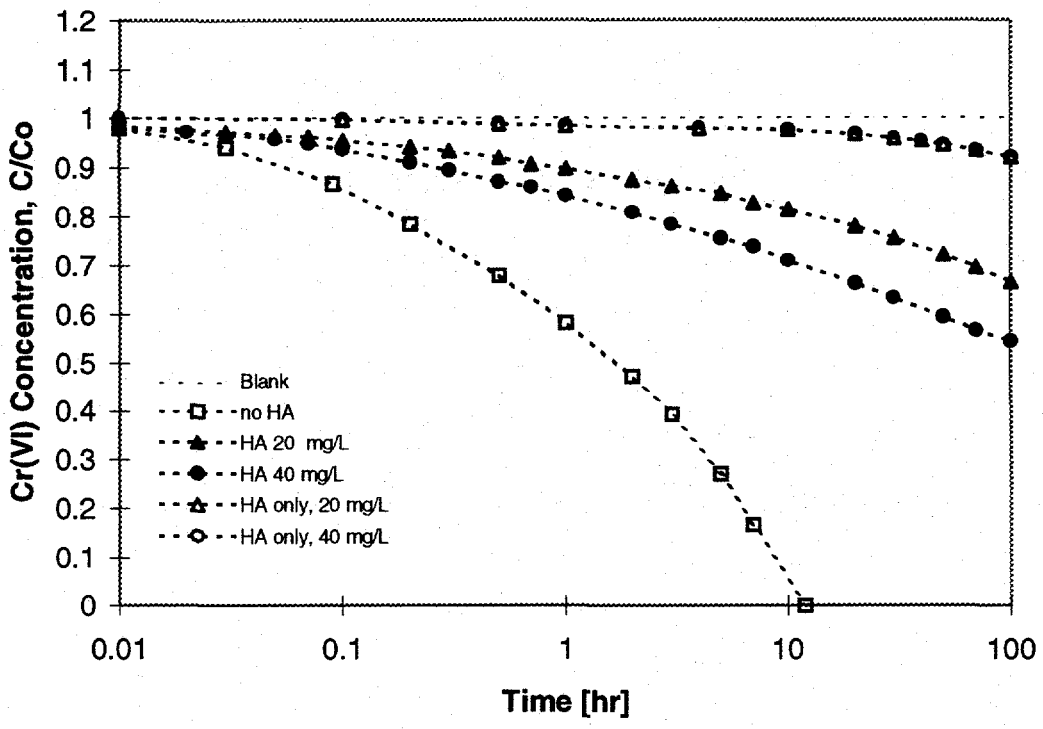

Figure 3. Cr(VI) Reduction by Humic Acid and/or by Fe(II) in the Presence and Absence of Humic Acid at pH 6.

The experiment to examine the reoxidation potential of chromium in Pantex soils has been continued during this quarter. Samples were taken at regularly-scheduled intervals from eight reactors containing reduced chromium and Pantex aquifer materials. Chromium quantification was not possible due to problems with the ICP-MS. The samples will be analyzed during next quarter after the instrument has been fixed. Because of our storage and analysis methodology, no deleterious effects are expected with the longer than normal storage times for these samples.

Anaerobic methods have been surveyed to better facilitate future chromium reduction experiments. An anaerobic chamber with palladium chloride catalysts will be used in our future reduction experiments. Depending on the performance of the chamber, an additional oxygen scavenging system such as a heated copper column or in-line oxygen absorber will be utilized to maintain oxygen concentrations in the chamber at very low concentrations (i.e., near ppb levels).

Zero Valent Metal Remediation of Chromium, Chlorinated Organics and High Explosives at the Pantex Site

A milestone report on zero valent metal (ZVM) remediation of chromium, chlorinated organics and high explosives was submitted during this quarter (January, 1997). Individual reduction experiments of TCE with low initial concentrations (~20 ppm) were conducted. In addition, a series of reduction experiments containing the two target contaminants, TCE and Cr(VI), was also conducted. Identical reactor conditions and analysis techniques that were developed during the previous quarters were used in all experiments. In the experiments containing only TCE, 27.32% of the initial 20 ppm TCE was removed by Fe^0 in 32 hours, and 87.5% was degraded by Pd/Fe^0 in 24 hours. Rate constants from these experiments predict half-lives (i.e., ln(2)/k) of 88 and 8 hours, respectively, for the low initial TCE concentrations.

The reduction of 20 ppm TCE by ZVMs in the presence of chromium is shown in Figure 4. The presence of chromium was found to be insignificant for TCE degradation by ZVMs in most of the experiments (i.e., rate constants remained unchanged). For a few experiments, small variations were observed which most likely resulted from nonuniform changes in the ZVMs over time.

The reduction of Cr(VI) was found to be rapid in the presence of TCE at both 20 ppm and 540 ppm. The reduction of Cr(VI) was almost unchanged in individual and combined contaminant experiments. Figure 5 shows the reduction of Cr(VI) over time in the mixture of TCE and Cr(VI). The Cr(VI) concentration was reduced below detection limit in 40 minutes for 3.22% Pd/Fe^0, and in 1 hour for Fe^0. The rate constants (details in Milestone report, submitted in January 1997) show an increase for Fe^0 and a decrease for Pd/Fe^0, both by factors of about 1.5. Considering the large excess of TCE present in the first hour of the reduction, it is clear that TCE has little effect on the reduction of Cr(VI) by either ZVM.

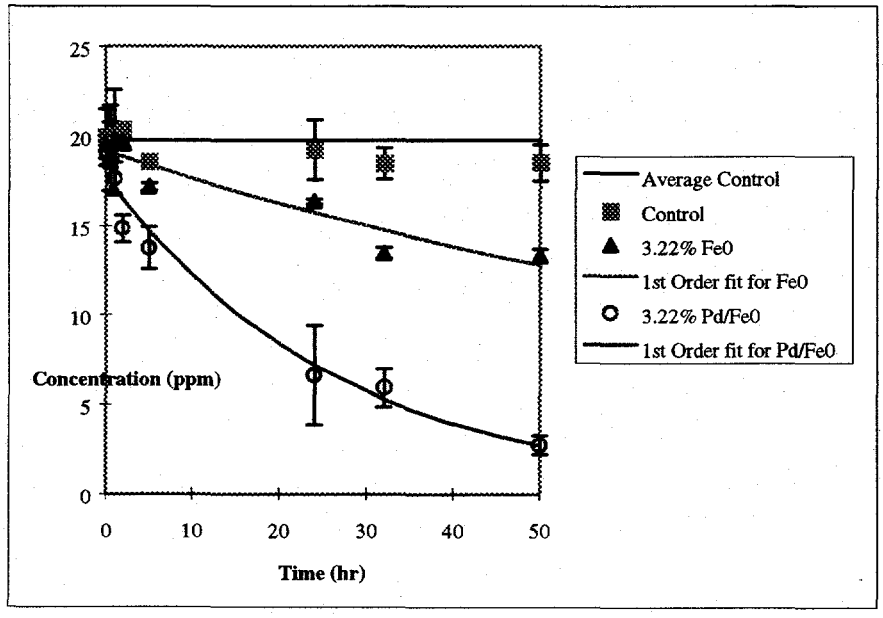

Figure 4. Reduction of TCE (20 ppm) by ZVMs in the presence of 2000 ppb Cr(VI).

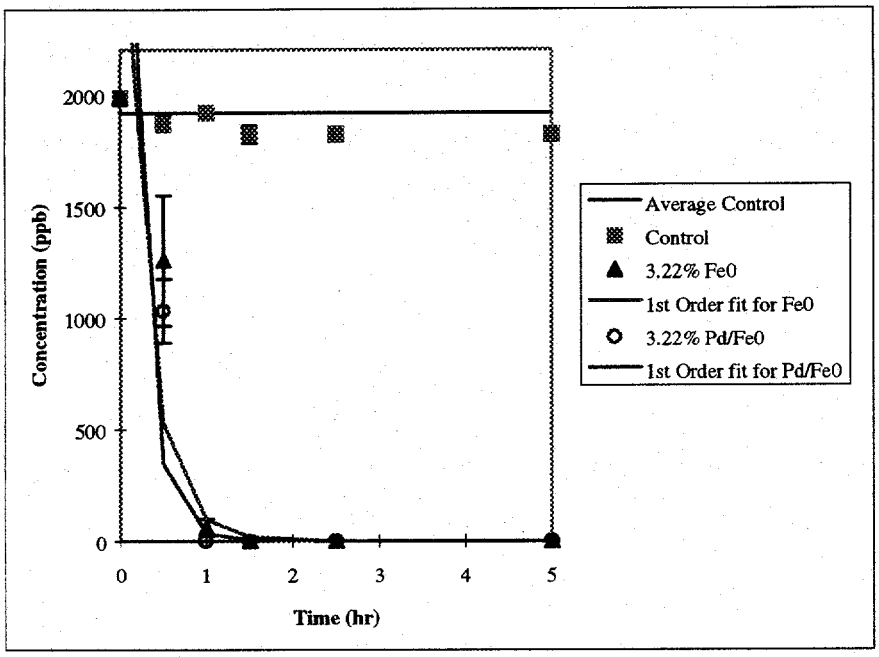

Figure 5. Reduction of Cr(VI) by ZVMs in the presence of 540 ppm TCE.

PROGRESS REPORT

Vadose Zone Remediation

Multicomponent Adsorption Isotherms and Effects of Water on VOC Adsorption

by

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December 1996

Summary

During this quarter we continued our studies on binary mixture adsorption using a well defined adsorbent, silica. After completing that we started our experimentation for isotherm measurements in presence of water. We realized that we could not complete our measurements with the equipment at hand, we developed a new measurement technique, ordered the necessary equipment parts, and are awaiting approval of our purchase order to complete the equipment and start the measurements.

We used binary mixtures of hexane/benzene (*non-polar/non-polar*), hexane/trichloroethylene (*non-polar/slightly-polar*) and chloroform/chlorobenzene (*polar/polar*) systems. Adsorption isotherms were measured using the frontal analysis chromatography technique. The adsorption isotherms for the single components were BET-type II isotherms as expected and showed an increasing uptake at the monolayer with increasing polarity of the components. The adsorption isotherms of the binary mixtures of n-hexane/benzene and n-hexane/trichloroethylene were BET-type II. For the chloroform/chlorobenzene mixture BET-type III isotherms were observed, consistent with our previous studies. On the other hand contrary to our studies on soil, the presence of a second organic increased the uptake of the other organic in all experiments. A predictive model, based on the potential theory, was evaluated for predicting mixture equilibria. For the *non-polar/non-polar* mixture the trend of increasing uptake with increasing concentration of the second component and the magnitude of the amount adsorbed could be predicted. For the *non-polar/polar* system only the trend could be predicted. The model predictions for the *polar/polar* system are not reliable.

Results and Discussion

A. Binary Isotherms on Silica Gel

Soil is a heterogeneous solid with a very complex matrix. Due mainly to the ill-defined nature of soil, and because of may simultaneous interactions between soil and polar organic compounds containing OH- groups, the prediction of adsorption isotherms of binary mixtures using soil as the adsorbent is inconclusive. To investigate only the influence of polarity on the adsorption equilibrium, a clear defined polar adsorbent such as silica gel and VOC's without OH-groups are used in this phase. Binary mixtures of hexane/benzene (*non-polar/non-polar*), hexane/trichloroethy-lene (*non-polar/slightly-polar*) and chloroform/chlorobenzene (*polar/polar*) were examined. The adsorption isotherm of one component is obtained whereas the concentration of the other component is kept constant. The important properties of the silica gel particles are listed in Table 1. All single component isotherms showed a BET II type shape. The isotherms showed a continuous progression from monolayer to multilayer adsorption and then to capillary condensation. The single component adsorption isotherms are modeled by the 3-parameter BET equation. The parameters obtained by fitting the experimental data with the *weighted least square* method are listed in Table 2. The consistency of the experimental data was checked by normalizing the uptake respectively to the amounts adsorbed by monolayer coverage. All isotherms collapsed onto the same curve, which indicates that the behavior of all compounds is similar with respect to their monolayer adsorption capacity.

For binary systems, the adsorption isotherm of one component was measured over the whole range of relative vapor pressures while the concentration of the second component was fixed. Different concentrations of the second component were considered. The mixture isotherms are shown in Figures 1 to 3. The isotherms of the pure components of the binary mixtures are also shown for comparison purposes.

For the *non-polar/non-polar* mixture of n-hexane and benzene the uptake in presence of one component was increased in presence of the second component compared to the pure component isotherms. Either the uptake of n-hexane in the presence of benzene and the uptake of benzene in the presence of n-hexane was higher than for the pure component isotherms. A similar trend is observed

for isotherms of the *non-polar/slightly-polar* adsorbate system of n-hexane and trichloroethylene. For the *polar/polar* adsorbate system of chloroform and chlorobenzene is the effect of increasing uptake due the presence of a second component even stronger.

The BET-type II shape observed for pure vapor adsorption was conserved for the sorption isotherms of *non-polar/non-polar* and *non-polar/slightly-polar* systems. For a binary mixture of *polar/polar* components, the shape of isotherms changed from type II to type III isotherms, which shows also that the interactions between silica gel and the organics were weakened.

For all binary systems it was observed that the amount adsorbed compared to the adsorption of the pure component increased in the presence of a second component. This effect is stronger for the *non-polar/slight-polar* system and even stronger for the *polar/polar* system.

