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THE DEVELOPMENT OF COAL-BASED TECHNOLOGIES FOR DEPARTMENT OF DEFENSE FACILITIES

Semiannual Technical Progress Report for the Period 03/28/1996 to 09/27/1996

By

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Energy and Fuels Research Center;
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Fuel Science Program;
Richard Hogg, Subhash Chander, Heechan Cho, M. Thaddeus Ityokumbul, Mark S. Klima, and Peter T. Luckie
Mineral Processing Section; and
Adam Rose, Timothy J. Considine, Richard L. Gordon, Ahmet E. Kocagil, Jeffrey Lazo, and Katherine McClain
Department of Mineral Economics

December 13, 1996

Work Performed Under Cooperative Agreement No. DE-FC22-92PC92162

For
U.S. Department of Energy
Pittsburgh Energy Technology Center
P.O. Box 10940
Pittsburgh, Pennsylvania 15236

By
The Consortium for Coal-Water Slurry Fuel Technology
The Pennsylvania State University
C211 Coal Utilization Laboratory
University Park, Pennsylvania 16802

"U.S. DOE Patent Clearance is NOT required for the publication of this document."

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DISCLAIMER

EXECUTIVE SUMMARY

The U.S. Department of Defense (DOD), through an Interagency Agreement with the U.S. Department of Energy (DOE), has initiated a three-phase program with the Consortium for Coal-Water Slurry Fuel Technology, with the aim of decreasing DOD's reliance on imported oil by increasing its use of coal. The program is being conducted as a cooperative agreement between the Consortium and DOE.

Activities this reporting period are summarized by phase.

PHASE I

Phase I was completed on November 1, 1995.

PHASE II

Work in Phase II focused on emissions reductions, coal beneficiation/preparation studies, and economic analyses of coal use.

Emissions reductions investigations included continuing bench-scale tests to identify an NO_X reduction catalyst which is appropriate for industrial boiler applications. In addition, installation of a ceramic filtering device on the demonstration boiler started. Also, a sodium bicarbonate duct injection system was procured for installation on the demonstration boiler.

Work related to coal preparation and utilization, and the economic analysis was primarily focused on preparing the final report.

PHASE III

Work in Phase III focused on coal preparation studies and economic analyses of coal use.

Coal preparation studies were focused on continuing activities on particle size control, physical separations, surface-based separation processes, and dry processing.

The economic study focused on community sensitivity to coal usage, regional/ national economic impacts of new coal utilization technologies, and constructing a national energy portfolio.

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1.0 INTRODUCTION

The U.S. Department of Defense (DOD), through an Interagency Agreement with the U.S. Department of Energy (DOE), has initiated a three-phase program with the Consortium for Coal-Water Slurry Fuel Technology, with the aim of decreasing DOD's reliance on imported oil by increasing its use of coal. The program is being conducted as a cooperative agreement between the Consortium and DOE. The first phase was completed; work is underway in the other two phases.

To achieve the objectives of the program, a team of researchers was assembled from Penn State (Energy and Fuels Research Center (EFRC), Mineral Processing Section, Department of Mineral Economics, Fuel Science Program, and Polymer Science Program), Energy and Environmental Research Corporation (EER), AMAX Research and Development Center, ABB Combustion Engineering, Inc., CeraMem Separations, Inc., Comprehensive Design Architects and Engineers, and Raytheon Constructors & Engineers.

Phase I activities were focused on developing clean, coal-based combustion technologies for the utilization of both micronized coal-water mixtures (MCWMs) and dry, micronized coal (DMC) in fuel oil-designed industrial boilers. Phase II research and development continued to focus on industrial boiler retrofit technologies by addressing emissions control strategies for providing ultra-low emissions when firing coal-based fuels in industrial-scale boilers. Phase III activities expands upon emissions reduction strategies through the use of deeply-cleaned coals as a means for reducing air toxics Each phase includes an engineering cost analysis and technology assessment. The activities and status of the phases are described below.

The objective in Phase I was to deliver fully engineered retrofit options for a fuel oil-designed watertube boiler located on a DOD installation to fire either MCWM or DMC. This was achieved through a program consisting of the following five tasks: 1) Coal Beneficiation and Preparation; 2) Combustion Performance Evaluation; 3) Engineering Design; 4) Engineering and Economic Analysis; and 5) Final Report/Submission of Design Package. Following is an outline of the project tasks that comprised Phase I:

Task 1: Coal Beneficiation/Preparation

Subtask 1.1	Identify/Procure Coals
Subtask 1.2	Determine Liberation Potential
Subtask 1.3	Produce Laboratory-Scale Quantities of Micronized Coal-Water Mixtures (MCWMs)
Subtask 1.4	Develop Dry Coal Cleaning Technique
Subtask 1.5	Produce MCWMs and Dry, Micronized Coal (DMC) From Dry Clean Coal
Subtask 1.6	Produce MCWM and DMC for the Demonstration Boiler
Subtask 1.7	Project Management and Support

Task 2: Combustion Performance Evaluation

- Subtask 2.1 Boiler Retrofit
- Subtask 2.2 Fuel Evaluation in the Research Boiler
- Subtask 2.3 Performance Evaluation of the MCWM and DMC in the Demonstration Boiler
- Subtask 2.4 Evaluate Emissions Reductions Strategies
- Subtask 2.5 Project Management and Support

Task 3: Engineering Design

- Subtask 3.1 MCWM/DMC Preparation Facilities
- Subtask 3.2 Fuel Handling
- Subtask 3.3 Burner System
- Subtask 3.4 Ash Removal, Handling, and Disposal
- Subtask 3.5 Air Pollution Control
- Subtask 3.6 Integrate Engineering Design
- Subtask 3.7 Project Management and Support

Task 4: Engineering and Economic Analysis

- Subtask 4.1 Survey Boiler Population/Identify Boilers for Conversion
- Subtask 4.2 Identify Appropriate Cost-Estimating Methodologies
- Subtask 4.3 Estimate Basic Costs of New Technologies
- Subtask 4.4 Process Analysis of MCWM and DMC
- Subtask 4.5 Analyze/Identify Transportation Cost of Commercial Sources of MCWM and Cleaned Coal for DMC Production
- Subtask 4.6 Determine Community Spillovers
- Subtask 4.7 Regional Market Considerations and Impacts
- Subtask 4.8 Integrate the Analysis
- Subtask 4.9 Project Management and Support

Task 5: Final Report/Submission of Design Package

The Phase I activities included:

Task 1: The coal beneficiation and preparation effort was conducted by Penn State's Mineral Processing Section with assistance from Penn State's Polymer Science Program and AMAX Research and Development Center. This task involved identifying and procuring six coals that could be cleaned to <1.0 wt.% sulfur and <5.0 wt.% ash which have been, or possess the characteristics to enable them to be, made into MCWMs. The coals were subjected to detailed characterization and used to produce laboratory-scale quantities of MCWM. A fundamental study of MCWM stabilization was conducted. Additional activities included developing a dry coal cleaning technique and producing MCWMs and DMC from the resulting cleaned coal.

Task 2: Penn State's EFRC conducted the combustion performance evaluation with assistance from EER and Penn State's Fuel Science Program. The technical aspects of converting a fuel oil-designed boiler at a DOD facility were identified in this task. All appropriate components were evaluated, including the fuel, the fuel storage, handling and delivery equipment, the burner, the boiler, the ash handling and disposal equipment, the emissions control system, and the boiler control system. Combustion performance as indicated by flame stability, completeness of combustion, and related issues such as system derating, changes in system maintenance, the occurrence of slagging, fouling, corrosion and erosion, and air pollutant emissions were determined. As part of this task, MCWM and DMC were evaluated in EFRC's 15,000 lb steam/h watertube boiler. EER provided a coal-designed burner for retrofitting Penn State's boiler. In addition, EER designed the burner for the DOD boiler identified for retrofitting.

Task 3: An engineering study was performed for a complete retrofit of a DOD boiler facility to fire either MCWM or DMC. The designs were performed by EER with input from the other project participants. The designs included the coal preparation, the fuel handling, the burner, the ash removal, handling, and disposal, and the air pollution control systems. The two designs were for the DOD boiler identified in Task 4. The retrofits were designed for community/societal acceptability. The deliverables for this task were a detailed design that could be used for soliciting bids from engineering/construction firms to retrofit the candidate DOD boiler.

Task 4: An engineering cost analysis and a technology assessment of MCWM and DMC combustion were performed by Penn State's Department of Mineral Economics and the EFRC with assistance from the industrial participants. The effort involved surveying the DOD boiler population, identifying boilers for conversion, identifying appropriate cost-estimating methodologies, estimating basic costs for new technologies, developing a process model, analyzing and identifying transportation costs for commercial sources of MCWM and cleaned coal, determining community spillovers, and determining regional market considerations and impacts.

Task 5: The results from each of the tasks were summarized in a final report. In addition, the design packages for the boiler retrofits were submitted. These included the engineering design and economic analysis.

The original objectives of Phase II were to: (a) extend the Phase I boiler retrofit options by including designs to achieve further reductions in gaseous and particulate emissions, (b) prepare and characterize fuels compatible with coal precombustors, and (c) investigate precombustion as a means of using high ash, high sulfur coals. Upon investigating precombustion options for installing a system on either the demonstration boiler (15,000 lb steam/h) or research boiler (1,000 lb steam/h), it became apparent that there were limited viable options and that the complexity of the systems would likely preclude their use on small-scale, industrial boilers. A similar conclusion was presented by the U.S. Corps of Engineers regarding the use of slagging combustors in the Army[1]. Consequently, the Phase II work was revised by eliminating the precombustion fundamental, pilot-scale, and demonstration-scale studies and focusing on fundamental, pilot-scale, and demonstration-scale emissions reduction strategies. An economic analysis of precombustion strategies was conducted, as originally planned, in order to compare precombustion strategies with (low ash) MCWM and DMC combustion retrofits. The revised Phase II consists of four tasks as outlined below:

- Task 1. Emissions Reduction
  - Subtask 1.1 Evaluation of Emissions Reduction Strategies
  - Subtask 1.2 Installation of an Emissions Reduction System on the Demonstration Boiler
  - Subtask 1.3 Evaluation of an Emissions Reduction System
  - Subtask 1.4 Conduct NO_x Emissions Study
  - Subtask 1.5 Conduct VOC Study
  - Subtask 1.6 Conduct Trace Element Study
  - Subtask 1.7 Conduct Nitrogen Occurrence Study
- Task 2. Coal Preparation/Utilization
  - Subtask 2.1 Optimization of Particle Size Consist for CWM Formulation
  - Subtask 2.2 Fine Grinding/Classification/Liberation
  - Subtask 2.3 Fine Gravity Concentration
  - Subtask 2.4 Agglomeration/Flotation Studies
  - Subtask 2.5 Fundamental Studies of Surface-Based Processes
  - Subtask 2.6 Column Flotation
  - Subtask 2.7 Dry Cleaning of Fine Coal
  - Subtask 2.8 CWM Density Control
  - Subtask 2.9 Stabilization of CWM
  - Subtask 2.10 Atomizer Testing
- Task 3. Engineering Design and Cost; and Economic Analysis
  - Subtask 3.1 Determination of Basic Cost Estimation of Boiler Retrofits
  - Subtask 3.2 Determination of Process Analysis
  - Subtask 3.3 Determination of Environmental and Regulatory Impacts
  - Subtask 3.4 Determination of Transportation Cost Analysis
  - Subtask 3.5 Determination of Technology Adoption
  - Subtask 3.6 Determination of Regional Economic Impacts
  - Subtask 3.7 Determination of Public Perception of Benefits and Costs
  - Subtask 3.8 Determination of Social Benefits
  - Subtask 3.9 Determination of Coal Market Analysis
  - Subtask 3.10 Engineering Design
  - Subtask 3.11 Integration of Analyses
- Task 4. Final Report/Submission of Design Package

Portions of Phase II have been completed. The Phase II activities include:

Task 1: Task 1 activities are ongoing. In Task 1, strategies are being developed to provide for ultra-low emissions when firing coal-based fuels in industrial-scale boilers. Emissions being addressed are SO_2, NO_x, fine particulate matter ($<10\ \mu m$), and air toxics (volatile organic compounds and trace metals). Post-combustion and during-combustion technologies to reduce SO_2 and NO_x emissions from coal-fired industrial boilers were surveyed. Novel technologies that are under development but are not commercially available were also surveyed as well as proven technologies such as limestone/lime injection, selective catalytic reduction, and nonselective catalytic reduction. Options for removing the submicron particulate were investigated. In addition, methods to remove air toxics from the flue gas, such as scrubbing, were investigated.