The mixture adsorption equilibria were predicted by the potential theory using parameters obtained by fitting the isotherm data of the pure components of the mixture. For the *non-polar/non-polar* adsorbate system the amounts adsorbed could be predicted in the magnitude of the experimental data. At low relative vapor pressures, under $p_i/p_s = 0.1$ the experimental data were under-predicted and at higher relative vapor pressures, over $p_i/p_s = 0.4$, over-predicted. The increase of the amount adsorbed with increasing relative vapor pressure of the second component was predicted. Examination of a *non-polar/slightly-polar* adsorbate system, showed that the error of the prediction of the isotherms increased. The amount adsorbed for both isotherms at different concentrations of the second component is under-predicted. However, the trend of the increasing amount adsorbed with increasing concentration of the second component can still be predicted. For the *polar/polar* system neither the magnitude nor the trend of the mixture isotherms could be predicted. These results indicate that under increasing polarity of the adsorbates, the prediction of the adsorption equilibria by adsorption on polar adsorbents looses accuracy. In general underpredicts the potential theory the equilibria of binary polar systems on silica gel. It can be concluded that the potential theory does not consider the adsorbate-adsorbate interactions sufficiently. It can clearly be seen for a *polar/polar* system, where the adsorbate-adsorbate interactions are as dominant as adsorbate-adsorbent interactions, that different compositions of the gas mixture do not effect the binary adsorption equilibrium.

B. Water Effect on Adsorption of VOCs

In our experimental system to measure binary adsorption we use an *SRI instruments* gas chromatograph (*model 8610*). The gas chromatograph is equipped both with a flame ionization detector (FID) and a thermal conductivity detector (TCD). The objective was to use the FID for organic component analysis and the TCD for water analysis in determining binary breakthroughs. In our preliminary studies in obtaining data on the co-adsorption of water and VOCs we observed that the sensitivity of the TCD on SRI-8610 is not sufficient to give reliable determination of the water concentration. A further investigation on the capabilities of the instrument led us to conclude that we cannot use the SRI-8610 for these measurements. We then moved our *HP 5986A* gas chromatograph on line with the system. There are detectors (TCD) available for HP which would yield reliable measurements. We decided to modify our HP by adding a TCD on line with the FID already available and install the necessary data acquisition software. In December we requested approval to purchase the necessary parts by transferring funds from "salaries" and the corresponding "fringe" and "overhead" to equipment category of the budget. At present we are still waiting for the approval. In addition we purchased a "humidity probe" which will give a more qualitative measurement of water content. We are concerned with the effect of the organic on the "humidity probe". The probe and the GC, combined, are expected to yield accurate measurements.

In addition, our current measurements mixes two streams (a VOC saturated one and a water saturated one) in frontal analysis measurements. In this technique the maximum concentrations that can be obtained is 50% of the saturation value for each species since two different saturated streams are mixed. Therefore, we designed a new system based on frontal analysis chromatography which enables us to investigate both the thermodynamics and kinetics of binary/ternary sorption of organic vapors and water across the *entire relative humidity range* and the *entire range of organics' partial pressures.* In this technique, the response of an initially clean adsorbent bed (i.e free of adsorbate) to a step change in the adsorbate concentration (organic and water) at the inlet of the bed is monitored to obtain the breakthrough curves of each species.

A schematic diagram of the experimental set-up is presented in Figure 4. The equipment is used to measure multicomponent adsorption isotherms in presence of water. First a nitrogen stream of desired relative humidity (0 - 100%) is prepared by saturating one stream with water and mixing

with a dry stream. A number of organic species are then injected into this stream employing a number of syringe pumps. The amount injected into the humid gas stream will always be less than equal to the amount corresponding to the vapor pressure at the operating conditions. Thus it is possible to obtain organic levels of 0 - P_{sat}. The stream humidity is monitored by a humidity probe (microprobes by Vaisala) in conjunction with the HP-5986A equipped with a series connected TCD and FID. First the soil bed is bypassed and the stream is monitored by GC until the desired concentrations are reached and stabilized. Then the stream is switched to flow over the soil bed and the breakthrough of each component (water and organic(s)) is obtained by GC in conjunction with the humidity probe. Both the GC output and the probe are connected to a PC for automated data acquisition. Water breakthrough from the column is determined by the humidity probe in conjunction with the TCD response whereas the organic(s) breakthrough is(are) determined by the FID.

Work in Progress

Currently we are waiting for the approval for purchase of the desired parts so that we can start the shake-down experiments. In addition, we are still working on our theoretical developments for the *a-priori* prediction of the adsorption isotherms. We do a fairly good job for prediction of binary isotherms for non-interacting systems but we are yet not successful in predicting the isotherms for polar systems, which will be important when we attempt to predict the water effect.

Table 1: Properties of Silica Gel.

Silica Gel	
Particle Size (m)	143 - 250
Average Pore Diameter (A)	150.6
Specific Surface Area (m^2/g)	381.6
Pore Volume (cm^3/g)	1.15
pH	7.0
Particle Density (g/cm^3)	1.99
Bed Density (g/cm^3)	0.36

Table 2: BET-Analysis Results for VOC's Adsorption on Silica Gel at 24◦C.

VOC	X_m (mg/g_{ad})	c	n
CCl_4	140.71	2.03	18.86
$CHCl_3$	139.61	8.38	11.31
C_2HCl_3	114.15	3.77	9.82
C_6H_5Cl	131.43	2.49	53.57
C_6H_6	57.35*	31.9*	1.79*
C_6H_{14}	41.88	4.67	101.77

*) from BET 4-parameter analysis

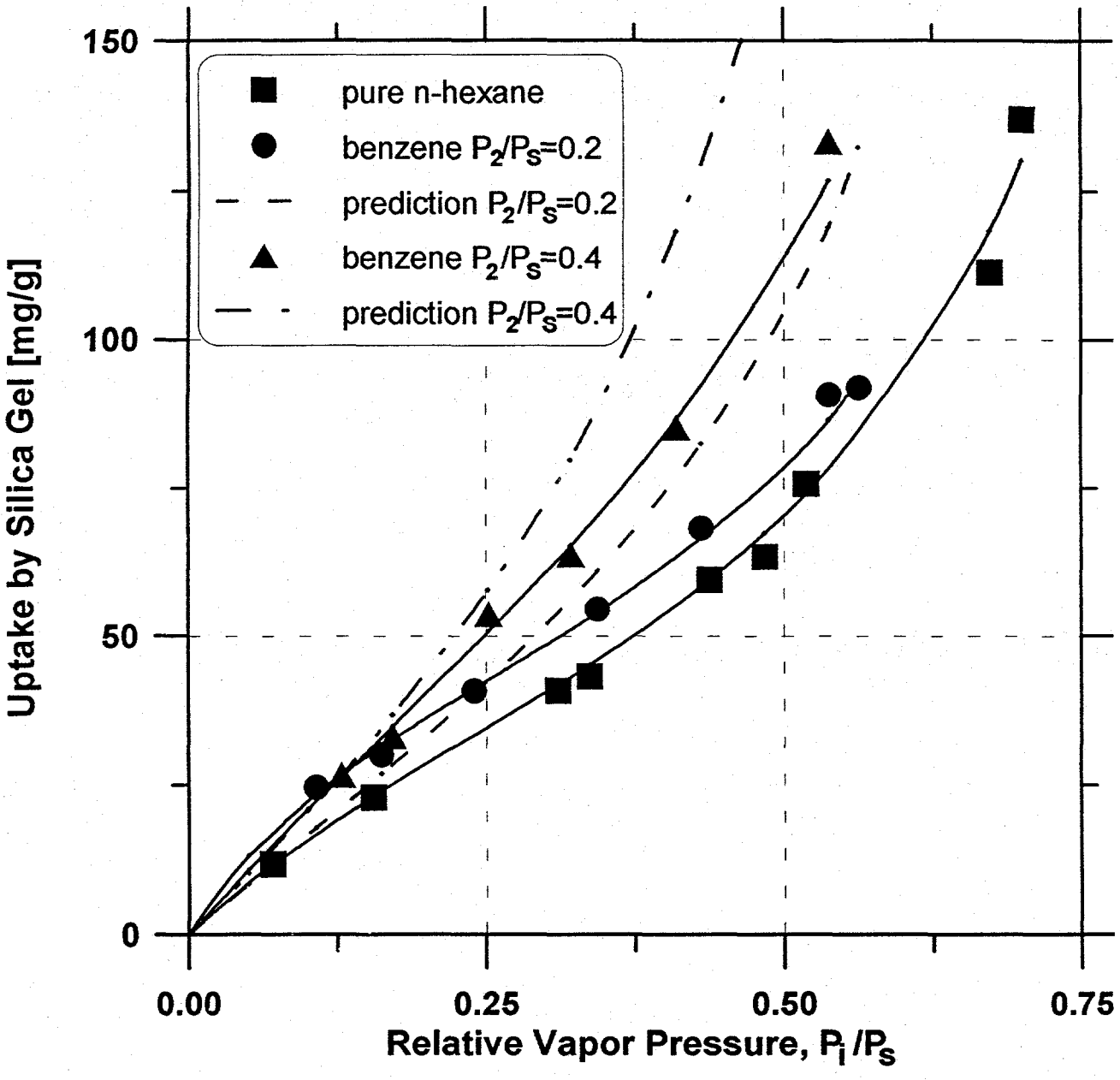

Figure 1: Measured and predicted mixture adsorption isotherms of n-hexane at different concentrations of benzene on dry silica gel at 24°C.

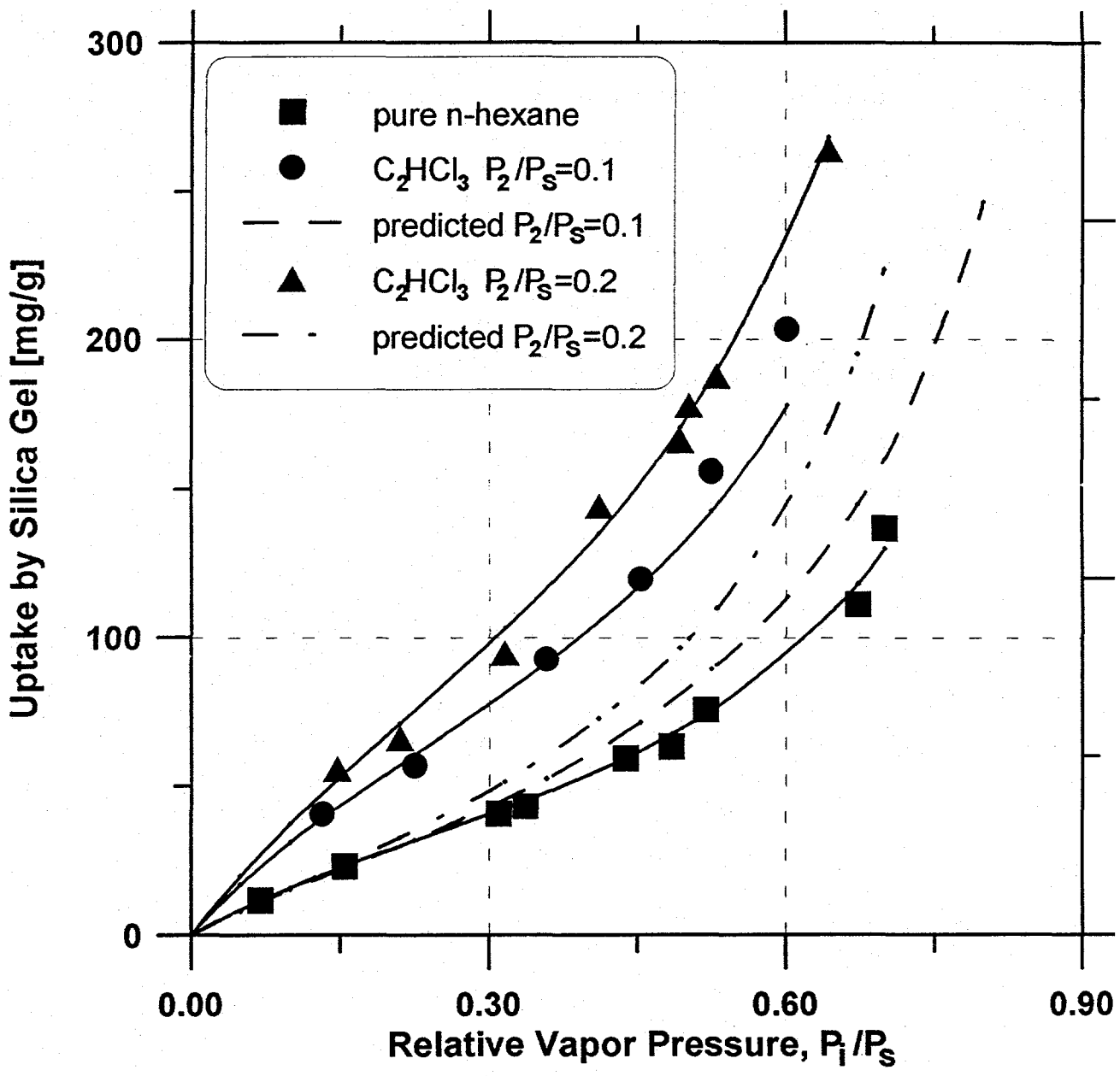

Figure 2: Measured and predicted mixture adsorption isotherms of n-hexane at different concentrations of trichloroethylene on dry silica gel at 24°C.

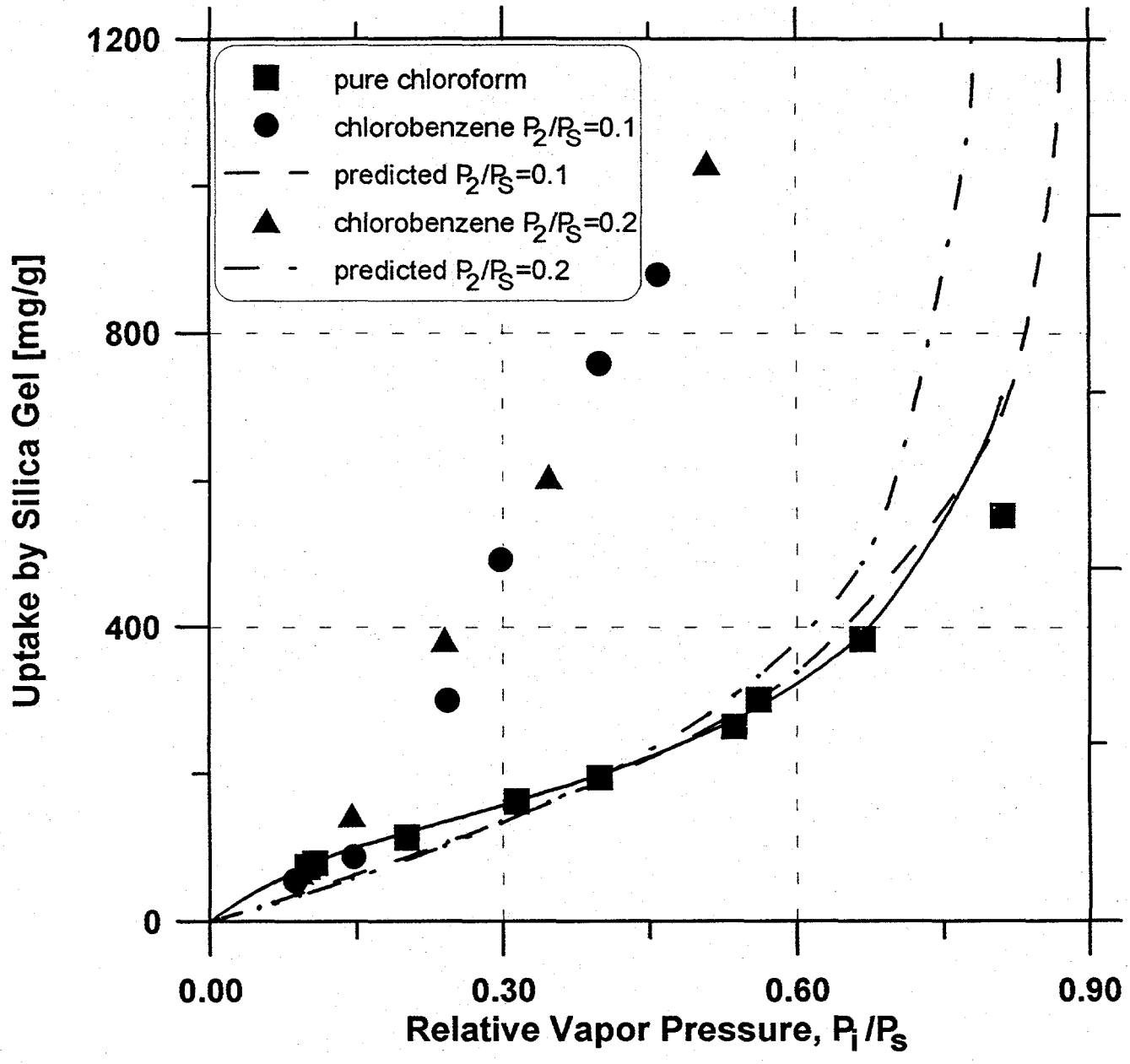

Figure 3: Measured and predicted mixture adsorption isotherms of chloroform at different concentrations of chlorobenzene on dry silica gel at 24°C.

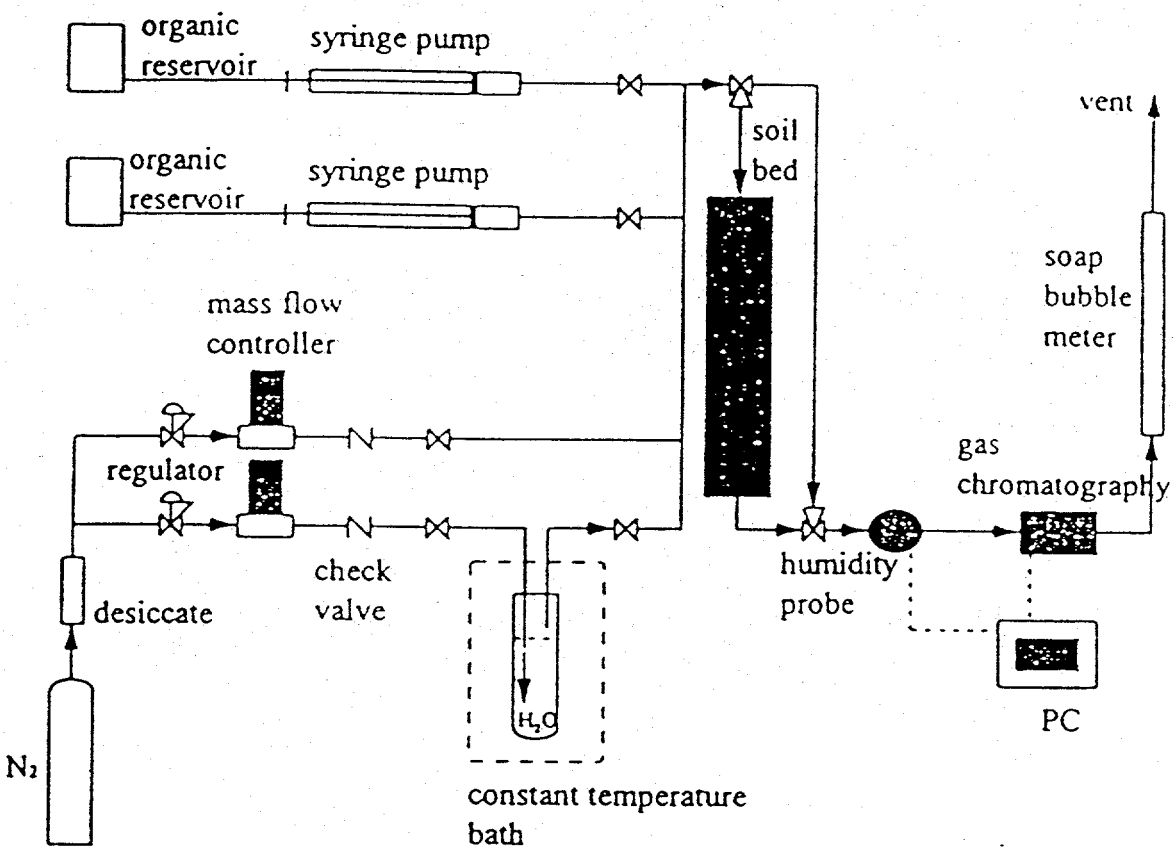

Figure 4. Experimental assembly for determining multicomponent adsorption isotherms in presence of water

DETAILED REPORT

Alternative Uses For Waste Explosives

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* Geoff Lindsay, Rich Hollins, Naval Air Warfare Center Weapons Division (NAWCWD), China Lake, CA

A fourth three dimensional compaction test was performed on November 8, 1996. This design consisted of a solid steel sphere as the workpiece. This design replaced the copper sphere encased in a steel shell used in the previous three experiments. The sample was introduced into the sphere by drilling a hole to the center of the sphere, loading the sample material, then tapping the hole with a threaded screw. The resulting workpiece was inserted into the spherical high explosive around which a brass shell was placed. The final assembly was buried in sand before detonation.

The result of the fourth shot was **complete recovery of the workpiece**. This result represents a major accomplishment toward the ultimate goal of this project. We now have a working design which allows for the study of materials under extreme temperatures and pressures. The workpiece was photographed and sent to UT for analysis. The sample was removed by cutting the sphere in half. In order to minimize sample loss during this machining, the sphere was cut from the outside to the edge of the sample cavity and then the piece was "cracked" in half. The sample was found in a powdered form which was easily removed from the sample cavity.

X-ray analysis was performed on the sample with no additional treatment. The X-ray spectra are shown in **Figure 1**. It is important to note that there is no evidence of C_{60} in the spectra. Simulations predicted the peak pressure pulse to be 300 GPa to 400 GPa. C_{60} is only stable to 20 GPa in shock compressions so there should be no presence of it in the detonation product, which is indeed the case. The scan clearly shows the presence of crystalline graphite (2θ=26.4) and copper metal (2θ=43.3). The presence of copper is due to its use as a quenching material in this experiment. The sample was not subjected to any acid treatment, therefore, the copper remained in the analysis. There is no indication of any crystalline diamond in the scan (2θ=43.9). In addition to X-ray diffraction, Raman spectroscopy was also used to determine the carbon phases present in the sample as shown in **Figure 2.** This scan supports the results of the X-ray analysis. Using a wavelength which does not cause copper to fluoresce, a very strong peak was found at about 1570 cm^{-1} and a weaker peak at around 1360 cm^{-1}. Characteristic graphite features include very strong peaks at 1360 cm^{-1}(graphite disorder induced mode) and 1574 cm^{-1} (graphite $E_{2g}{}^2$ mode)[3]. These match the results of the scan. Diamond is

characterized with a single strong peak at 1333 cm^{-1} while C_{60} shows a strong peak at 1468 cm^{-1} with weaker peaks occurring at 496 cm^{-1} and 272 cm^{-1}, none of which are present in the scan.

Possible explanations for the formation of solely graphite from C60 include: not enough quenching material, the wrong quenching material, and too drastic of conditions. For this experiment, a one to one ratio (by weight) of copper to buckyball was used. It may be the case that there was not enough quenching material to "freeze" the carbon in the diamond phase. Another possibility is copper is inadequate as a quenching material and other materials, namely nanometer grade nickel, will allow for the recovery of diamond from such a compression. An array of experiments has been established which will test these hypotheses. Also, the intense pressure and temperature reached in this experiment may be too extreme too allow for proper quenching regardless of the quenching material used or the amount used. One dimensional experiments should help in this regard.

Three one-dimensional tests were performed in early December to test changes in the 1-D setup. Tests were done using a 1/4 inch and 1/8 inch impacting plates placed on top of the sample holder in addition to a detonation with no impacting plate. Removal of the sample consisted of dissolving the brass plug in nitric acid and scraping the sample out of the sample chamber using a spatula. The presence of crystalline C_{60} is obvious in the X-ray spectra taken for the compressions using the 1/4 inch and 1/8 inch plates. However, the compression using no impacting plate appears to be completely amorphous aside from residual copper. Raman spectroscopy was then used to confirm the presence of C_{60} in all three cases. Thus, the pressure pulse delivered to the sample was not substantial enough to cause destruction of the C_{60}. A new design is needed to increase the pressure pulse delivered to the sample so that a condition is reached where C_{60} is no longer stable. This will be achieved using a threaded steel plug instead of a brass plug which will decrease the amount of sample cavity deformation, thereby, increasing the pressure pulse. Copper will again be used as a quenching material in the same amount used in the three dimensional compaction. This will allow a materials comparison to be made using the results of the very high pressure of the 3-D compression to the less drastic conditions of the 1-D compression.