Task 2: Task 2 activities have been completed except for Subtask 2.10, which is an atomization study being conducted by Carnegie Mellon University, which was recently added to the program. Emphasis in Task 2 was on the refinement and optimization of coal grinding and CWM preparation procedures, and on the development of advanced processes for beneficiating high ash, high sulfur coals. CWM formulation is still an art and there was a clear need for scientifically-based guidelines for slurry design. This involved determining the optimum particle size distribution, how and why the optimum particle size distribution varies from coal to coal, and the specific roles of chemical dispersing and stabilizing agents. Extensive, physical pre-cleaning of coal is especially important in small-boiler applications. The research effort built on work conducted in Phase I.

Task 3: Task 3 economic analysis activities are nearly complete and focus on determining the basic cost estimation of boiler retrofits, evaluating environmental, regulatory, and regional economic impacts, and analyzing the coal market.

Task 4: The results from each of the tasks will be summarized in a final report.

The original objectives of Phase III were to: (a) develop coal-based fuel/waste cofiring technologies, and (b) assist DOD in improving the combustion performance and reducing emissions from existing stoker-fired boilers. Since the initial development of the program's statements of work (Phases I through III), there has been a change in military boiler plant operating philosophy. This, coupled with recent developments in cofiring technologies and DOE coal preparation programs, necessitates the revision of the Phase III statement of work. Consequently, the Phase III work has been revised by eliminating coal-based fuel/waste cofiring and stoker combustion performance analysis and evaluation, and focusing these efforts toward evaluating deeply-cleaned coals as industrial boiler fuels, and investigating fundamental, pilot-scale, and demonstration-scale emissions reduction strategies. The revised Phase III consists of five tasks as outlined below:

Task 1. Coal Preparation/Utilization

Subtask 1.1	Particle Size Control
Subtask 1.2	Physical Separations
Subtask 1.3	Surface-Based Separation Process
Subtask 1.4	Dry Processing
Subtask 1.5	Stabilization of Coal-Water Mixtures

Task 2. Emissions Reduction

Subtask 2.1 SO_2 Reduction
Subtask 2.2 NO_x Reduction
Subtask 2.3 Study of VOC and Trace Element Production, Reduction, and Capture

Task 3. Economic Evaluation

Subtask 3.1 Cost and Market Penetration of Coal-Based Fuel Technologies
Subtask 3.2 Selection of Incentives for Commercialization of the Coal-Using Technology
Subtask 3.3 Community Sensitivity to Coal Fuel Usage
Subtask 3.4 Regional Economic Impacts of New Coal Utilization Technologies
Subtask 3.5 Economic Analysis of the Defense Department's Fuel Mix
Subtask 3.6 Constructing a National Energy Portfolio which Minimizes Energy Price Shock Effects
Subtask 3.7 Proposed Research on the Coal Markets and their Impact on Coal-Based Fuel Technologies
Subtask 3.8 Integrate the Analysis

Task 4. Evaluation of Deeply-Cleaned Coal as Boiler Fuels

Subtask 4.1 Modify MCWM Preparation Circuit
Subtask 4.2 Fuels Characterization
Subtask 4.3 Pilot-Scale Combustion Tests
Subtask 4.4 Demonstration-Scale Combustion Tests

Task 5. Final Report

The Phase III activities include:

Task 1: Research conducted under Phase I and Phase II of this project has revealed a number of specific areas where continued and/or more focused effort is required in order to develop more effective and more reliable coal processing systems. Specific objectives of Task 1 are centered around:

- focused investigations into specific coal-cleaning options and their associated ancillary operations; and
- integration of processing/cleaning operations for overall system optimization.

As in the previous phases, emphasis is on fine-coal processing for the production of high-quality, micronized coal for dry coal and coal-water mixture (CWM) applications.

Task 2: Task 2 is a continuation of the emissions reduction work started in Phase II, and involves fundamental studies, pilot-scale investigations, and full-scale demonstrations. The low-temperature NO_x reduction catalyst identified in Phase II will be tested at the pilot and demonstration scale. The effect of coal cleaning, particulate removal devices, and boiler operating conditions on air toxics emissions from coal-fired industrial boilers will also be investigated.

Task 3: The activities in Task 3 focus on determining cost and market penetration, selection of incentives, and regional economic impacts of coal-based fuel technologies. In addition, DOD's fuel mix is being determined and a national energy portfolio constructed.

Task 4: The results from each of the tasks will be summarized in a final report.

The status of Phase I is presented in Section 2.0. The accomplishments and status of Phase II, Tasks 1, 2, 3, and 4 are presented in Sections 3.0, 4.0, 5.0, and 6.0, respectively. The accomplishments and status of Phase III, Tasks 1, 2, 3, and 4 are presented in Sections 7.0, 8.0, 9.0, and 10.0, respectively. Section 11.0 discusses miscellaneous activities that were conducted. Activities planned for the next semiannual period are listed in Section 12.0. References and acknowledgments are contained in Sections 13.0 and 14.0, respectively. The project schedule for Phases II and III is given in Figures 1-1 and 1-2, respectively, with a description of the milestones contained in Tables 1-1 and 1-2, respectively.

2.0 PHASE I, TASK 5: FINAL REPORT/SUBMISSION OF DESIGN PACKAGE

The draft final report for Phase I was completed on November 1, 1995.

3.0 PHASE II, TASK 1: EMISSIONS REDUCTION

The objective of this task is to develop strategies to provide for ultra-low emissions when firing coal-based fuels in industrial-scale boilers. Emissions being addressed are SO_2, NO_x, fine particulate matter (<10 µm), and air toxics (volatile organic compounds and trace metals).

3.1 Subtask 1.1 Evaluation of Emissions Reduction Strategies

Subtask 1.1 was previously completed.

3.2 Subtask 1.2 Install System on the Demonstration Boiler

Activity is underway to install an SO_2 reduction system and a ceramic filter on the demonstration boiler to reduce SO_2 emissions, and remove ultrafine particulate and increase the particulate collection efficiency, respectively. The SO_2 reduction system and a ceramic filter are discussed in Sections 2.2.1 and 2.2.2, respectively.

3.2.1 SO_2 Reduction System

A sodium duct injection system was procured during this reporting period. The system, shown schematically in Figure 3-1, consists of a bag (sodium bicarbonate) unloading station, hopper with weigh cells, eductor, and piping to a port located in the ducting upstream of the baghouse and ceramic filter. The system will be installed during the next reporting period.

Task 2. Coal Preparation / Utilization

Subtask 2.1 - Optimization of Particle Size Consist for Slurry Formulation

Subtask 2.2 - Fine Grinding / Classification / Liberation

Subtask 2.3 - Fine Gravity Concentration

Subtask 2.4 - Agglomeration / Flotation Studies

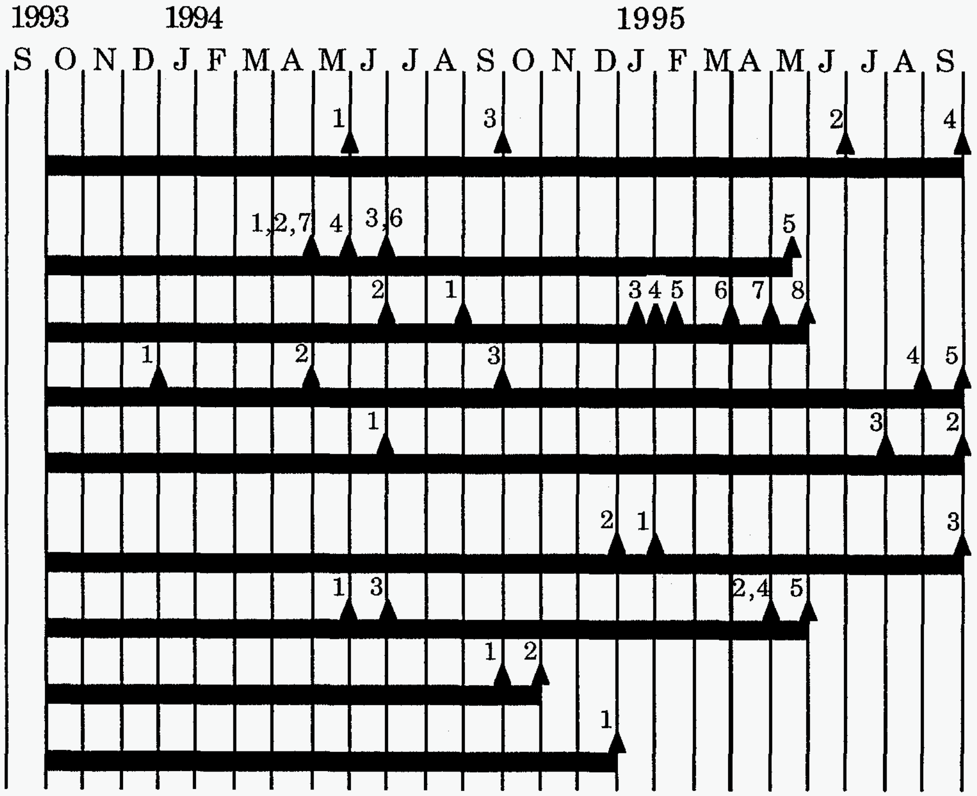
Subtask 2.5 - Fundamental Studies of Surface-Based Processes

Subtask 2.6 - Column Flotation

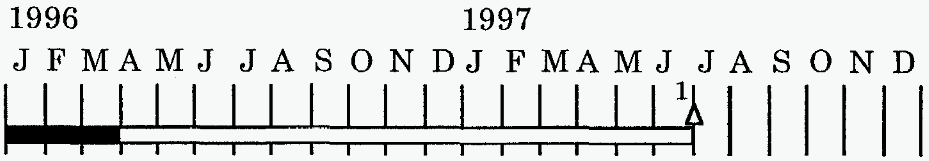
Subtask 2.7 - Dry Cleaning of Fine Coal

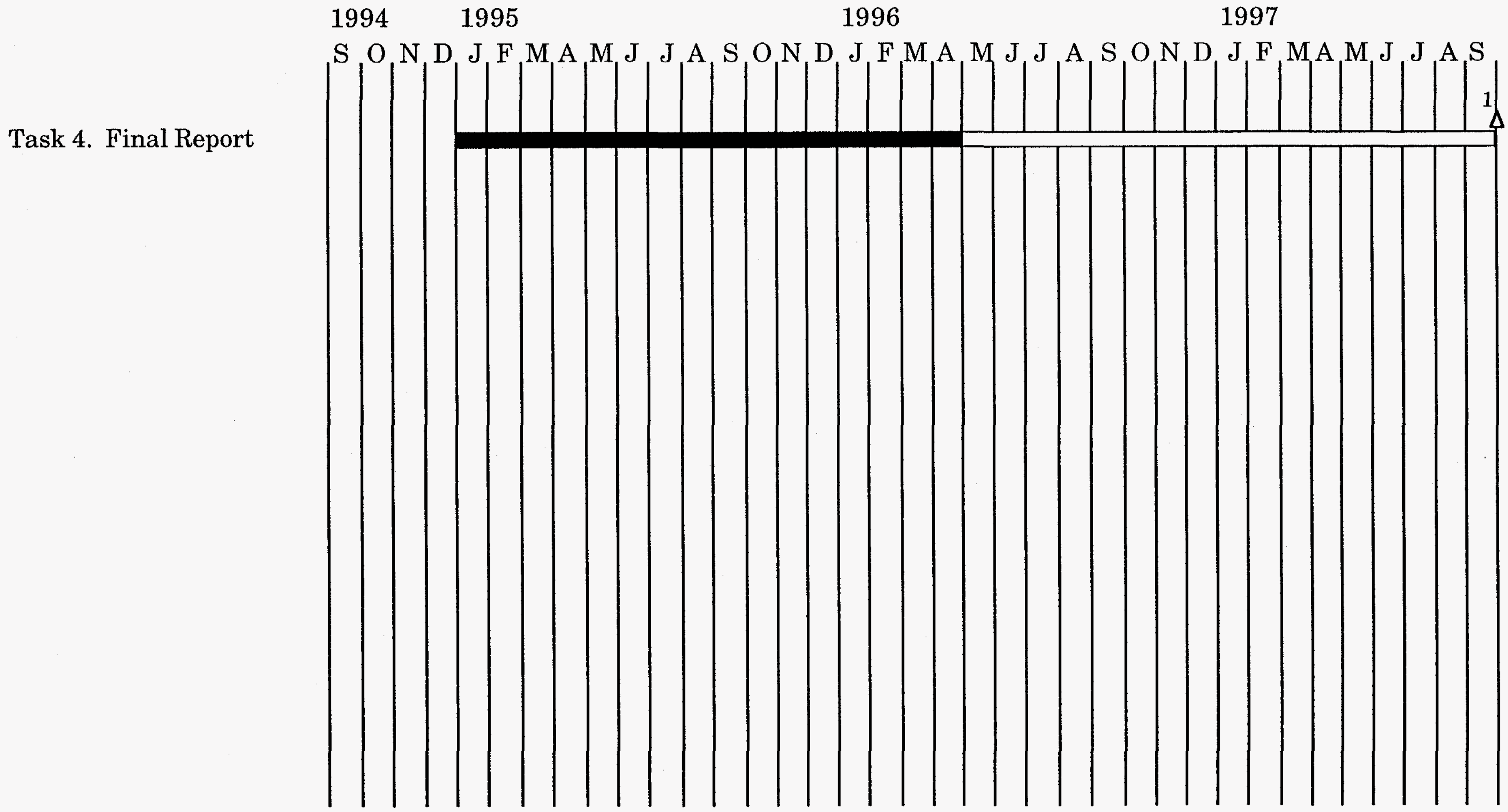
Subtask 2.8 - Slurry Density Control

Subtask 2.9 - Stabilization of CWSF



Subtask 2.10 - Atomizer Testing

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Task 4. Final Report
1

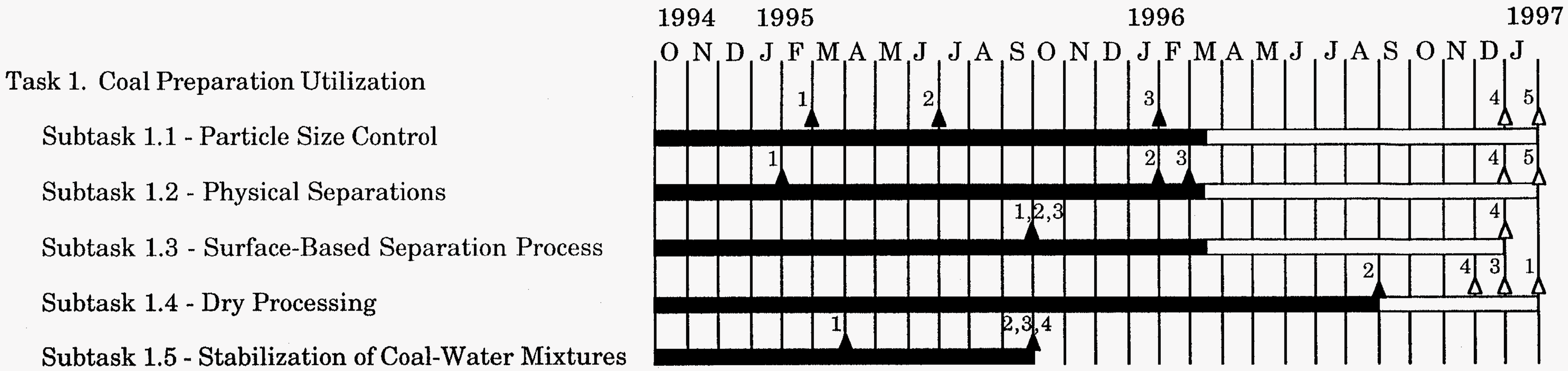
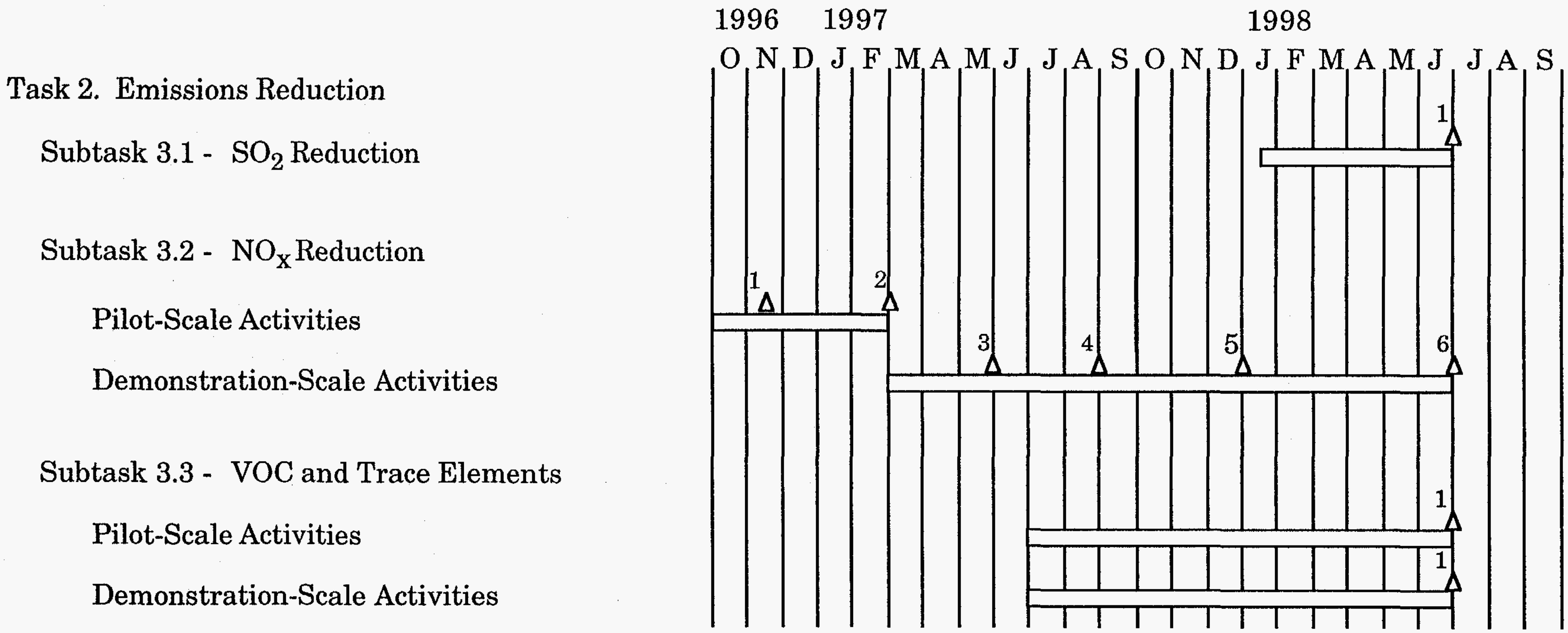


Figure 1-2. DOD Phase III Milestone Schedule


1996
1997
1998
O N D J F M A M J J A S O N D J F M A M J J A S
Task 2. Emissions Reduction
Subtask 3.1 - SO2 Reduction
1
Subtask 3.2 - NOx Reduction
Pilot-Scale Activities
1
2
Demonstration-Scale Activities
3
4
5
6
Subtask 3.3 - VOC and Trace Elements
Pilot-Scale Activities
1
Demonstration-Scale Activities
1

Task 3. Economic Evaluation

Subtask 3.1 - Cost and Market Penetration of Coal-Based Fuel Technologies

Subtask 3.2 - Selection of Incentives for Commercialization of the Coal Using Technology

Subtask 3.3 - Community Sensitivity of Coal Fuel Usage

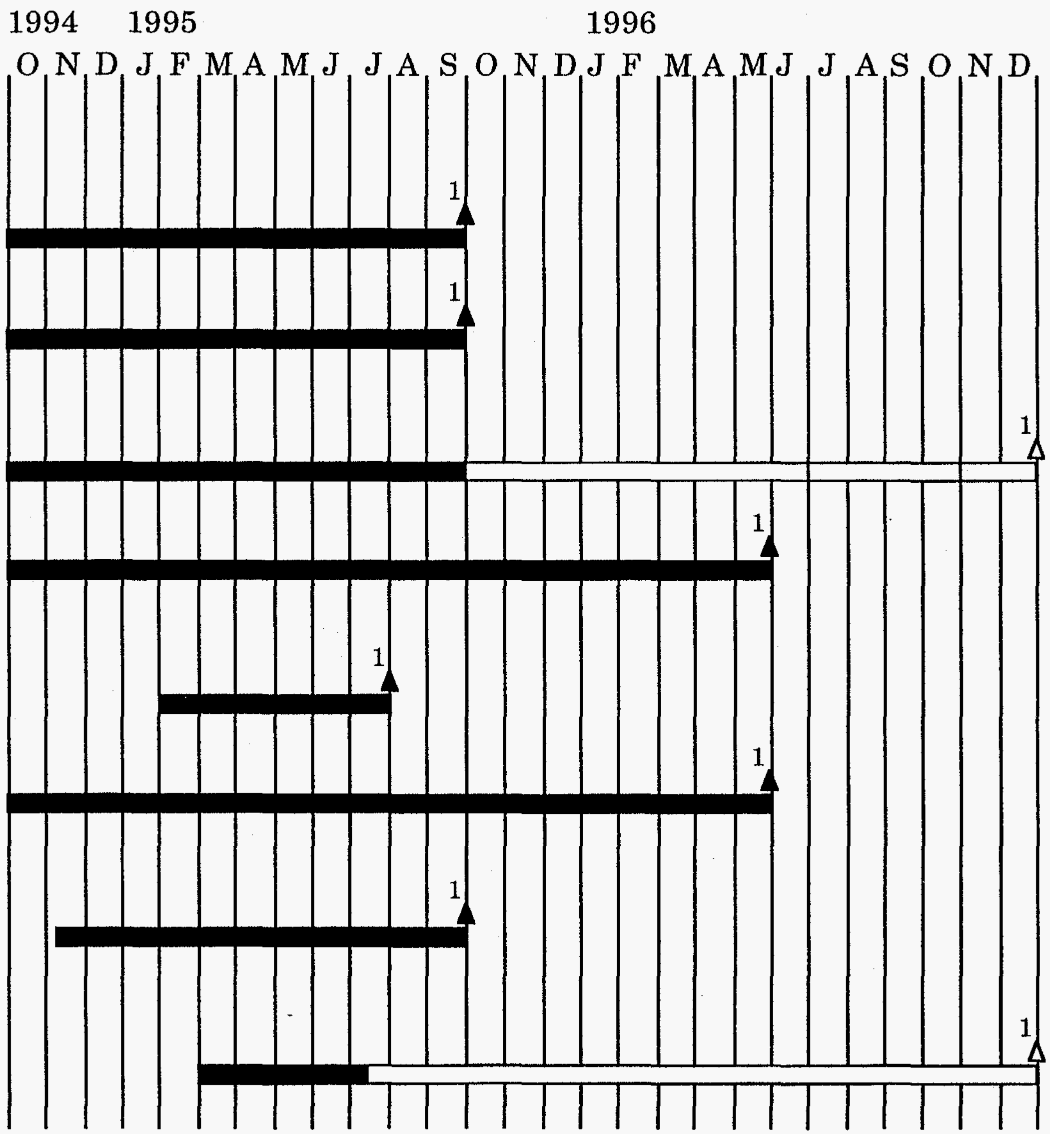
Subtask 3.4 - Regional-National Economic Impacts of New Coal Utilization Technologies