Figure 1

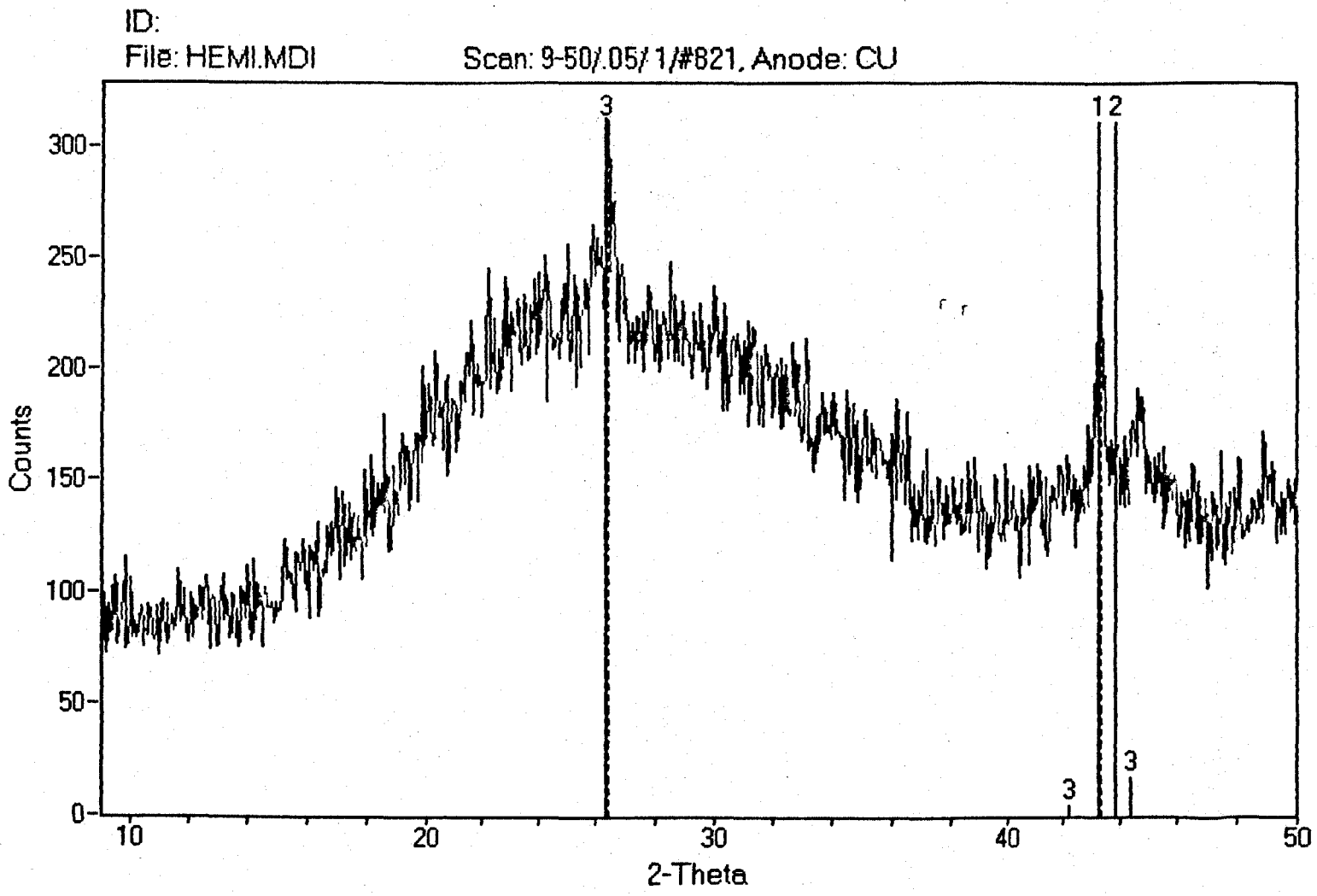
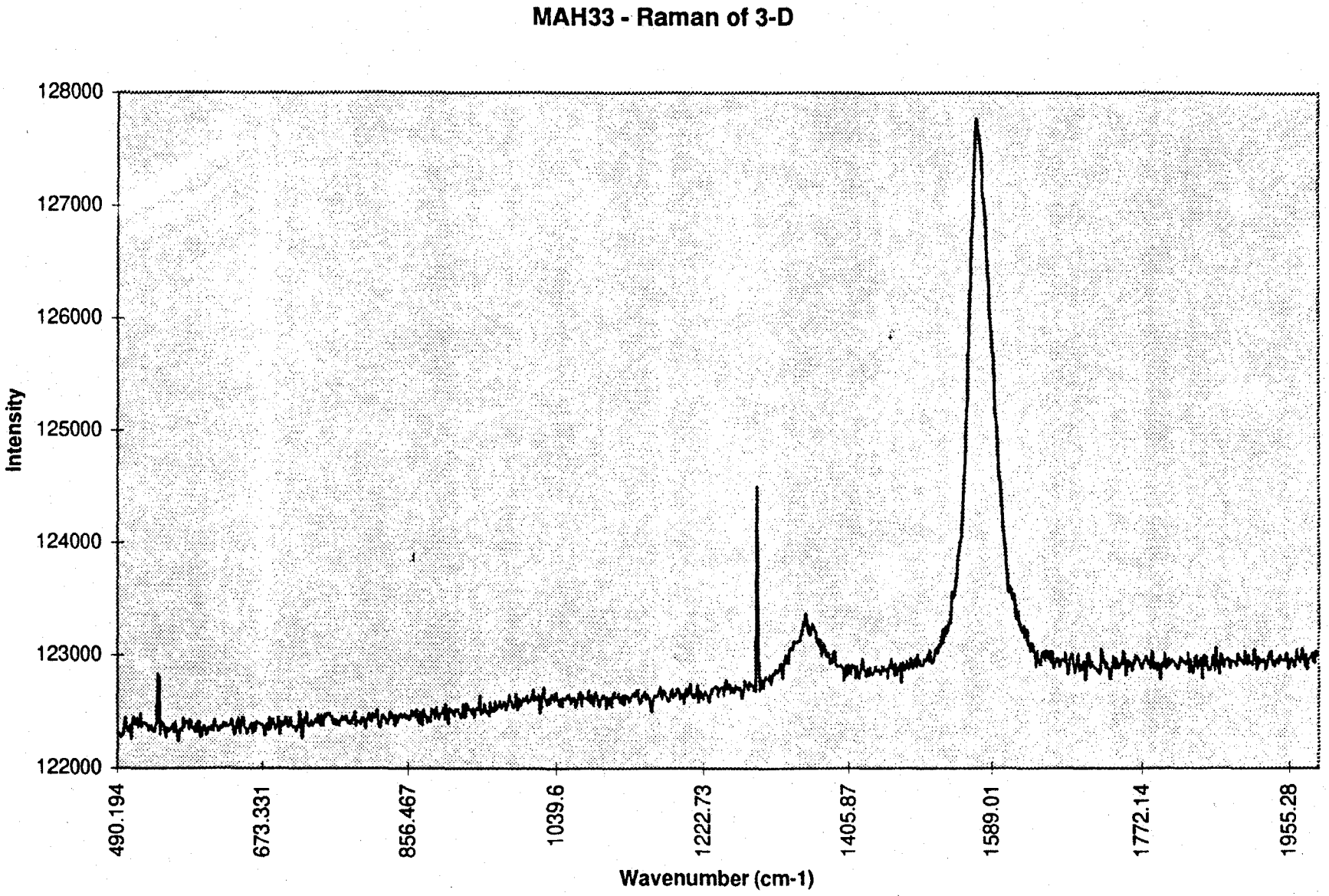


Figure 2


MAH33 - Raman of 3-D
Intensity
128000
127000
126000
125000
124000
123000
122000
490.194
673.331
856.467
1039.6
1222.73
1405.87
1589.01
1772.14
1955.28
Wavenumber (cm-1)

COMMUNICATION, EDUCATION, AND TRAINING

A Community Service

The Center operates under a cooperative agreement between the U.S. Department of Energy and the State of Texas. A Governing Board, made up of a representative from each university and one from the Amarillo area community, oversees the Center's operations. In addition to the work of the consortium, Amarillo College and other area academic institutions are participating in several of the Center's programs.

The Center's Commitment

The Center is committed to ensuring that options for the use and disposition of materials from dismantled nuclear weapons are thoroughly studied, competently evaluated, and safely implemented. We further commit to do our part to ensure that excess plutonium is made secure from proliferation, carefully evaluated for productive peace-time uses, ultimately disposed of in a safe and environmentally sound manner, and made forever inaccessible for use in weapons of mass destruction.

Communication, Education, and Training

The Center is committed to communicating its programs to the public, government officials, business leaders, scientific and technical organizations, academicians, and the news media. Open dialog and communication are essential because the Center's mission has implications for public safety, environmental quality, international relations, nuclear materials disposition, and the continued growth of the Amarillo community.

The Center is actively involved with community programs that promote the study of science, mathematics, and engineering. The Center's goal is to help the community develop the technical and scientific talent that is needed in today's competitive business environment.

Governing Board

By locating its staff in Amarillo, and conducting as many of its programs as possible in the Panhandle, the Center strives to be a valuable addition to the area. If you have questions or concerns, or if you would like to have a speaker for your civic group or community organization, please contact us at:

Amarillo National
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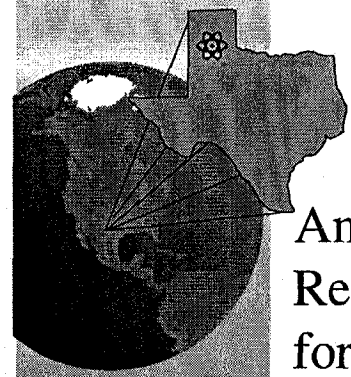


Amarillo National Resource Center for Plutonium

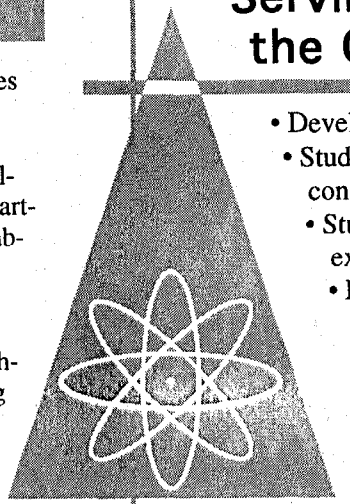
A Global Challenge

With the end of the Cold War, the United States and Russia are reducing their weapons stockpiles. What to do with the materials from thousands of nuclear weapons is an important international challenge. To help address this question, the U.S. Department of Energy (DOE) and the State of Texas established the Amarillo National Resource Center for Plutonium. The Center is a scientific and technical resource for the storage, disposition, potential use and transportation of plutonium, high-explosives, and the hazardous materials remaining after the disassembly of nuclear weapons.

The Center, Pantex, and the Amarillo Community

The Center is a research consortium made up of The Texas A&M University System, Texas Tech University, and The University of Texas System. The universities have separately conducted research related to Pantex operations for years, but the Center now integrates and focuses those efforts in the Amarillo area, giving area citizens a voice in their future. The Center is funded by DOE through a cooperative agreement with the State of Texas.

The Center has a full-time staff based in Amarillo, where community leaders have strongly supported the DOE's mission at Pantex. In 1989, the Amarillo City Commission appointed Amarillo leaders to organize an effort that would culminate in the expansion of Pantex. This project became Panhandle 2000, which is comprised of regional business, civic, and education leaders. The Commission also authorized the Amarillo Economic Development Corporation to provide appropriate financial support for activities related to Pantex's expansion. During this time, the idea for the Center was born, and Panhandle 2000 was instrumental in seeing the Amarillo National Resource Center for Plutonium brought to fruition.



Serving regional, national and international needs, the Center's programs include:

- Developing peaceful uses for the materials removed from dismantled weapons.
- Studying the effects of nuclear materials on the environment and public health, and contributing to remediation of contaminated soils and water.
- Studying issues related to storage, disposition, and transportation of plutonium, high explosives, and other hazardous materials removed from weapons.
- Providing research and counsel to the U.S. government in carrying out weapons reductions and coordinating these activities with Russia.
- Conducting education and training programs.
- Communicating the results of these programs.

Program Highlights

U.S.-Russian Joint Working Group

The Center is coordinating efforts of the U.S.-Russian Joint Working Group on the storage and disposition of fissile materials. Technical and policy experts from the U.S. and Russia are exchanging information and developing mutual policies on disarmament and the ultimate storage and disposition of these weapons.

Electronic Data Base

As a part of its resource role, the Center has designed a state-of-the-art electronic library with information retrieval capability that will serve as the national archives of historical, policy, and technical information about weapons material. The archives will make this information readily available to all parties.

Environment, Health, and Safety

The Center's responsibilities include counseling a wide range of people on environment, health, and safety issues related to weapons materials handling and recycling. The Center also participates in environmental studies related to surplus fissile materials. This role includes performing evaluations, planning, and carrying out environmental work.

Nuclear Studies

The Center is studying the use and storage of materials from nuclear weapons disassembly and providing support to the Office of Fissile Materials Disposition and the Office of Defense Programs of the U.S. Department of Energy.

The Center's long-term storage and disposition studies include:

- Use of weapons plutonium as a fuel to generate electricity.
- Immobilization of plutonium.
- Robotics, and monitoring technologies.

Senior Technical Review Group

A Senior Technical Review Group of top experts in science, engineering, industry, public health, and foreign policy helps the Center evaluate the disposition options for fissile materials. The group evaluated DOE's process for selecting methods for plutonium disposition and made recommendations on a number of related issues. The Senior Technical Review Group includes the Nobel Laureate who discovered plutonium, a former U.S. Ambassador, and six members of the National Academies of Science and Engineering.

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

rth Quarter 1996 Newsletter

Volume II
Issue IV

Microscopic Army Can "Eat" Contamination

Researchers at Texas A&M University and Texas Tech University, working on behalf of the Amarillo National Resource Center for Plutonium, have shown that bacteria found naturally in the soil can be used to "eat" high explosive contaminants in soils, and render them harmless.

Traces of high explosives have been found in soils beneath the Pantex Plant. Though contaminants were found in minute concentrations, Pantex has launched an all-out effort to remove or disable the contaminants through several means.

> ". . . Pantex, environmentally, has gone to incredible lengths to be a good neighbor in recent times."
>
> Dr. Randall Charbeneau -- UT Austin

The latest research is good news because the bacteria that "eat up" high explosive contamination are already present in the soil beneath Pantex. They just need artificial stimulation to get the job done.

Research conducted by Drs. Autenrieth and Bonner at Texas A&M University focuses on determining what factors influence or control the degradation of high explosives by microorganisms found in the soil.

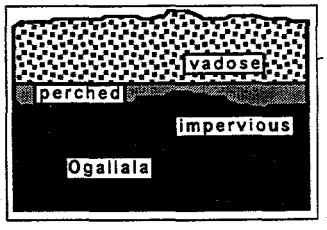
Microorganisms isolated from soils taken from Pantex and from an urban playa in Lubbock have been mixed with essential nutrients and carbon sources to degrade HMX and RDX (the types of high explosives found in trace amounts in Pantex soil). The microorganisms primarily use the explosive compounds as a source of nitrogen, likely because the chemical structures of explosive compounds are relatively rich in nitrogen and much less so in carbon.

In laboratory tests, these organisms are able to degrade up to 97 percent of the supplied RDX from solution in 18 days. The organisms require conditions between the aerobic (with oxygen) and anaerobic (without oxygen) environments. HMX is harder to remediate through biodegradation, but it is possible. HMX degrades at much slower rates than RDX, and neither compound can be degraded adequately with unstimulated microorganisms.

This research is part of an ongoing effort to verify Pantex's remediation efforts and help with cleanup efforts. When Pantex was built in 1942, environmental concerns took a back seat to winning the war, according to Dr. Randall Charbeneau, director of the Center for Research in Water Resources at the University of Texas at Austin and environmental program coordinator for the Amarillo National Resource Center for Plutonium. Even so, Pantex is a remarkably clean industrial site, he said. "From our vantage point, Pantex, environmentally, has gone to incredible lengths to be a good neighbor in recent times," Charbeneau said.

To understand contamination at Pantex, imagine the ground beneath Pantex as a big sponge resting on a plate. Water collecting on the surface "migrates" downward, seeps through the pores of the sponge and carries contaminants with it. When water reaches the plate (the impervious zone), it becomes trapped in the sponge. At this point, water begins to flow sideways, saturating the bottom of the sponge.

This saturated area is known as the perched aquifer, and tests revealed parts of this aquifer are slightly contaminated with high explosive materials, chromium, and chlorinated solvents. Because water has a tendency to flow across this zone, it is being cleaned up to ensure it doesn't eventually find a way into the Ogallala Aquifer, which is separated from the perched aquifer by the impervious layer. The area above the saturated zone, the vadose zone, is wet but not saturated. It contains both air and water, and traces of high



Continued on page 3

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STRG Recommends Planning for Mixed-Oxide Fabrication Now

Some of the world's best scientific minds have tackled the issue of plutonium disposal and, in September, released a report outlining their recommendations. The Senior Technical Review Group (STRG), a group organized to help the Center evaluate disposition options for fissile materials, outlined its recommendations for disabling weapons plutonium by using the plutonium in fuel for nuclear electric generating plants. The report said the U.S. Department of Energy to should begin government-industry dialog on the subject.