Subtask 3.5 - Economic Analysis of the Defense Department's Fuel Mix

Subtask 3.6 - Constructing a National Energy Portfolio which Minimizes Energy Price Shock Effects

Subtask 3.7 - Proposed Research on the Coal Markets and their Impact on Coal-Based Fuel Technologies

Subtask 3.8 - Integration of Economic Analysis



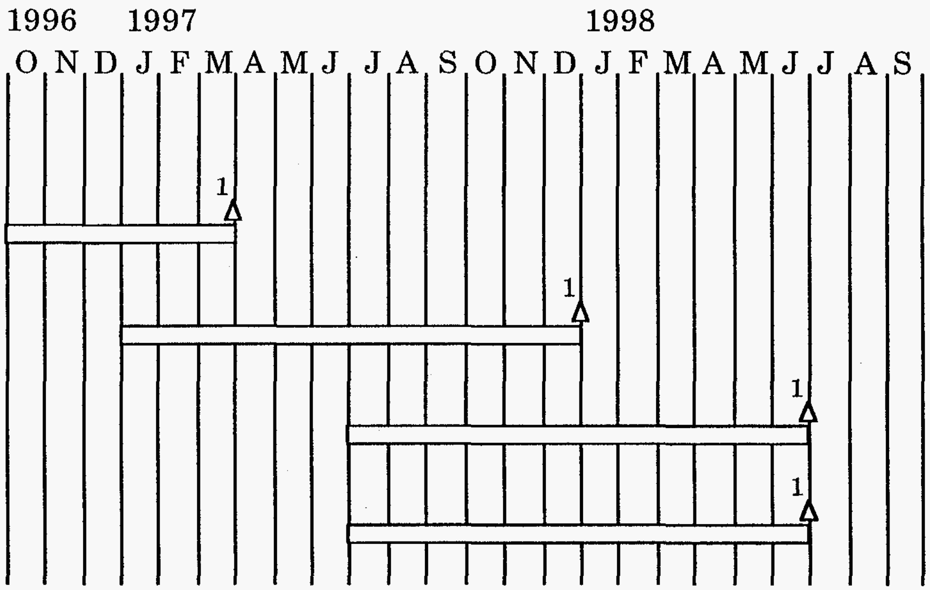
Task 4. Evaluation of Deeply-Cleaned Coal as Boiler Fuel

Subtask 4.1 - Modify MCWM Preparation Circuit

Subtask 4.2 - Fuels Characterization

Subtask 4.3 - Pilot-Scale Combustion Tests

Subtask 4.4 - Demonstration-Scale Combustion Tests



Task 5. Final Report / Submission of Design Package

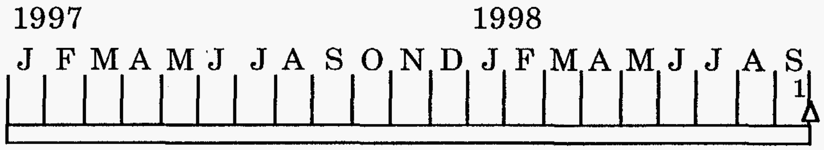


Table 1-1. Phase II. Milestone Description

Milestone	Description	Planned Completion Date	Actual Completion Date
Task 1. Emissions Reduction			
Subtask 1.1. Evaluation of Emissions Reduction Strategies			
Subtask 1.1, No. 1	Receive proposals for pollution control system	12/01/93	12/01/93
Subtask 1.1, No. 2	Complete summary report of pollution control technologies	03/31/95	03/31/95
Subtask 1.1, No. 3	Select pollution control system	12/31/95	12/31/95
Subtask 1.2. Install System on Demonstration Boiler			
Subtask 1.2, No. 1	Design pollution control system	05/01/96	07/01/96
Subtask 1.2, No. 2	Complete installation of system	11/22/96	
Subtask 1.3. Evaluate Emissions Reduction System			
Subtask 1.3, No. 1	Shakedown system	12/31/96	
Subtask 1.3, No. 2	Complete system evaluation	06/30/97	
Subtask 1.4. Conduct NO_X Emissions Study			
Subtask 1.4, No. 1	Review state-of-the art in NO_X catalysts	10/01/94	10/01/94
Subtask 1.4, No. 2	Design bench-scale flow reactor	02/01/95	03/01/95
Subtask 1.4, No. 3	Design FTIR gas analysis system for the flow reactor	04/01/95	04/18/95
Subtask 1.4, No. 4	Construct flow reactor and data acquisition system	10/01/95	12/15/95
Subtask 1.4, No. 5	Shake down system and calibrate FTIR spectrometer	03/01/96	03/15/96
Subtask 1.4, No. 6	Select and acquire catalysts for testing	04/01/96	04/01/96
Subtask 1.4, No. 7	Develop catalyst characterization database	06/15/96	08/01/96
Subtask 1.4, No. 8	Design selective catalytic NO_X reduction system	11/01/96	
Subtask 1.5. Conduct VOC Study			
Subtask 1.5, No. 1	Modify research boiler	12/31/95	01/15/96
Subtask 1.5, No. 2	Literature survey on trace organic emissions and analytical procedures	03/31/96	04/01/96
Subtask 1.5, No. 3	Evaluate the GC/MS equipment and upgradation	12/31/96	
Subtask 1.5, No. 4	Procurement of Method 5 apparatus and auxiliaries	10/31/96	
Subtask 1.5, No. 5	Shakedown of the sampling procedures	01/31/97	
Subtask 1.5, No. 6	Conduct test program and analyze samples	04/30/97	
Subtask 1.5, No. 7	Analysis of the results	06/30/97	
Subtask 1.6. Conduct Trace Element Study			
Subtask 1.6, No. 1	Conduct literature survey on trace element emissions and analysis techniques	11/30/96	
Subtask 1.6, No. 2	Procure sampling equipment	11/30/96	
Subtask 1.6, No. 3	Shake down sampling procedure	12/31/96	
Subtask 1.6, No. 4	Characterize emissions from industrial boiler	05/31/97	
Subtask 1.6, No. 5	Analysis of results	06/30/97	
Subtask 1.7. Conduct Nitrogen Occurrence Study			
Subtask 1.7, No. 1	Optimization of sample preparation for ^{15}N NMR on coals and chars	01/31/95	01/31/95
Subtask 1.7, No. 2	First solid-state ^{15}N NMR spectra at natural ^{15}N abundance of coals obtained	11/30/94	11/30/94
Subtask 1.7, No. 3	First solid-state ^{15}N NMR spectra at natural ^{15}N abundance of chars obtained	01/31/95	01/31/95

Milestone	**Description**	**Planned Completion Date**	**Actual Completion Date**
Subtask 1.7, No. 4	Examination of diagenetic changes of the N-functionality in oil shale and its precursors by means of ^{15}N and ^{13}C NMR spectroscopy	08/30/96	
Subtask 1.7, No. 5	Examination of the N-functionality in vitrinite coals as a function of maturation degree by means of ^{15}N and ^{13}C NMR spectroscopy	06/30/95	06/30/95
Subtask 1.7, No. 6	Examination of changes of the N-functionality in chars as a function of retention time in combustion chamber by means of ^{15}N and ^{13}C NMR spectroscopy	08/30/96	
Task 2. Coal Preparation/Utilization			
Subtask 2.1. Optimization of Particle Size Consist for Slurry Formulation			
Subtask 2.1, No. 1	Samples of fine and coarse slurry components prepared	04/30/94	05/30/94
Subtask 2.1, No. 2	Rheological characterization of components completed	04/30/95	06/30/95
Subtask 2.1, No. 3	Models for rheology of binary mixtures developed	09/30/94	09/30/94
Subtask 2.1, No. 4	Optimization studies complete	06/30/95	09/30/95
Subtask 2.2. Fine Grinding/Classification Liberation			
Subtask 2.2, No. 1	Grinding kinetics data for wet ball milling obtained	04/30/94	04/30/94
Subtask 2.2, No. 2	Wet classifier performance evaluated	04/30/95	04/30/95
Subtask 2.2, No. 3	Dry classifier performance evaluated	04/30/94	06/30/94
Subtask 2.2, No. 4	Grinding kinetics data for stirred media milling obtained	05/31/94	05/31/94
Subtask 2.2, No. 5	Closed-circuit jet-milling data obtained	05/15/95	05/15/95
Subtask 2.2, No. 6	Slurry production simulations initiated	06/30/94	06/30/94
Subtask 2.2, No. 7	Liberation data on Type III coal obtained	04/30/94	04/30/94
Subtask 2.3. Fine Gravity Concentration			
Subtask 2.3, No. 1	Initiate magnetic fluid separation of Type III coal	07/31/94	08/15/94
Subtask 2.3, No. 2	Complete batch centrifuge testing	04/30/94	06/30/94
Subtask 2.3, No. 3	Continuous centrifuge test rig set-up	09/30/94	01/15/95
Subtask 2.3, No. 4	Initiate magnetite classification studies	10/15/94	01/31/95
Subtask 2.3, No. 5	Initiate separations of Type III coals	02/28/95	02/28/95
	Initiate micronized coal classification studies	04/30/95	03/31/95
Subtask 2.3, No. 6			
Subtask 2.3, No. 7	Evaluate dense-medium separation data	04/30/95	04/30/95
Subtask 2.3, No. 8	Evaluate size classification data	05/31/95	05/31/95
Subtask 2.4. Agglomeration/Flotation Studies			
Subtask 2.4, No. 1	Set-up device to size separate flotation products of micronized coal	12/31/93	12/31/93
Subtask 2.4, No. 2	Set-up equipment for larger scale tests using 2.2 cu.ft. flotation cells	04/30/94	04/30/94
Subtask 2.4, No. 3	Conduct agglomeration-flotation tests for micronized Type III coal	09/30/94	09/30/94
Subtask 2.4, No. 4	Conduct agglomeration-flotation tests in larger cells	03/31/95	08/31/95
Subtask 2.4, No. 5	Determine parameters for scale-up	06/30/95	09/30/95
Subtask 2.5. Fundamental Studies of Surface-Based Processes			
Subtask 2.5, No. 1	Conduct interface characterization studies to determine flotation reagent-coal interactions	06/30/94	06/30/94
Subtask 2.5, No. 2	Measure contact angles in the coal-oil-surfactant-water system	06/30/95	09/30/95
Subtask 2.5, No. 3	Determine effect of surfactants on slurry stability	05/31/95	07/31/95