The STRG recommendations are based on a "hybrid" approach to disabling excess plutonium removed from nuclear weapons. According to the STRG:

- Plutonium metal should be converted to mixed-oxide fuel for commercial nuclear power plants. Plutonium residues and other forms of plutonium should be encased in glass logs and disposed of in underground repositories.
- Mixed-oxide fuel may be the only option that will induce the Russians to dispose of their excess plutonium. Russia is skeptical of U.S. proposals to vitrify (encase in glass for disposal) all its weapons plutonium because it is much easier to retrieve and use once again in weapons.
- The U.S. government must define and form relationships with businesses and utilities who would play a role in the mixed-oxide fuel process. Arranging these ties will be one of the principal challenges to the mixed-oxide fuel option.

Though 17 U.S. and Canadian utilities have expressed interest in using mixed-oxide fuel, potential fabricators and utilities have some concerns that must be addressed.

Three European firms — Belgonucleaire, BNFL, and COGEMA, have extensive experience in fabricating mixed-oxide fuel. Even so, these firms are cautious about working with the U.S. government because of past reversals of nuclear policy.

The STRG report recommends that the U.S. provide contractual arrangements that assure adequate reimbursement of costs and investments if the government changes its policy.

The concerns of nuclear utilities are more complicated. While fabricators of mixed-oxide fuel stand to make a profit, utilities might not. By participating in the program, utilities could face additional costs, regulatory requirements, and public interventions. In spite of these risks, however, DOE has received 15 Expressions of Interest from 17 U.S. and Canadian utilities (two responses were submitted jointly by two utilities).

The STRG study says that some utilities see profit potential in mixed-oxide fuel, while others see using the fuel as a public service. In either case, utilities are under extreme cost-cutting pressures and are likely to expect full compensation for their costs, time, effort, and risk, in addition to a fee for their service. The STRG recommends that DOE cover all costs and liabilities incurred from using mixed-oxide fuel and offer appropriate incentives.

Other STRG recommendations:

- DOE should focus only on nuclear power plants that are currently in operation and have adequate time remaining on their operating licenses.
- DOE must assure utilities that using mixed-oxide fuel will impose a minimum of new operating regimes or requirements, and that utilities will be able to switch back to uranium-oxide fuel without additional cost or delay.
- Disassembly of plutonium pits and removal of classified characteristics should remain government functions and should be performed on secured and protected government property. Existing nuclear reservations such as Hanford, Pantex or Savannah River would be most appropriate.
- Conversion of plutonium could take place at either a government facility

Continued on p. 3

The Senior Technical Review Group

A Senior Technical Review Group comprised of top experts in science, engineering, industry, public health, and foreign policy has helped the Center evaluate the disposition options for fissile materials. The group is evaluating DOE's process for selecting methods for plutonium disposition and providing advice and making recommendations on a number of related issues. The STRG includes a Nobel Laureate, a former U.S. Ambassador, and six members of the National Academies of Science and Engineering. The members are:

John Ahearne, Sigma Xi, The Scientific Research Society; **Floyd L. Culler, Jr.**, Electric Power Research Institute; **Paul Doty**, Harvard University; **E. Linn Draper, Jr.**, American Electric Power Service; **Shirley A. Fry**, Oak Ridge Institute for Science; **Norman Hackerman**, Rice University, University of Texas at Austin; **Richard T. Kennedy**, Former Ambassador; **Myron Kratzer**, Former Assistant Secretary of State; **John W. Landis**, Stone & Webster Engineering; **Harry Mandil**, MPR Associates; **L. Manning Muntzing**, Morgan, Lewis & Bockius; **Paul Nelson**, Texas A&M University; **Wolfgang Panofsky**, Stanford University; **Genevieve Roessler**, University of Florida; **Glenn T. Seaborg** (discoverer of plutonium), Lawrence Berkeley National Laboratory- University of California; **John Taylor**, Electric Power Research Institute; and **Kenneth L. Woodfin**, Retired Admiral and Former NASA Assistant Administrator.

Center Points

Math & Science Conference

More than 700 educators participated in the third annual Panhandle Area Mathematics and Science Conference on Saturday, Sept. 28 at West Texas A&M University. The day-long conference drew mathematics and science teachers from the Texas Panhandle, South Plains, Eastern New Mexico, and other surrounding areas.

"Science and math teachers depend on this conference to share information with each other, to learn more about science and math, and to see new methods for helping students learn science and math concepts," said Judy Kelley, conference chairperson and associate director of the Texas Engineering Experiment Station at WTAMU.

The Center arranged to have Presidential Award-winning teachers from Las Vegas, Nevada present sessions dealing with nuclear issues.

Peer Review

Eleven experts in nuclear engineering, environmental engineering, and education spent two and a half days in Amarillo in September reviewing the Center's research proposals for fiscal year 1997. Representing business, industry, academic institutions, and the national labs, these men and women analyzed and critiqued proposals over the three-day period, offering valuable guidance to the Center as funding decisions were being made.

STRG Report from p. 2

or mixed-oxide fuel fabrication facility, depending on variables such as cost, transportation, and safety.
- Fabrication should be performed on a commercial contract basis, but the government may need to provide the facility for the oxide fabrication.
- Government must support this operation from the highest levels.
- The schedule of Russian and U.S. disposition programs should be established by treaty or executive agreement.
- Before this framework is in place, DOE should move ahead quickly with detailed planning, contracting, advance licensing work, and informational programs.

Cleanup from p. 1

explosives, chromium, and chlorinated solvents.

Techniques to disable contamination through biological means are known as bioremediation. Though bioremediation is a promising tool, Pantex has launched other cleanup efforts aimed at removing contaminants from soil and groundwater.

The Pantex Plant has established a groundwater treatability system for pumping underground water to the surface, treating it, and re-injecting it into the ground. Center researchers are involved in projects that support these activities through the following tasks:
- Investigation of ion exchange for removal of chromium from the water pumped from the aquifer.
- Investigation of zero valent metals for reduction of high explosives, chromium, and chlorinated solvents.
- Investigation of adsorption of high explosives on granular-activated carbon, and bioregeneration of the activated carbon for reuse.
- Investigation of soil vapor extraction for removal of volatile chemicals from the vadose zone.

Protection of groundwater is the most pressing environmental issue the region faces, according to results from a recent Pantex Plant Citizens Advisory Board poll. Through its environmental research, the Center is watching after the environment and fulfilling its mission to serve the people of the Texas Panhandle.

Chemistry Road Show

Erik Walke, with the Texas A&M University Chemistry Road Show, opens his talk with a flaming book during a public presentation Sept. 25 in downtown Amarillo. The program was sponsored by the Center, and included stops at area middle schools. It was designed by A&M's Department of Chemistry to interest young people in science by entertaining them with scientific wonders.

Texas Regulators Hear About Mixed-Oxide Fuel

The Amarillo National Resource Center for Plutonium facilitated a meeting on mixed-oxides regulatory and waste stream issues for representatives of Texas regulatory agencies on Aug. 29-30.

The purpose of the meeting was to inform regulators on what would be involved in providing regulatory oversight if the U.S. Department of Energy chooses Pantex as a site to dispose of excess plutonium by converting it to mixed-oxide fuel, a blend of uranium oxide and plutonium oxide. The Center coordinated the meeting at the request of Roger Mulder, Pantex Project Manager in the Governor's Office.

DOE is expected to announce its disposal preference before the end of the year. Mixed-oxide fuel fabrication is a promising option that would disable plutonium while offering something of value in return -- electricity for millions of Americans.

As the nation's only nuclear weapons disassembly site, Pantex has about 60 percent of the nation's excess weapons plutonium in temporary storage. In addition to Pantex, DOE is considering Hanford, Savannah River, and Idaho as possible sites for mixed-oxide fabrication.

Close to 55 people attended the meeting, including representatives of the Texas Department of Health -- Radiation Control, the Department of Public Safety's Division of Emergency Management, Texas Low Level Radiation Waste, Texas Natural Resource Conservation Commission, The Attorney General's Office, and the Bureau of Economic Geology.

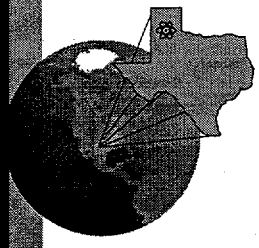
Dr. Dale Klein, chairman of the Amarillo National Resource Center for Plutonium, opened the meeting. A number of Amarillo and area civic leaders attended the meetings, including Panhandle 2000 co-chairs Jerome Johnson and Wales Madden.

Electronic Resource Library Goes On-Line

Amarillo College and Texas Tech University have unveiled the Electronic Resource Library (ERL) to Center personnel and the press in anticipation of the formal November launch.

The ERL is an interactive library of government documents and other material related to plutonium. It can be accessed through a variety of ways, including the Internet. The goal of the ERL is to encourage students and life-long learners to engage the subjects of math and science, as well as to perpetuate and sustain a knowledge base for new scientific researchers.

The ERL eventually will contain government documents, scientific journals, scientific and technical reports, and articles from the popular press. At its startup, 100 documents will be on-line.



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LETTERS

OTHER OPINION

Sunday, November 17, 1996

Kudos to WTAMU

I want to commend West Texas A&M University, and particularly Dr. Shearle Furnish, for their outstanding work with the third annual Student Research Conference that was held at WTAMU on Nov. 1.

One of the chief efforts of the Amarillo National Resource Center for Plutonium, the organization I represent, is to advance mathematics, science and engineering education throughout the Texas Panhandle. Though the Student Research Conference encompassed many disciplines, we were happy to join Southwestern Bell in sponsoring the conference because WTAMU does so much to help us further our educational objectives.

Students from more than 30 universities submitted research abstracts and proposals for their work, then presented their ideas to a panel of judges. Cash prizes were awarded to the research teams with the best proposals in categories ranging from agriculture to computer science. It was probably one of the few times many of these students have ever been rewarded publicly, and financially, for their excellent work.

This year's event deserves further commendation for including research categories such as nuclear energy, radiation and robotics – areas of research that could benefit U.S. Department of Energy operations, the Pantex Plant, and the people who live around these sites.

I can't overstate the need to support research. Scientific reasoning and unbiased analysis of global challenges will make life worth living in the years to come.

As a university consortium working on the tough issues of plutonium disposition and nuclear proliferation, we rely on the innovative ideas emanating from our universities.

We must support the hundreds of students at institutions such as WTAMU who are meeting the challenges of the future and helping to solve problems of the present. We must continue to support and recognize the value of events such as the Student Research Conference.

ELDA D. ZOUNAR
Assistant Director for
Communication, Education
& Training
Amarillo National Resource
Center for Plutonium
Amarillo

Column on Pantex repeats errors

The Nov. 3 guest column by Paul Leventhal and Jim Adams, "Pantex: A plutonium dump for the nation?," is an example of the misinformation that can occur when East Coast activists try to tell Amarilloans what to do.

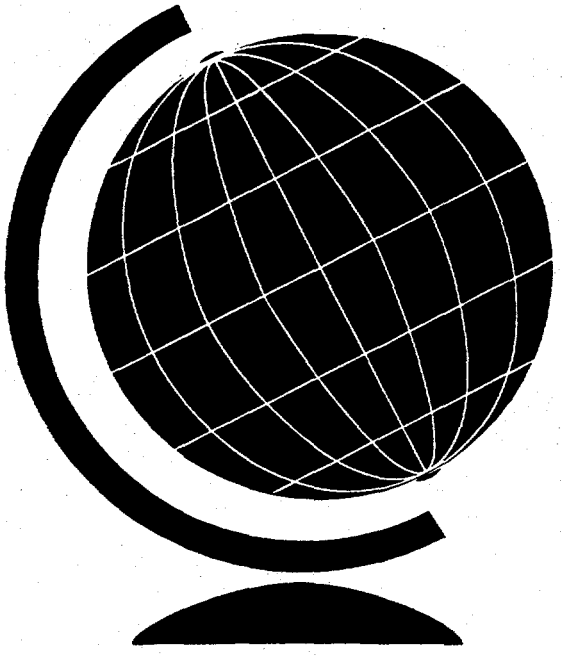
These gentlemen clearly do not understand (or intentionally misstate) the role of the Amarillo National Resource Center for Plutonium.

As a consortium of Texas A&M University, Texas Tech University and the University of Texas, a primary role is to bring scientific and engineering expertise to bear on issues of concern to Amarillo. We are researching and applying environmental protection technologies for using and disposing of the excess plutonium stored at Pantex, and providing the public with independent assessments and information about Pantex operations and proposed future activities.

The Amarillo community will decide for itself which proposed future activities should be implemented here. We at the Center are working to provide solid, scientific information so Amarillo citizens can make those decisions based on fact.

BILL HARRIS
Director
Amarillo National Resource
Center for Plutonium
Amarillo

Call for Papers



The Third Annual Student Research Conference

at
West Texas A&M University
Canyon, Texas
Nov. 1, 1996

The Student Research Conference is a unique opportunity for undergraduate and graduate students to actively participate in the pursuit of scholarly achievement and to share the results of their pursuits with fellow academicians. The student experience involves two phases—

- preparation of a 500-word abstract/proposal, in format according to discipline standards. (Submissions must include judging category, title of abstract, name and address of research adviser, name of department and university, and author's mailing address and telephone number.)
- a 15–20 minute presentation before jurors and colleagues.