Milestone	**Description**	**Planned Completion Date**	**Actual Completion Date**
Subtask 2.6. Column Flotation			
Subtask 2.6, No. 1	Test work on Type II coals	11/30/94	01/31/95
Subtask 2.6, No. 2	Test work on Type III coals	09/30/94	12/31/94
Subtask 2.6, No. 3	Determine scale-up parameters	05/31/95	09/30/95
Subtask 2.7. Dry Cleaning of Fine Coal			
Subtask 2.7, No. 1	Complete evaluation of Type III coal in batch separator	04/30/94	05/31/94
Subtask 2.7, No. 2	Integration of closed dry grinding circuit with TES	04/30/95	04/30/95
Subtask 2.7, No. 3	Initiate investigation of continuous TES	04/01/94	06/30/94
Subtask 2.7, No. 4	Complete charge measurements on Type II coal	04/30/95	04/30/95
Subtask 2.7, No. 5	Complete charge measurements on Type III	05/31/95	05/31/95
Subtask 2.8. Slurry Density Control			
Subtask 2.8, No. 1	Evaluate procedures for reversible flocculation of fine coal	09/30/94	09/30/94
Subtask 2.8, No. 2	Establish process engineering for thickening of fine-coal slurries	10/31/94	10/31/94
Subtask 2.9. Stabilization of CWSF			
Subtask 2.9, No. 1	Complete stabilization study	12/31/94	12/31/94
Subtask 2.10. Atomizer Testing			
Subtask 2.10, No. 1	Complete atomization study	06/30/97	
Task 3. Engineering Design and Cost; and Economic Analysis			
Subtask 3.1. Determine Basic Cost Estimation of Boiler Retrofits		02/01/95	02/01/95
Subtask 3.2. Determine Process Analysis		02/01/95	02/01/95
Subtask 3.3. Determine Environmental and Regulatory Impacts		02/01/95	02/01/95
Subtask 3.4. Determine Transportation Cost Analysis		04/01/95	04/01/95
Subtask 3.5. Determine Technology Adoption		06/01/95	06/01/95
Subtask 3.6. Determine Regional Economic Impacts		12/31/96	
Subtask 3.7. Determine Public Perception of Benefits and Costs		04/01/95	04/01/95
Subtask 3.8. Determine Social Benefits		06/01/95	06/01/95
Subtask 3.9. Determine Coal Market Analysis		02/01/95	02/01/95
Subtask 3.10. Complete Integration of Analyses		12/31/96	
Task 4. Final Report		09/30/97	

Table 1-2. Phase III. Milestone Description

Milestone	Description	Planned Completion Date	Actual Completion Date
Task 1. Coal Preparation/Utilization			
Subtask 1.1. Particle Size Control			
Subtask 1.1, No. 1	Evaluate conventional ball milling circuit	02/28/95	02/28/95
Subtask 1.1, No. 2	Evaluate stirred-media milling circuit	06/30/95	06/30/95
Subtask 1.1, No. 3	Complete baseline testing of attrition milling for the production of broad size distributions	01/31/96	01/31/96
Subtask 1.1, No. 4	Complete preliminary evaluation of dry grinding/ classifier circuit	12/31/96	
Subtask 1.1, No. 5	Initiate investigation of an integrated grinding/cleaning circuit	01/31/97	
Subtask 1.2. Physical Separations			
Subtask 1.2, No. 1	Complete preliminary investigation of magnetic fluid-based separation for fine coal cleaning	01/31/95	01/31/95
Subtask 1.2, No. 2	Complete baseline testing of dense-medium separation using the continuous, solid-bowl centrifuge	01/31/96	01/31/96
Subtask 1.2, No. 3	Initiate investigation of magnetic fluid cyclone separations	02/29/96	02/29/96
Subtask 1.2, No. 4	Complete baseline testing of solid-bowl centrifuge for micronized coal classification	12/31/96	
Subtask 1.2, No. 5	Initiate testing of integrated centrifugal/flotation system	01/31/97	
Subtask 1.3. Surface-Based Separation Processes			
Subtask 1.3, No. 1	Set up and evaluate continuous flotation circuit	05/31/95	09/30/95
Subtask 1.3, No. 2	Evaluate effectiveness of alternative bubble generators in flotation column	06/30/95	09/30/95
Subtask 1.3, No. 3	Baseline testing on selected coal	08/31/95	09/30/95
Subtask 1.3, No. 4	Evaluate flotation system performance	12/31/96	
Subtask 1.4 Dry Processing			
Subtask 1.4, No. 1	Complete deagglomeration testing using the batch triboelectrostatic separator	01/31/97	
Subtask 1.4, No. 2	Complete baseline testing of continuous triboelectrostatic separator unit	05/31/96	08/31/96
Subtask 1.4, No. 3	Initiate investigation of alternative approaches to charging/deagglomeration	12/31/96	
Subtask 1.4, No. 4	Complete preliminary testing of integrated grinding and triboelectrostatic separator unit	11/30/96	

Milestone	Description	Planned Completion Date	Actual Completion Date
Subtask 1.5 Stabilization of Coal-Water Mixtures			
Subtask 1.5, No. 1	Complete PSD model extension	04/01/95	04/01/95
Subtask 1.5, No. 2	Complete construction of computer program	09/27/95	09/27/95
Subtask 1.5, No. 3	Complete PSD model comparison to experimental results	09/27/95	09/27/95
Subtask 1.5, No. 4	Complete coal oxidation study	09/27/95	09/27/95
Task 2. Emissions Reduction			
Subtask 2.1. SO_2 Reduction			
Subtask 2.1, No. 1	Evaluate SO_2 reduction system in coordination with NO_x reduction system	07/01/98	
Subtask 2.2. NO_x Reduction			
Subtask 2.2, No. 1	Assemble pilot-scale testing system	11/15/96	
Subtask 2.2, No. 2	Perform pilot-scale tests of NO_x reduction system	03/01/97	
Subtask 2.2, No. 3	Design selective catalytic NO_x reduction system	06/01/97	
Subtask 2.2, No. 4	Design demonstration boiler modifications for NO_x reduction system	09/09/97	
Subtask 2.2, No. 5	Modify demonstration boiler system for NOx reduction system	12/31/97	
Subtask 2.2, No. 6	Complete testing of NOx reduction system	07/01/98	
Subtask 2.3. Study VOC and Trace Element Production, Reduction, and Capture			
Subtask 2.3, No. 1	Complete pilot-scale testing of deeply-cleaned coals	07/01/98	
Subtask 2.3, No. 2	Complete demonstration-scale testing of deeply-cleaned coals	07/01/98	
Task 3. Economic Evaluation			
Subtask 3.1. Cost and Market Penetration of Coal-Based Fuel Technologies			
Subtask 3.1, No. 1	Complete study of cost and market penetration of coal-based fuel technologies	06/01/95	09/27/95
Subtask 3.2. Selection of Incentives for Commercialization of the Coal Using Technology			
Subtask 3.2, No. 1	Complete selection of incentives for commercialization of the coal-using technology	09/27/95	09/27/95
Subtask 3.3. Community Sensitivity to Coal Fuel Usage			
Subtask 3.3, No. 1	Complete evaluation of community sensitivity to coal fuel usage	12/31/96	

Milestone	Description	Planned Completion Date	Actual Completion Date
Subtask 3.4 Regional Economic Impacts of New Coal Utilization Technologies			
Subtask 3.4, No. 1	Complete study of regional economic impacts of new coal utilization technologies	06/01/96	06/01/96
Subtask 3.5 Economic Analysis of the Defense Department's Fuel Mix			
Subtask 3.5, No. 1	Complete economic analysis of the defense department's fuel mix	09/27/95	06/30/95
Subtask 3.6 Constructing a National Energy Portfolio which Minimizes Energy Price Shock Effects			
Subtask 3.6, No. 1	Complete construction of a national energy portfolio which minimizes energy price shock effects	06/01/96	06/01/96
Subtask 3.7 Proposed Research on the Coal Markets and their Impact on Coal-Based Fuel Technologies			
Subtask 3.7, No. 1	Complete research on the coal markets and their impact on coal-based fuel technologies	09/27/95	09/27/95
Subtask 3.8 Integrate the Analysis			
Subtask 3.8, No.1	Complete integration of the analysis	08/01/96	
Task 4. Evaluation of Deeply-Cleaned Coals as Boiler Fuels			
Subtask 4.1 Modify MCWM Preparation Circuit			
Subtask 4.1, No. 1	Complete modifications to MCWM preparation circuit	04/01/97	
Subtask 4.2 Fuels Characterization			
Subtask 4.2, No. 1	Complete fuels characterization	01/01/98	
Subtask 4.3 Pilot-Scale Combustion Tests			
Subtask 4.3, No. 1	Complete pilot-scale testing of deeply-cleaned coals	07/01/98	
Subtask 4.4 Demonstration-Scale Combustion Tests			
Subtask 4.4, No. 1	Complete demonstration-scale testing of deeply-cleaned coals	07/01/98	
Task 5. Final Report/Submission of Design Package		09/27/98	

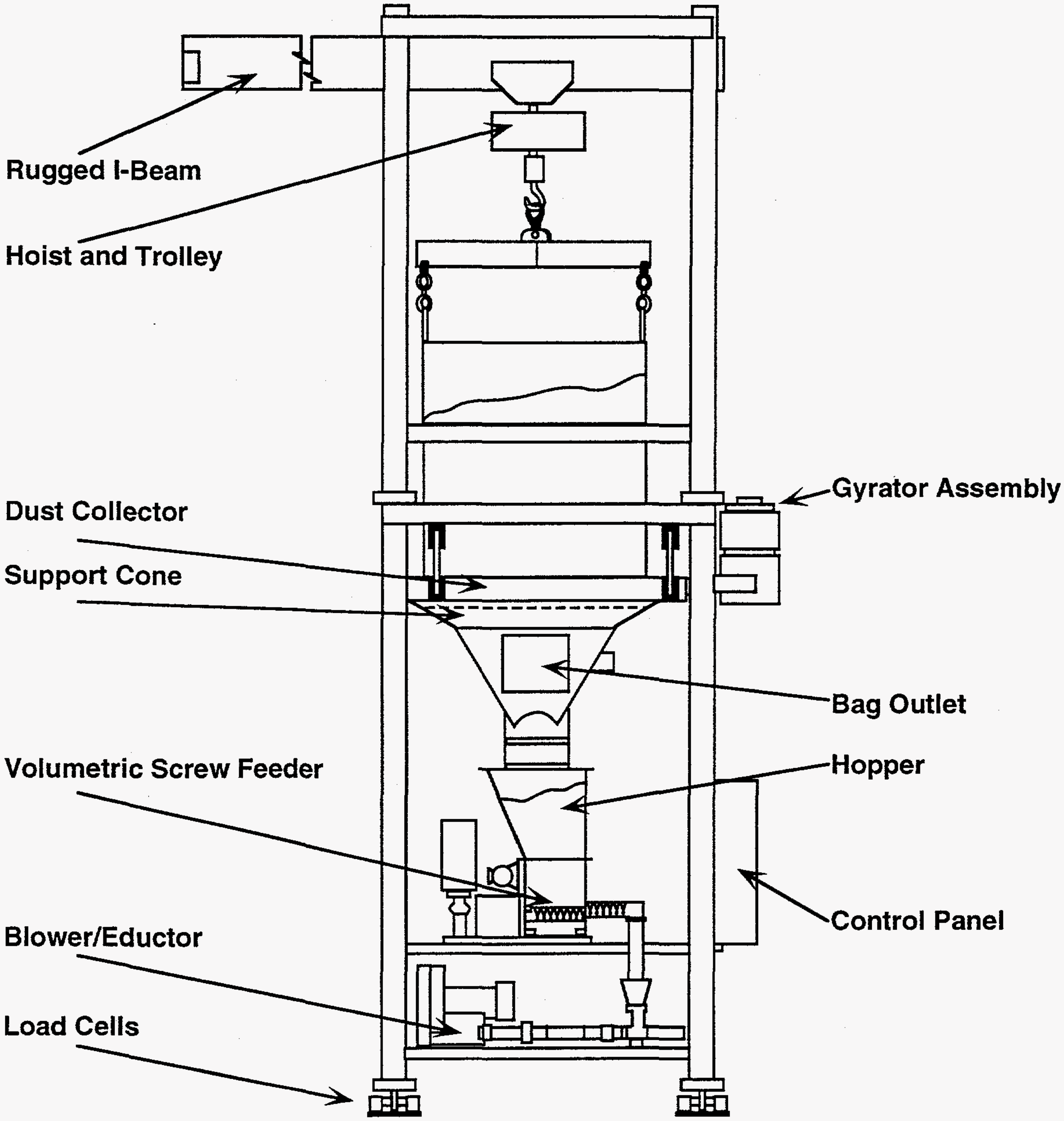


Figure 3-1. SCHEMATIC DIAGRAM OF THE SODIUM BICARBONATE DUCT INJECTION SYSTEM FOR SO_2 REDUCTION

3.2.2 Ceramic Filter

The ceramic filter will be installed adjacent to the existing baghouse and will be capable of filtering the entire flue gas stream. The system has been engineered such that the flue gas stream can be passed either through the baghouse or ceramic filter. The construction of the new system, which includes the chamber to house the ceramic filters, structural supports, walkways, steps and ladders, ducting, valves, induced draft fan, and associated controls, was started in September 1996. Installation of the system will be completed in November, 1996. Figures 3-2 and 3-3 are plan and side views, respectively, showing the location of the ceramic filter chamber with respect to the boilerhouse and baghouse. Figure 3-4 is a schematic diagram of the ceramic filter chamber internals showing the 80 filters, inlet baffles, and arrow baffles. Details of the ceramic filter chamber were given in the previous semiannual report[2].