Cash prizes will be awarded to top presenters in categories among the following:

- Agriculture
- Business
- Communications
- Computer Science
- Education
- Engineering Technology
- Fine Arts, Literature and Languages
- Health Sciences
- Humanities
- Mathematics
- Natural Sciences
- Social and Behavioral Sciences

Deadline for Submission of Abstracts/Proposals: Sept. 13, 1996

For more information, contact your research adviser or

Dr. Shearle Furnish
Student Research Conference Chair
West Texas A&M University
WTAMU Box 908
Canyon, Texas 79016-0001
furnish@wtamu.edu

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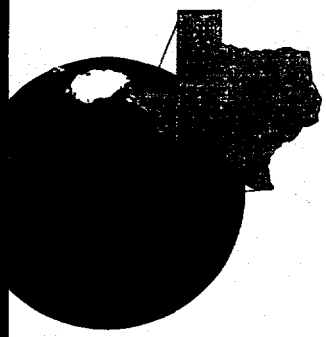

Amarillo National Resource Center for Plutonium

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

Date: December 2, 1996

To: Elda Zounar

From: Effie Harle

Subject: National Association of Partners in Education (NAPE) Conference

The NAPE Conference was held November 19 - 23, 1996 at the Chrystal Gateway Marriott in Arlington, Virginia. Workshops were scheduled on November 19 and 20 and the formal conference started November 21 with the final session held on November 23. Conference attendees represented partnership directors, corporate decisionmakers, educators, volunteers and public policymakers from the United States, Canada, and several other countries.

The Conference carried out the 1996 theme, *Children at the Center; Partnerships Linking Education, Community & Economic Development,* by presenting workshops focused on new, emerging and established education issues, motivational general sessions, and Professional skills Development sessions.

I attended the NAPE sponsored two-day workshop, Organizing Effective School To Career Partnerships. The workshop was designed to teach the process for developing a School-to-Career program in any school/business partnership program. Instructors from successful programs in Maryland, California and New York shared information about their school-to-career programs and a NAPE training manual based on two highly successful school-to-career models was provided. Information learned and publications provided will be valuable in starting a school-to-career program in local schools.

The opening plenary session of the conference was held on Thursday, November 21 with Hedrick Smith, Pulitzer Prize-winning journalist and author of *Rethinking America* sharing his observations of a "paradigm shift" in corporate America and the effect of this shift on education. His discussion focused on the urgent need for America to train, educate, and motivate people differently, with emphasis on the use of partnerships to develop and implement strategies for preparing students for the job world of the 21st. Century. After the opening session on Thursday and Friday concurrent one-hour sessions were held concerning technology, school-to-career, economic development/business needs, parent/family/community involvement, and new learning systems. I attended several sessions about technology and parent/family/community involvement. A common theme in the technology sessions was the importance of technology labs in middle and high school.

The closing plenary session featured William Strickland, Executive Director of the Manchester Craftsman Guild and recent recipient of the prestigious 1996 MacArthur Fellowship "Genius" Award. Strickland founded the Craftsman Guild to improve the quality of life within the inner-city. Through Guild programs in art appreciation and vocation training, inner-city "at-risk" public school children are redirected and empowered to become self-sufficient citizens.

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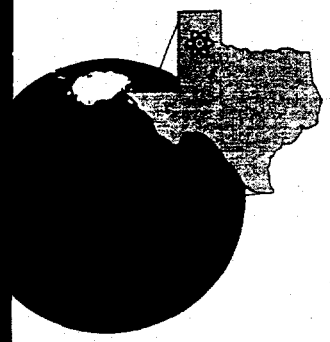

Amarillo National Resource Center for Plutonium

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

The conference helps me stay current with education issues and provides networking opportunities for learning about programs around the country. In addition, the conference provided an opportunity to become better acquainted with Amarillo partnership people. Others attending from Amarillo were Lori Cizon, AISD; Annette Carlisle, AISD School Board; Gwen Treat, AISD; and Becky Zenor, Amarillo Chamber of Commerce.

While at the NAPE conference, I visited the American Association for the Advancement of Science (AAAS) new headquarters building in downtown Washington. Information I took from the Internet stated there would be interactive exhibits on loan from well-known museums and science centers around the country located in the building atrium. These exhibits were touted as being a focal point for visiting scientists, students, business leaders, and tourists. The three exhibits on display were not what I expected and I gained little from the experience.

Thank you for allowing me to attend the 1996 NAPE Conference. Information I gathered from the workshop, motivational speakers, and professional development sessions will help keep our education programs current and me informed about education trends.

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West Texas Environmental Project (WTEP)
for Integrative Studies in Science and Mathematics (K-12)
June 16-26, 1997
(selected sites in West Texas and New Mexico)

BRINGING SCIENCE AND MATHEMATICS TOGETHER IN RELEVANT WAYS

WTEP is looking for highly creative, flexible, and innovative K-12 teachers who enjoy developing new ways of teaching.

DEADLINE FOR APPLICATIONS: MARCH 10, 1997

What WTEP is about:

- skills and strategies for motivating K-12 students in new ways
- cutting-edge national trends in curriculum development
- innovative ways for teaching state-mandated knowledge and skills
- integrative and interdisciplinary science and mathematics
- pressing environmental issues related to semi-arid regions, most especially environmental & social sustainability

What WTEP gives you:

- $800 honorarium
- new ways of working with colleagues, and new ways of teaching content
- informative and extensive five-day field trip (all expenses paid)
- participation in one of the most innovative curriculum projects in the nation
- books, materials, supplies
- all travel expenses, including lodging and food
- professional development credit, ESC 17 (available upon request)
- college credit (optional, not paid by grant, available upon request)

WTEP

What WTEP asks you to do:

- attend summer workshop and participate in field trip, June 16-26, 1997; make presentation to peers during trip
- attend orientation meeting in Spring, 1997, and follow-up meeting in fall, 1997 (possibly a Saturday meeting)
- create integrative classroom curriculum materials for science and mathematics
- create a classroom set of AV materials for your classroom curriculum (all film and processing will be provided)
- complete all project readings
- demonstrate professional flexibility and openness to new ideas

For more information about WTEP and the extended field trip, contact:

Richard Powell, Ph.D., Tx Tech Univ, College of Education, Lubbock, TX (phone 806.742.1997 ext 298)
Amanda Miller, Floydada High School, Floydada, TX (phone 806.983.2340)
Mary Hobbs, Dunbar Middle School, Lubbock, TX (phone 806.766.1300)
Judy Kelley, WTAMU, Canyon, TX (phone 806.656.2271)

***FUNDING AVAILABLE FOR ONLY 20 TEACHERS**

For WTEP application, fill in the information below and send or fax immediately to:
Richard Powell, Texas Tech University, Box 41071, Lubbock TX 79409-1071 (fax 806.742.2179)

Name:_____ fax number _____
School, grade level, & subjects taught:_____
address:_____
home phone: _____ work phone: _____
e-mail address:_____

WTEP funding provided by
Amarillo National Resource Center for Plutonium

NUCLEAR AND OTHER MATERIAL PROGRAMS

Numerical Simulations of Tracer Gas Concentration in Mixing Elbow and Straight Pipe

H. Gong, A. Langari and A.R. McFarland
Aerosol Technology Laboratory
Department of Mechanical Engineering
Texas A&M University

Progress Report for the Period of Nov 1, 1996 - Jan 31, 1997
Subtask of ANRCP Air Monitoring Group

A tracer gas technique using sulfur hexafluoride (SF_6) was used to evaluate the mixing efficiency of a 90° elbow and a straight pipe. In the experiment with the elbow, SF_6 was released 4 diameters upstream of the elbow and the development of tracer gas concentration profiles (in terms of the concentration coefficients of variation, *COV*s) were measured starting from 1 diameter downstream of the elbow. In the experiments with a straight pipe, SF_6 concentration *COV* development was analyzed starting from a location 3 diameters downstream of the SF_6 release point. All experiments were performed at a Reynolds number of 70,000. The diameters of the pipe and elbow were both 203 mm (8 inches), and the elbow had a curvature ratio (bend radius/tube radius) of two.

Numerical simulations of the mixing of SF_6 in the elbow and straight pipe were performed and the results compared with the experimental resuslts. Two different approaches were used in numerical computations. One was to treat air and SF_6 as a two species gas. The mixing and transport of SF_6 was simulated by solving the momentum and mass conservation equations that describe the turbulent convection and diffusion for SF_6. A commercial code, FLUENT, was used to solve the governing equations, which provided the results in terms of the mass fraction of SF_6 in the flow field.The tracer gas concentration *COV* at various locations downstream the release point were calculated by:

$$COV = \frac{1}{\bar{c}} \sqrt{\frac{1}{A} \int_A (c-\bar{c})^2 dA} \qquad (1)$$

where: c is the SF_6 concentration; and, $\bar{c}$ is overall mean SF_6 concentration across the duct cross section.

The other numerical approach was based on the Lagrangian method. In this approach, individual SF_6 particle trajectories were calculated and the SF_6 concentration *COV* was obtained by tracking a large number of SF_6 particles released into the flow field at the same location where the tracer gas was introduced in the experiments. It was assumed the SF_6 particles were inertial-less points, which followed the flow perfectly and which had negligible thermal diffusion. The computation procedure included calculation of air flow field and SF_6 particle trajectories. The air flow field was solved using FLUENT with a Reynolds stress turbulence model. Turbulent eddy fluctuation was generated using

a "random walk" model. In the random walk model, a random fluctuating velocity was sampled during a period of eddy life time from a Gaussian process with a zero mean and a standard deviation of $\sqrt{\overline{u_i'u_i'}}$. The trajectories of particles were calculated and recorded to give the SF6 concentration in the flow field statistically when 10000 particles were used. The concentration COV was then computed from Equation 1.

With reference to Figures 1 and 2, the experimental and numerically predicted COVs are shown as functions of downstream distance (expressed as tube diameters, z/d, where z is axial distance, and d is the tube diameter) for the straight tube and 90°elbow, respectively. The particle tracking code and the FLUENT two-species gas model both correctly predict the trend of mixing as exhibited by the experiments. Predictions by the particle tracking code more closely approximate the experimental results.

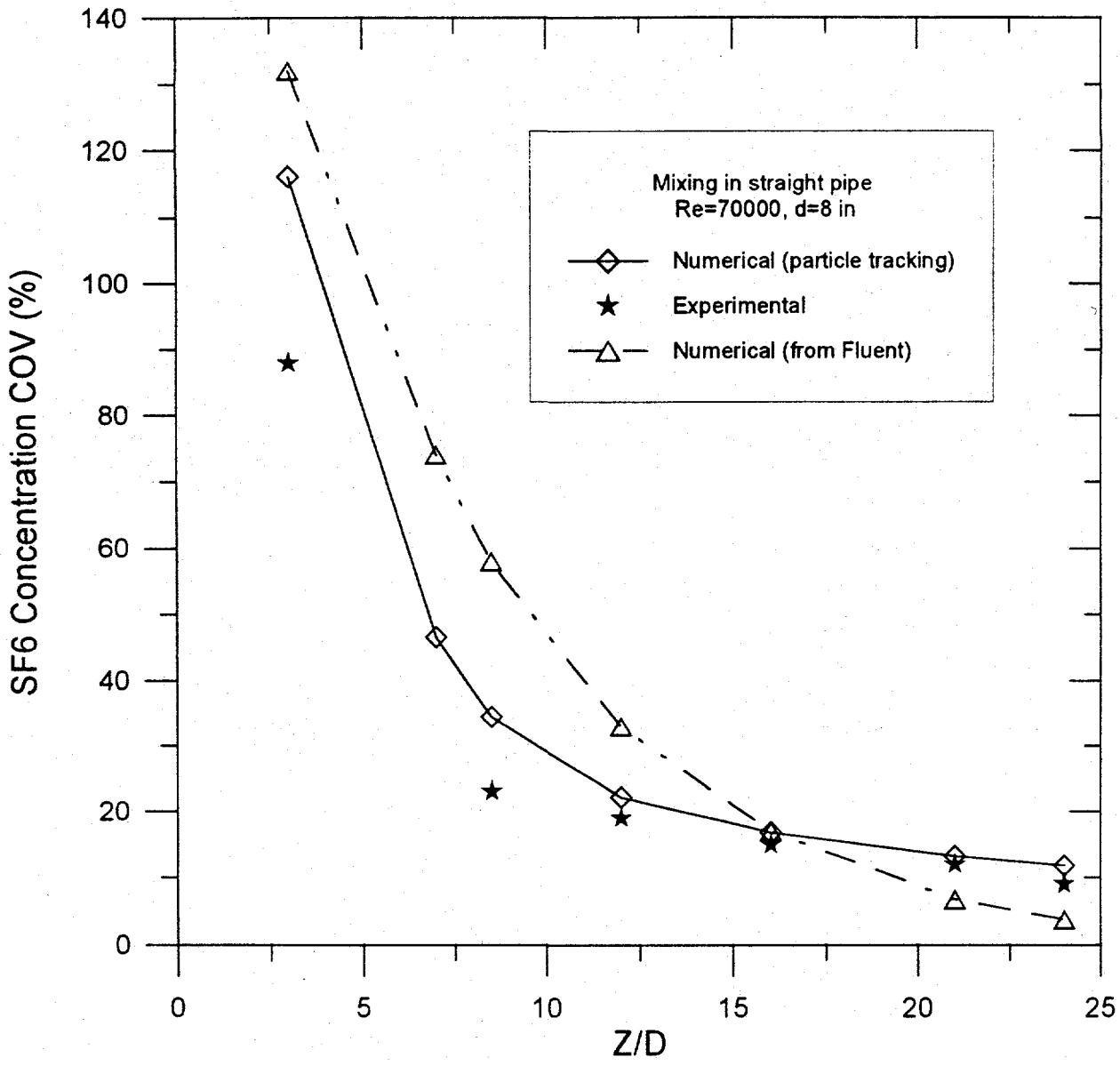

Figure 1. Development of tracer gas concentration profiles in a straight pipe.