The ceramic filter chamber was designed by Penn State. Comprehensive Design Architects and Engineers (CDAE), of State College, Pennsylvania, designed the structural supports, walkways, steps and ladders, ducting, valves, induced draft fan, and associated controls.

3.3 Subtask 1.3 Evaluate Emissions Reduction System

No work was conducted on this subtask.

3.4 Subtask 1.4 Conduct NO_x Emissions Study

The objectives for this subtask are as follows:

- To identify and/or develop a NO_x reduction catalyst that is compatible with the typical operating conditions and the economic constraints of industrial boilers, specifically:
    1. Flue gas temperatures of 550°F (288°C);
    2. O_2 concentrations of 3-5 vol %;
    3. H_2O concentration of 10-20 vol %;
    4. SO_2 concentrations of 500-1,000 ppm;
    5. NO concentrations of 100-500 ppm;
    6. No regeneration of sorbent/catalyst required; and
    7. Low maintenance and operating costs.
- To establish the limitations of the candidate NO_x reduction catalyst so that its implementation in pilot and demonstration-scale tests will be straightforward, for example, determining the relationship between space velocity and NO_x conversion efficiency for scale-up purposes; and
- To identify maximum allowable transients that the catalyst can be exposed to before losing effectiveness, such as swings in flue gas temperature and sulfur and unburned hydrocarbon concentrations.

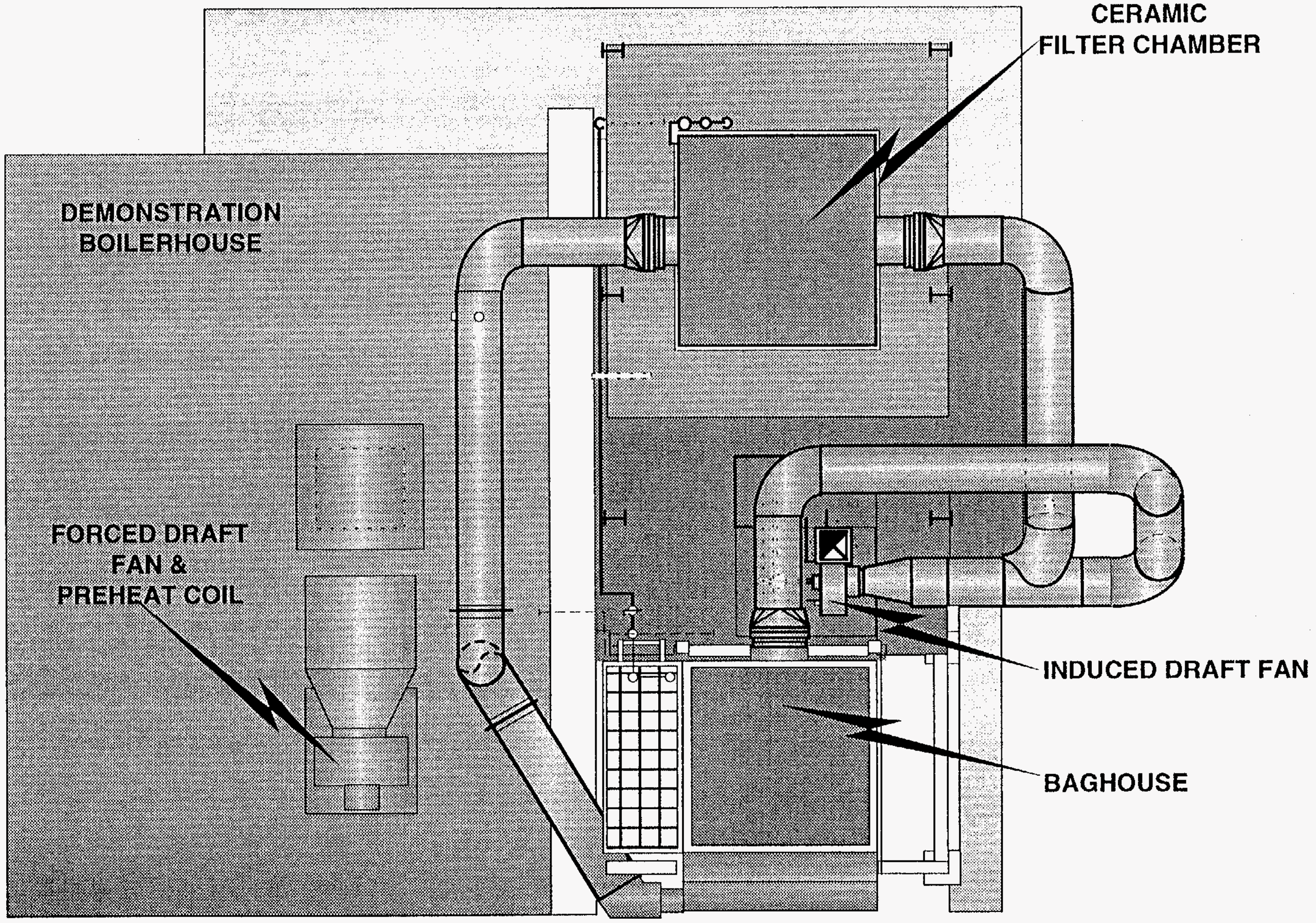


Figure 3-2. PLAN VIEW SHOWING THE LOCATION OF THE CERAMIC FILTER CHAMBER WITH RESPECT TO THE BAGHOUSE AND DEMONSTRATION BOILERHOUSE

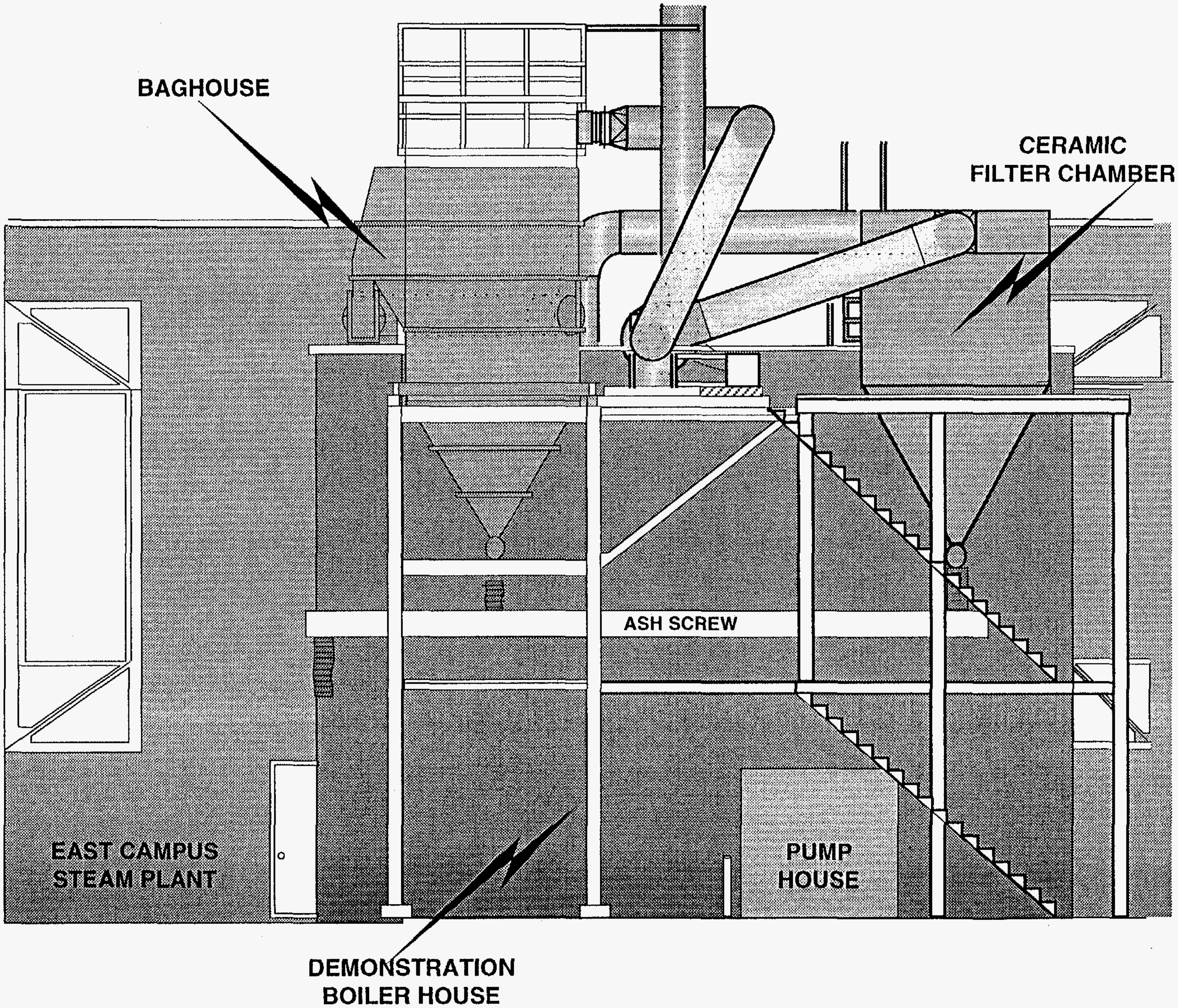


Figure 3-3. SIDE VIEW OF THE EAST CAMPUS STEAM PLANT SHOWING THE LOCATION OF THE CERAMIC FILTER CHAMBER WITH RESPECT TO THE DEMONSTRATION BOILERHOUSE AND BAGHOUSE