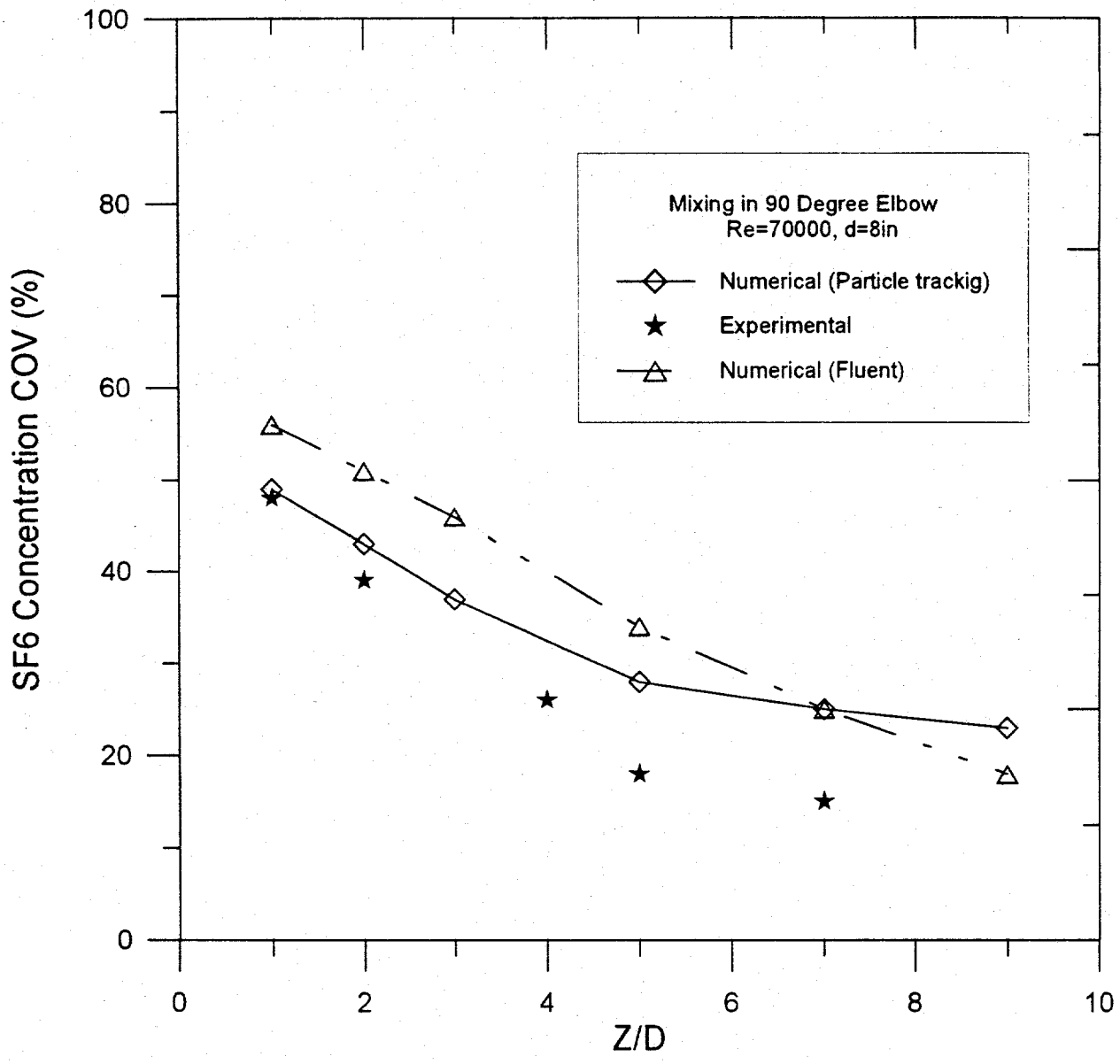

Figure 2. Development of tracer gas concentration profiles in a 90° elbow.

Quarterly Progress Detailed Report

11/1/96-1/31/97

Project: Development of Nondestructive Assay
Methods for Weapons Plutonium and
Mixed Oxide Fuel Safeguards

SUBMITTED TO THE
AMARILLO NATIONAL RESOURCE CENTER FOR PLUTONIUM

Naeem M. Abdurrahman, PI
Bernard W. Wehring, CO-PI
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DEPARTMENT OF MECHANICAL ENGINEERING
THE UNIVERSITY OF TEXAS AT AUSTIN
AUSTIN, TEXAS 78712

1. DESCRIPTION OF RESEARCH ACTIVITIES

1.1 Neutronics Calculations

We continued our research program to investigate the lead and graphite slowing down time spectrometers. In this period, we devoted more effort to the graphite spectrometer assay device because of its desirable features and because of the shortage of funds to continue the investigation of the lead spectrometer. A graphite spectrometer with its lighter weight, smaller volume, and lower neutron source-intensity requirements, would be more transportable and more affordable than its lead counterpart. We extended our computational program to investigate the neutronics of the proposed device. These calculations would provide us with a better understanding of the neutronics behavior and expected assay performance. The following is a summary of some of the calculations.

1. A simplified assay model was developed in which the graphite spectrometer was housing a BWR fuel assembly. The graphite pile was square cylinder with a diameter of 100 cm. The fuel assembly had a square cross section (15x15 cm) and an active length of 100 cm. The assembly contained 64 fuel pins in an 8x8 matrix arrangement. The fuel assembly was interrogated by a 14-MeV isotropic point neutron source located at the mid plane 20 cm off the cylinder axis. The fission neutron counting signatures of U^{235} and Pu^{239} inside the fuel assembly as a function of the slowing down time were calculated and compared. As our calculations showed, the U^{235} and Pu^{239} signatures were quite distinct from each other over the time interval from 10 μs to 100 μs. Therefore, these two fissile isotopes can be determined separately by the proposed graphite device.

2. The effect of self shielding in bulky fuel assemblies was studied using the same assay model described above, in which the signatures of U^{235} and Pu^{239} were tallied at four different positions in the radial direction (from center to surface) inside the fuel assembly. These calculations showed that the effect of self shielding is not expected to pose a series problem for the graphite spectrometer.

3. As an extension of our assay model, a graphite spectrometer is now being modeled in which threshold fission detectors and fissile fission chambers are simulated explicitly. The threshold fission detectors are located around the middle of the fuel assembly and the fission chambers are located inside it. In this calculation we will be looking at the signatures of individual fissiles as measured by the fission chambers inside the assembly as well as the assay signature consisting of contributions from all the fissiles in the assembly as seen by the assay (threshold) detectors located around the fuel assembly.

1.2 Pulsed Neutron Generator

As presented in the preceding quarterly report, we have acquired a pulsed 14-MeV neutron generator from The University of Michigan. We have successfully transferred the generator from Ann Arbor to Austin and are currently working on setting it up. As part of this setup effort, we designed and have started fabrication of the various steel bases needed to support the neutron generator and its beam lines. In addition, we have completed the assessment of the vacuum requirements for the new system and are now in the process of procuring the required pumps and controllers.

To ensure that the transfer of the neutron generator from Michigan to Texas is done in a timely and orderly manner, Dr. Ayman Hawari and Raul Radulescu went to Michigan and spent approximately two weeks dismantling and packaging the neutron generator, keeping a detailed record of the generator setup at Michigan, and gathering pertinent documents (manuals, drawings, procedures, safety requirements, journal articles, papers, dissertations). The neutron generator was then loaded and transported to Austin a truck. One minor damage (which can be repaired in our laboratory) to an auxiliary component occurred during the transportation of the generator. Our effort is now focused on setting up the neutron generator (which includes fabricating the steel tables) and upgrading some of its subsystems including vacuum and vacuum controller. Figure 1 shows the planned layout of the neutron generator in NETL.

2.

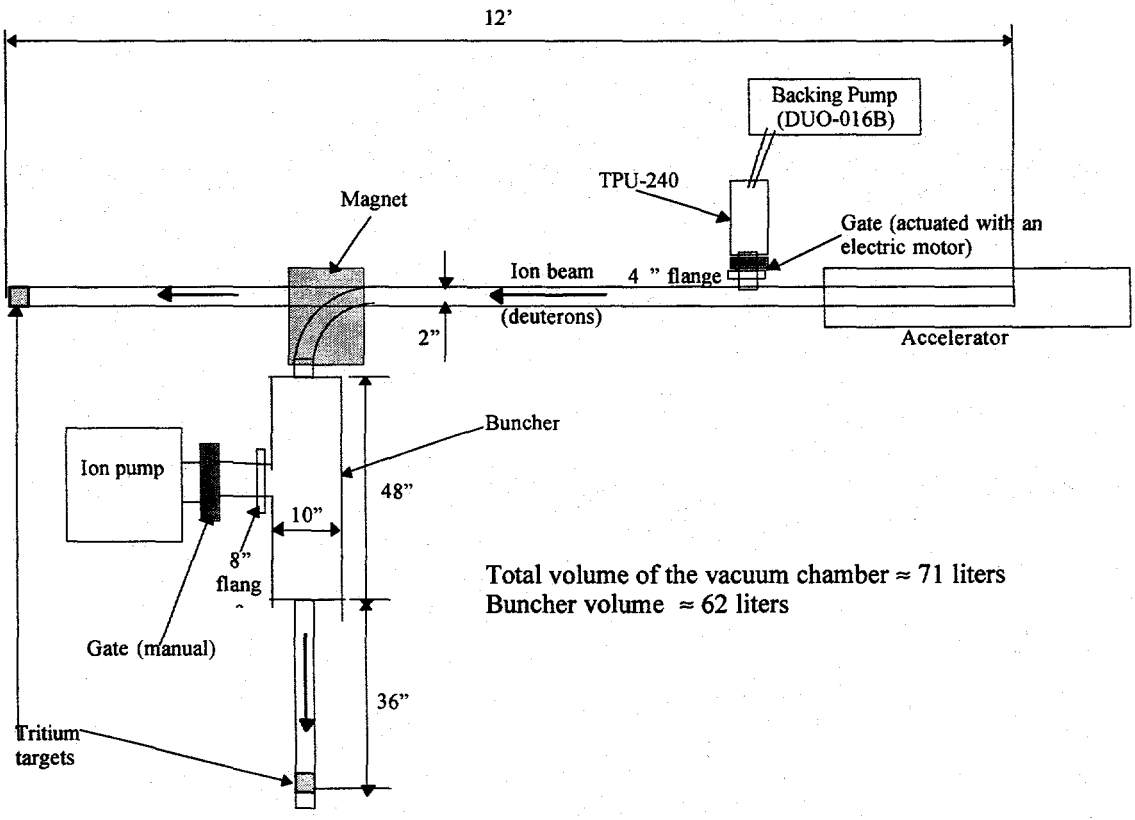

Figure 1. Neutron Generator Layout

3. MILESTONES AND DELIVERABLES

We have submitted two papers for presentation at the coming American Nuclear Society Annual Meeting to be held in Orlando, Florida in June 1997. If accepted for publications, the summaries of the papers will appear in the ANS Transactions of the meeting. The two papers are:

1. M. A. Elsawi, N. M. Abdurrahman, A. I. Hawari, and B. W. Wehring, "Use of Graphite for Slowing Down Time Spectrometry."

2. A. I. Hawari, N. M. Abdurrahman, and B. W. Wehring, "Neutron Sources for Nondestructive Assay of Nuclear Materials Using Slowing Down Time Spectrometry."

No.	*Description*	*Completion Date*		*Comments*
		Planned	*Actual*	
1	Transferring the new pulsed neutron generator from Michigan to Texas	11/96	11/96	Revised task
2	Writing paper on our preliminary investigations of the graphite slowing down time spectrometer		1/97	Revised task
3	Writing paper documenting the review of candidate pulsed neutron sources for SDT and NDA applications		1/97	Revised task

Tasks 2 and 3 represent revisions to our original task plan. Task 2 is a revised task of the original task to investigate a pulse power neutron generator concept. The revision is motivated by our recent findings that a number of novel neutron sources have either been developed or under active developments by different research groups in the US and abroad. Task 3 is a new one related to tasks 2 and 3 in our original plan which were focused on the lead spectrometer. This new task was a result of our discussions with Kenneth Coop of LANL (NIS-6) and our preliminary calculations which indicated that a graphite based slowing down time spectrometer might be a viable assay device. Shortage of funds for FY 97 was another reason behind some of the above revisions.

Immobilization of Plutonium in Ceramic Materials

Quarterly Report

to

Amarillo National Resource Center for Plutonium

by

Abraham Clearfield, PI
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College Station, TX 77843

Collaborators

Paul Sylvester, Research Associate
Rick Carroll, Research Assistant

February 1997

Plutonium Immobilization in Ceramic Materials

This past quarter has involved continued work on the analysis of samples of Zirconolite ($CaZrTi_2O_7$). Zirconolite is an ideal material for immobilization due to its ability to form a broad range of solid solution ($CaZr_xTi_{2-x}O_7$, where $0.8 < x < 1.37$). A large number of ions can be incorporated into this solid solution, including up to twenty-seven weight percent of UO_2. The latter is crucial, since much of the plutonium waste is contaminated with UO_2. In these samples, cerium has been used as a model for plutonium. Samples containing calculated substitution of 5, 10, 15, 25, and 35 weight percent cerium in Zirconolite have been synthesized. Previously it was reported that Rietveld analysis of the Zirconolite samples was impossible due to poor crystallinity of the samples. Samples had previously been calcined at only 1200° C due to equipment limitations. A new 1500° C furnace has been installed and the samples have been recalcined at 1300° C. The crystallinity of the samples has improved immensely. (Figures 1 and 2) Rietveld analysis is in progress at this time. The patterns clearly show the characteristic fingerprint of Zirconolite. However, there are also a number of peaks in the pattern not accounted for by the Zirconolite model. These may possibly be due to an impurity phase in the mixture or to a loss of C symmetry due to the inclusion of cerium in the matrix. As yet, this has not been determined. It should be noted, that these substituted Zirconolites were synthesized by sol-gel methods. Experiments are proceeding to repeat the synthesis by solid state methods, as the immobilization procedure favored at present is an all dry method.