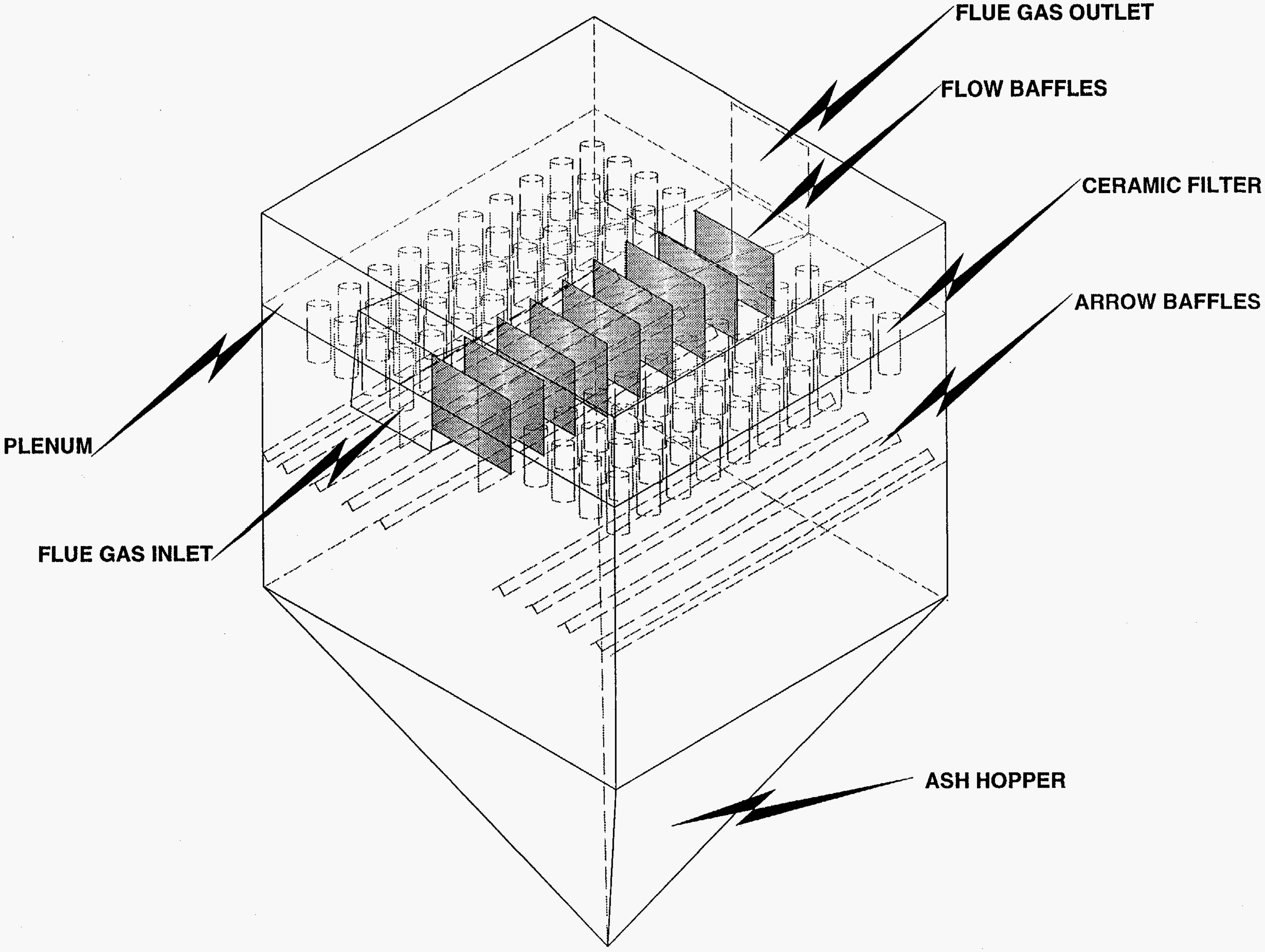


Figure 3-4. INTERIOR OF THE CERAMIC FILTER CHAMBER SHOWING BAFFLES AND FILTERS

3.4.1 Current Status of the Bench-Scale Catalyst Tests

The bench-scale testing apparatus has been operational since April, 1996. Recently, some important results have been obtained regarding catalyst selectivity and activity that may permit activity to be maximized under conditions where selectivity is optimal. These and other recent observations are summarized below.

Reactor Design

The basic design of the reactor is shown in Figure 3-5. The gases flow through mass flow controllers to a mixing manifold. The three corrosive/toxic gases pass through a solenoid valve for emergency shutdown. Water is injected close to the entrance of the furnace, and a bypass line with a four-way valve is present so that either the inlet or the outlet flow may be sent to the Fourier Transform Infra-Red (FTIR) spectrometer for quantitative gas analysis.

The reactor consists of a quartz tube 24 mm ID and 1 mm wall thickness, placed in a three zone furnace of total length 300 mm. The section of the tube enclosed by the furnace is filled with quartz beads to improve heat transfer to the gas. The catalyst bed is loaded in the section of the quartz tube where the tube emerges from the downstream end of the furnace. Monolith catalysts 25.4 mm long and ~20 mm in diameter were used. The catalyst temperature was monitored using thermocouple probes inserted at the entry, center and exit of the monolith. This configuration allows precise temperature monitoring and control of the catalyst bed.

Computer control and reading of temperatures, pressure, and gas flow rates was made possible by interfacing all measuring instruments to a pentium computer through a DAS 8- PGA (for analog inputs), an EXP-16 (Amplifier and multiplexer for thermocouple inputs) and a DDA-06 (for analog outputs as control signals for devices). All the data acquisition systems, along with the software drivers were purchased from Keithley Metrabyte. The total flow is set for a maximum of 9 L/min.

FTIR spectroscopy is used for quantitative analysis of the inlet and outlet gases. FTIR was chosen as the characterization technique because other techniques are unsuited for this particular set of requirements. Chemiluminescence detectors can measure NO_x compounds and can differentiate between NO and NO_2, but cannot identify other oxides of nitrogen, in particular N_2O. On-line flame ionization detectors measure total hydrocarbons and cannot distinguish between individual hydrocarbons. Gas-Chromatography/Mass Spectrometry (GC-MS) is relatively slow. FTIR is the only technique which, in conjunction with the 100 MHz pentium computer, can provide real-time on-line quantitative analysis. Because it is equipped with an MCT detector, it can detect in the far - infrared

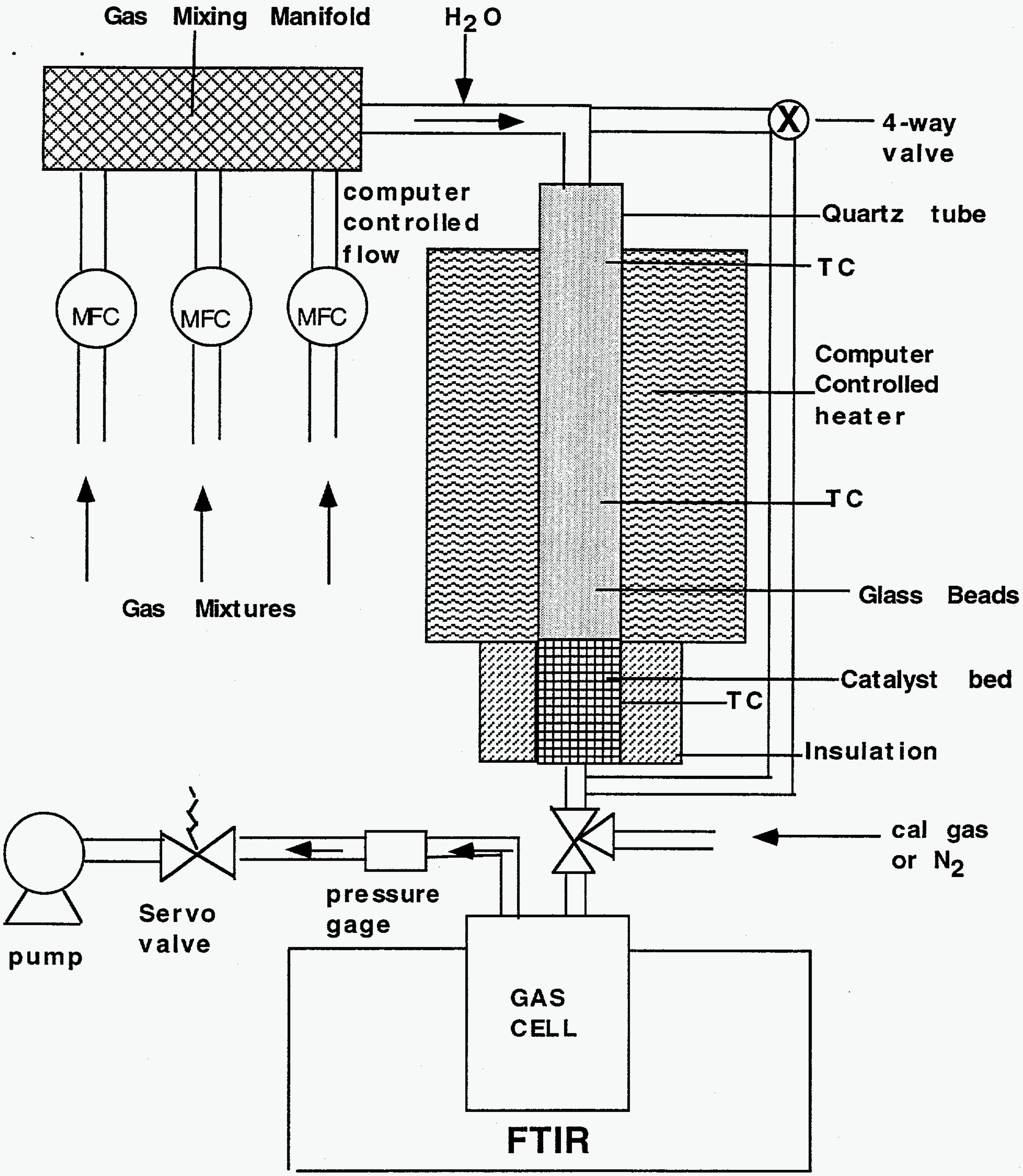


Figure 3-5. SCHEMATIC DIAGRAM OF THE BENCH-SCALE FLOW REACTOR

region as well as the near - infrared region, so there is no need to change detectors for different spectral regions. Liquid nitrogen cooling is necessary for detector operation.

Water is injected into the synthetic exhaust stream in liquid form using a syringe pump. The transfer lines are heated to prevent condensation. The 2 M gas cell is also heated by a heating blanket which has its own temperature control system. FTIR calibration, alignment, and spectrum collection is carried out using the Omnic software provided by Nicolet, and quantitative analysis is carried out using the QuantSetup and QuantPad software, also supplied by Nicolet. The rest of the data acquisition hardware is controlled by code written in Microsoft Visual Basic (Version 3), which also acts as a trigger for spectrum collection through Omnic. This language was chosen because of its excellent user interface and ease of programming.

Bench-Scale Reactor Results

To date, the studies of catalyst behavior have focused on a low temperature, precious metal-based, ammonia SCR catalyst supplied by Engelhard. No other catalyst technology currently available can provide conversion of NO on the order of 90% in the temperature range that the demonstration boiler baghouse operates (350 - 400°F). Work has focused on the influence of three primary parameters on activity and selectivity of the catalyst: (1) space velocity; (2) catalyst temperature; and (3) feedstream composition. The results from this testing is shown in Figures 3-6 through 3-9. During the course of FTIR calibration and initial catalyst testing, it was observed that substantial infrared absorption band interference severely affects the ability of the FTIR to quantify gas composition for certain species before and after the catalyst bed, particularly SO_2. This difficulty has degraded the quality of some of the measurements and consequently has added to experimental uncertainties in the results. Nonetheless, the behavior of the catalyst is made clear by the recent studies.