In addition to the analysis of the Zirconolite samples, work has been continuing on the barium zirconate ($BaZrO_3$) phase. In the prior quarter, it was reported that the Perovskite barium zirconate phase will incorporate up to twenty-two weight percent (forty-eight mole percent) cerium (corresponding to thirty-three weight percent plutonium) into its crystal lattice. Experiments are under way using hafnium as a potential neutron poison. Currently synthesis of $BaZr_{0.3}Hf_{0.3}Ce_{0.4}O_3$ is under way. The natural occurrence of hafnium in

zirconium makes purifying zirconium an expensive process. If the barium zirconate phase will still incorporate twenty-two weight percent cerium with the hafnium present, the less pure, less expensive sources of zirconium may potentially be used for the synthesis of the ceramic on the large scale. This possibility, in addition to hafnium's activity as a neutron poison, make this an attractive compound for immobilization of the waste plutonium.

Plans are under way to duplicate our experiments using PuO_2. Our year end report has been transmitted to Leonard Gray at Lawrence Livermore National Laboratory along with the first set of designed experiments. Plans for further collaboration will await their outcome.

Figure 1. Sample PS1-C 15% Cerium substituted Zirconolite, calcined at 1200° C

Figure 2. Sample PS1-C 15% Cerium substituted Zirconolite, calcined at 1300° C

Figure 1

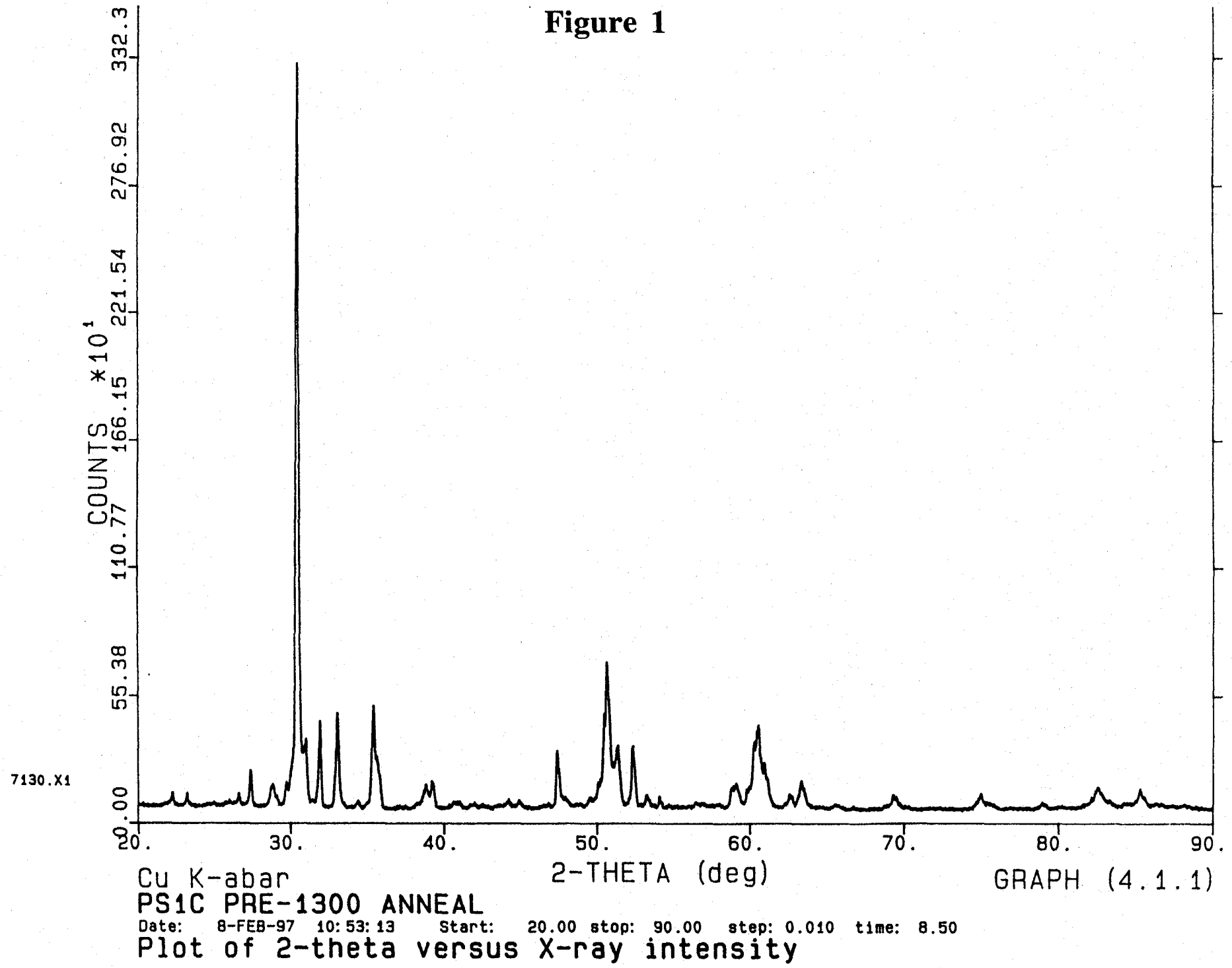
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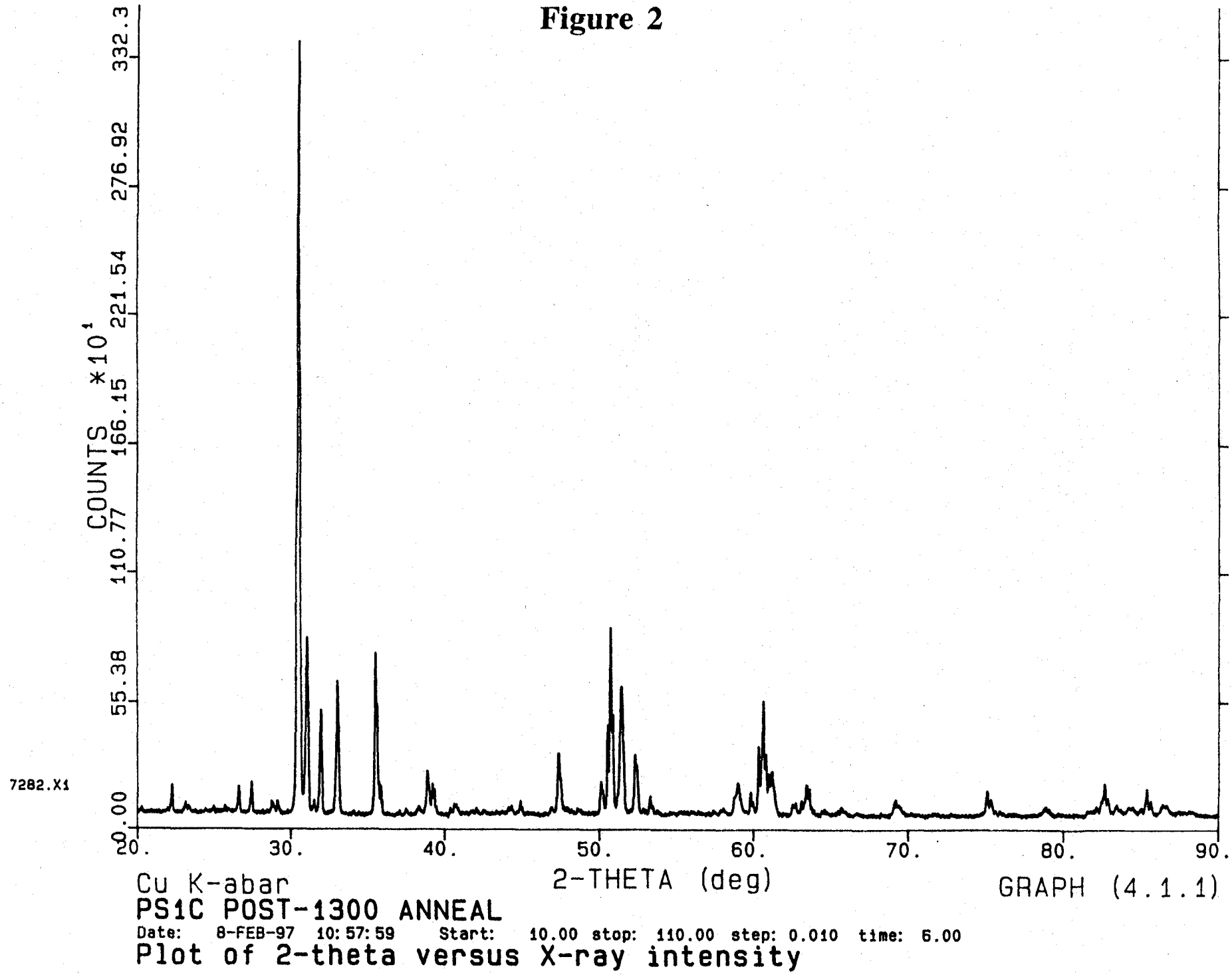
Figure 2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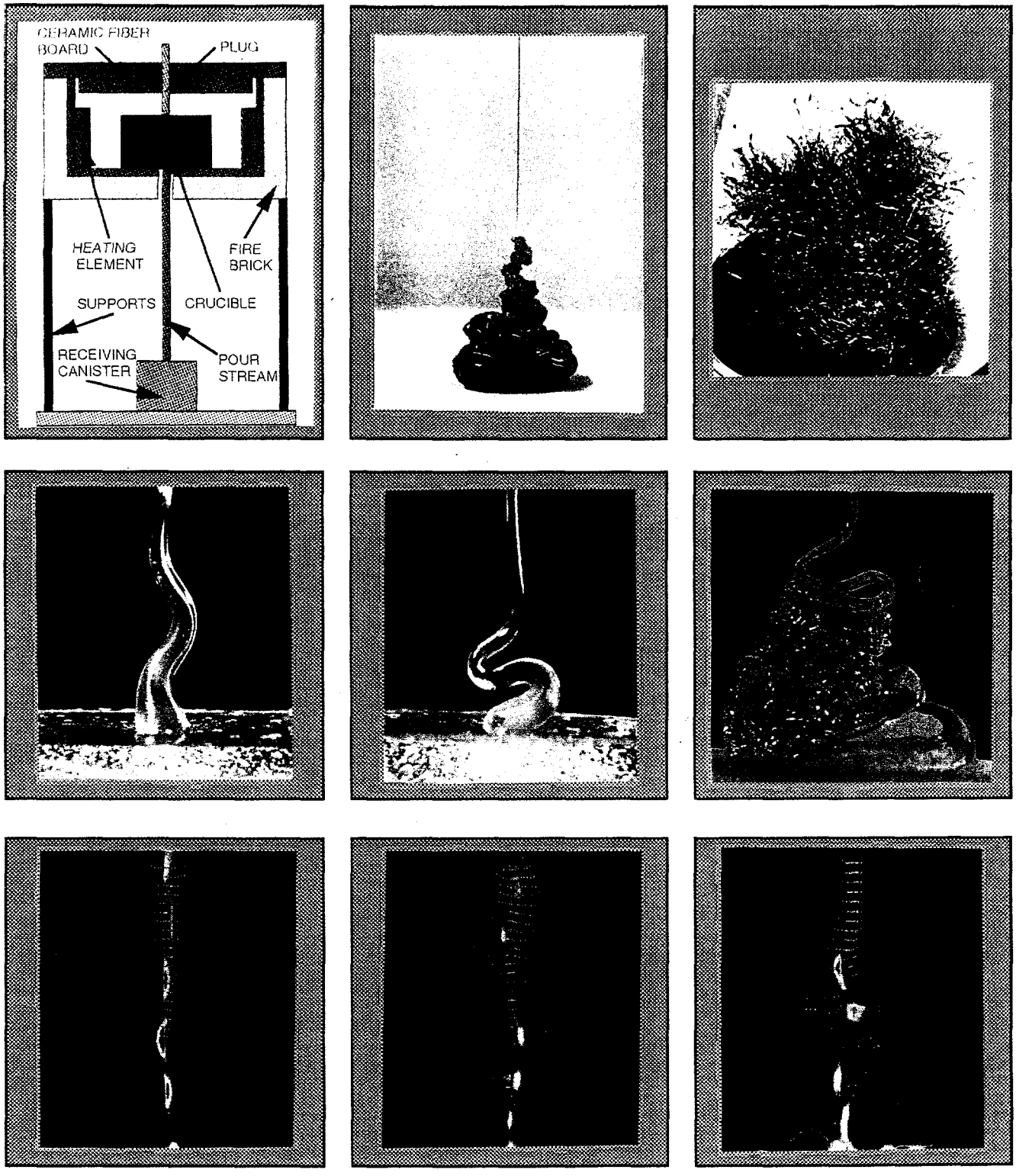

Canister Filling with a Molten Glass Jet

K. S. Ball, M. Song, M. Gomon, and M. W. Silva, Department of Mechanical Engineering,
E. L. Taleff and B. M. Powers, Department of Aerospace Engineering and Engineering Mechanics,
The University of Texas at Austin, Austin, TX 78712;
T. L. Bergman, Department of Mechanical Engineering, University of Connecticut, Storrs, CT 06269

Top row: high-temperature molten glass experiment (furnace temperature: 1050° C): (l) schematic of pouring apparatus, (m) buckling of impinging jet, (r) bird's nest formation. Middle row: room-temperature analogous fluid experiment (corn syrup): (l) initial impact of jet, (m) immediately after impact, (r) pile-up after approximately 1 s. Bottom row: finite element/volume of fluid simulation (FIDAP) of analogous fluid experiment: velocity vectors and air/liquid interface location superimposed on pressure field (bright red indicates compression, dark blue indicates tension).