The results obtained thus far are for synthetic flue gas mixtures containing various amounts of CO_2, O_2, H_2O, SO_2, NO, and NH_3 in N_2. In presenting these results, two definitions are required, conversion efficiency and catalyst selectivity. Conversion efficiency represents the percentage of the incoming NO that has been converted, regardless of the product species to which it is converted. Thus, conversion in and of itself does not sufficiently represent how effective the catalyst is. Selectivity can be defined in a number of ways; for this program, the following definition has been chosen:

$$\%\ Selectivity = \frac{NO\ reacted - N_2O\ produced}{NO\ reacted} \cdot 100\% \tag{3-1}$$

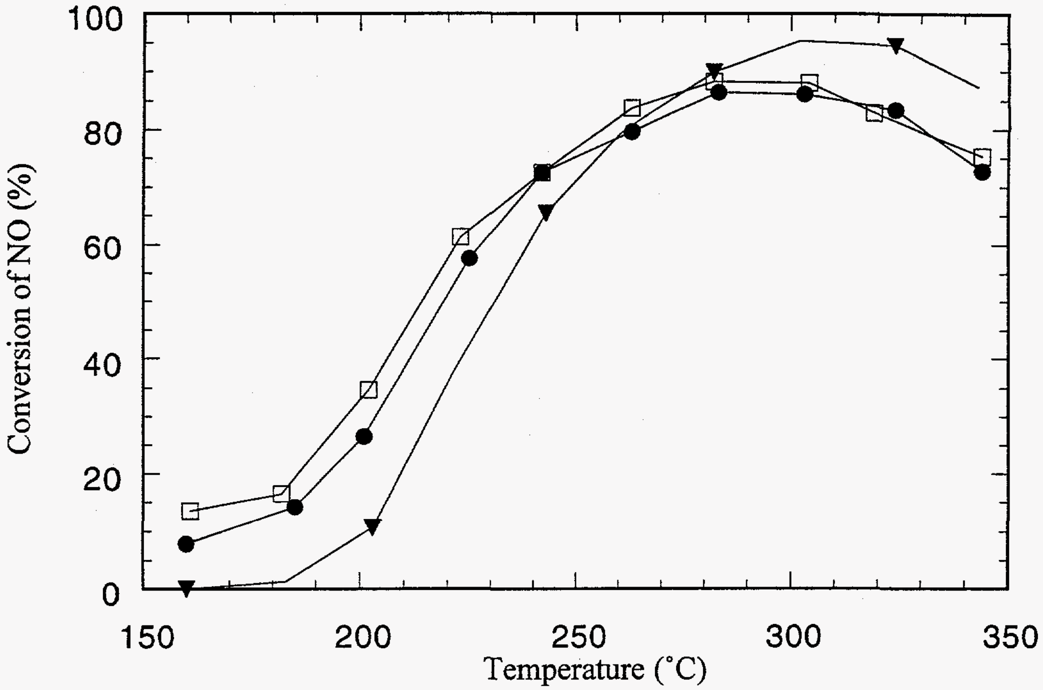


Figure 3-6. **NO CONVERSION VERSUS CATALYST TEMPERATURE FOR AMMONIA CONCENTRATIONS OF 400 (●), 500 (□) and 600 (▼) ppm at 2.5 SLM TOTAL FLOWRATE.**

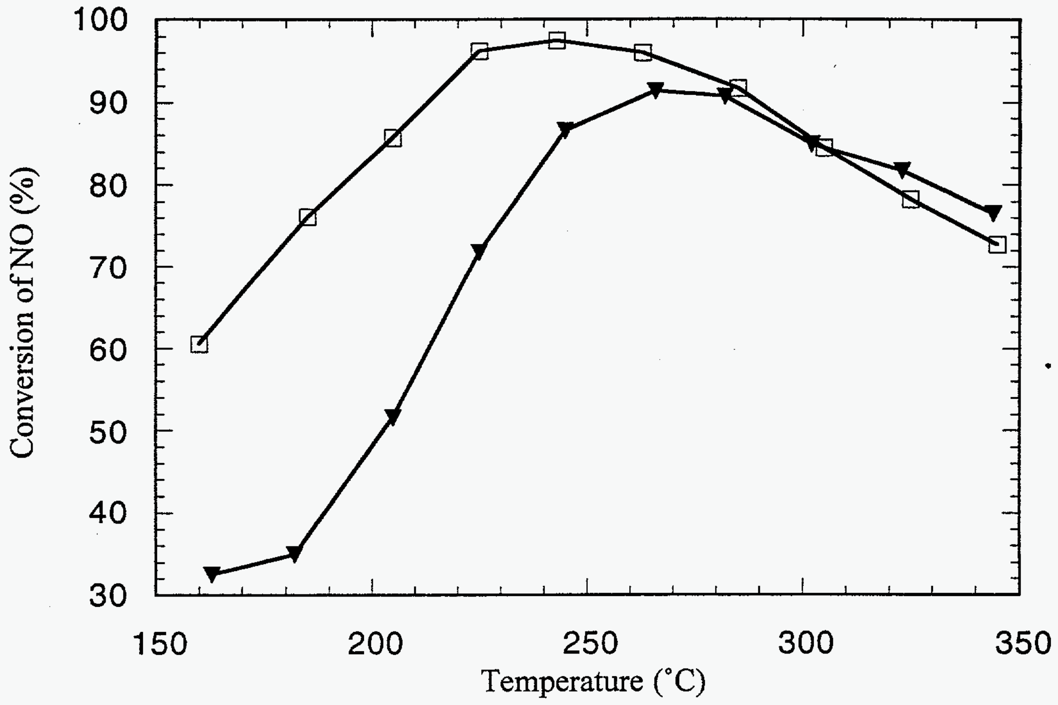


Figure 3-7. NO CONVERSION VERSUS CATALYST TEMPERATURE FOR SO_2 CONCENTRATIONS of 20 (☐) and 100 (▼) ppm at 1.25 SLM TOTAL FLOWRATE.

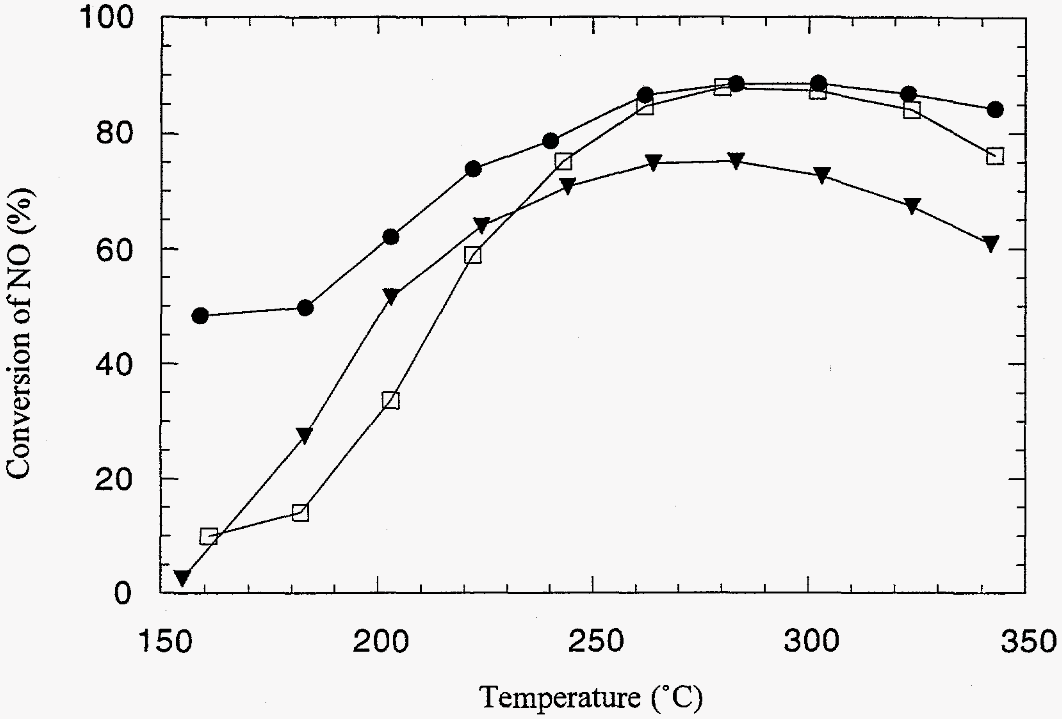


Figure 3-8. **NO CONVERSION VERSUS CATALYST TEMPERATURE FOR FLOWRATES OF 1.25 (●), 2.5 (☐) and 5.0 (▼) SLM.**

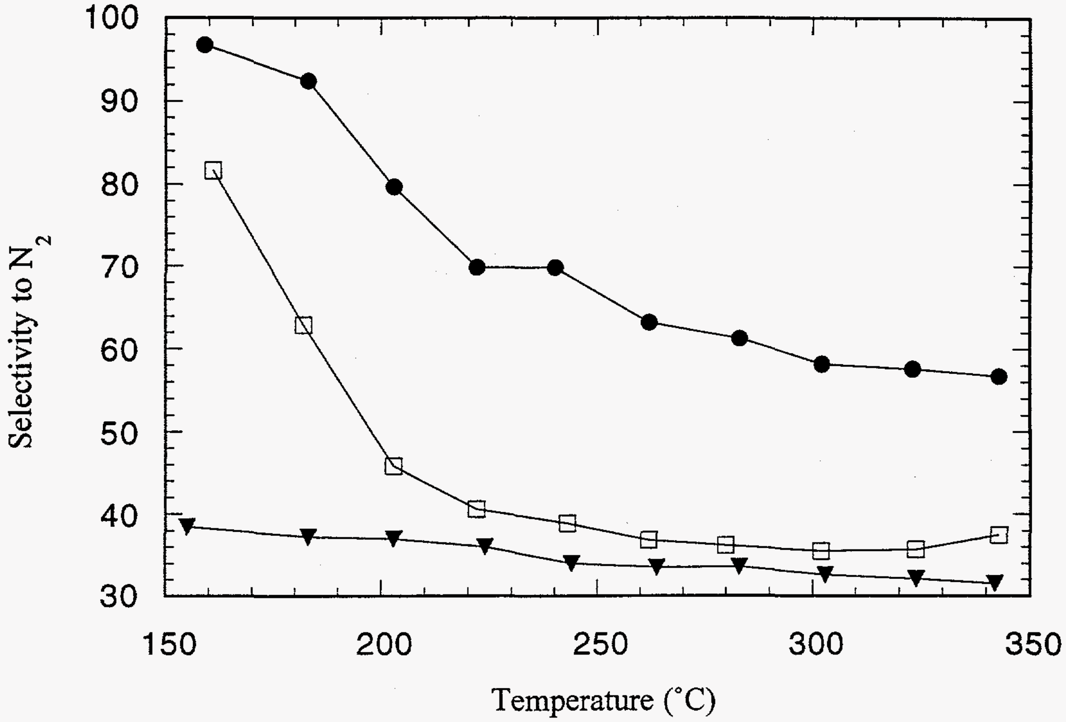


Figure 3-9. SELECTIVITY TO N_2 VERSUS CATALYST TEMPERATURE FOR FLOWRATES OF 1.25 (●), 2.5 (❑) and 5.0 (▼) SLM.

where amount of NO reacted = Initial [NO] - Final [NO]

Given these definitions, the following observations of Engelhard's catalyst can be made:

1. With modest SO_2 in the feedstream, the conversion efficiency typically reaches a maximum value of 90% at 240°C (464°F) at low space velocity;
2. Additional SO_2 in the feedstream acts to reduce the peak conversion and the conversion at lower temperatures, while not substantially affecting high temperature conversion;
3. Increased space velocity suppresses conversion and degrades selectivity to N_2; and
4. At lower temperatures (~ 160°C i.e., 320°F), conversion is low but selectivity is high. As temperature increases, the reaction pathway that produces the undesirable product, N_2O, and the NH_3 oxidation reaction become more prevalent. At an intermediate temperature, NO conversion is high but selectivity worsens as increasing amounts of N_2O are produced by the conversion process. At high temperatures, the dominant reaction pathway is the oxidation of NH_3, and any conversion of NO is hidden by the production of NO from NH_3.

Another useful description of catalyst behavior is provided by the product of the conversion of NO and the selectivity to N_2, shown in Figure 3-10. This product directly shows the conditions where both important features of catalyst performance are high. Figure 3-10 makes clear that low space velocity enhances the desirable features of the catalyst. In combination with Figures 3-8 and 3-9, a clear conclusion can be drawn about the catalyst: that lower temperatures promote the conversion pathway to N_2 and that enhancing activity in the lower temperature range could provide the optimal performance for this catalyst. Increasing the loading of precious metal on this catalyst may provide increased low temperature activity, while preserving a high selectivity to N_2.

3.5 Subtask 1.5 Conduct VOC Study

During this reporting period, a sampling train suitable for collecting samples for subsequent analysis of polycyclic aromatic hydrocarbons (PAHs) has been purchased. The sampling system can be easily modified to appropriately sample for many other species when necessary.

The targeted PAHs, listed in the previous semiannual technical progress report [2], should be found in concentrations above the detection limit obtainable with existing GC/MS techniques. PAHs have been found in detectable levels in utility boiler ash samples with carbon conversion values close to 99.9%. If PAHs are not found in detectable amounts, the chemical families containing dioxins and furans that are listed as HAPs would be a logical alternative to PAHs investigations.

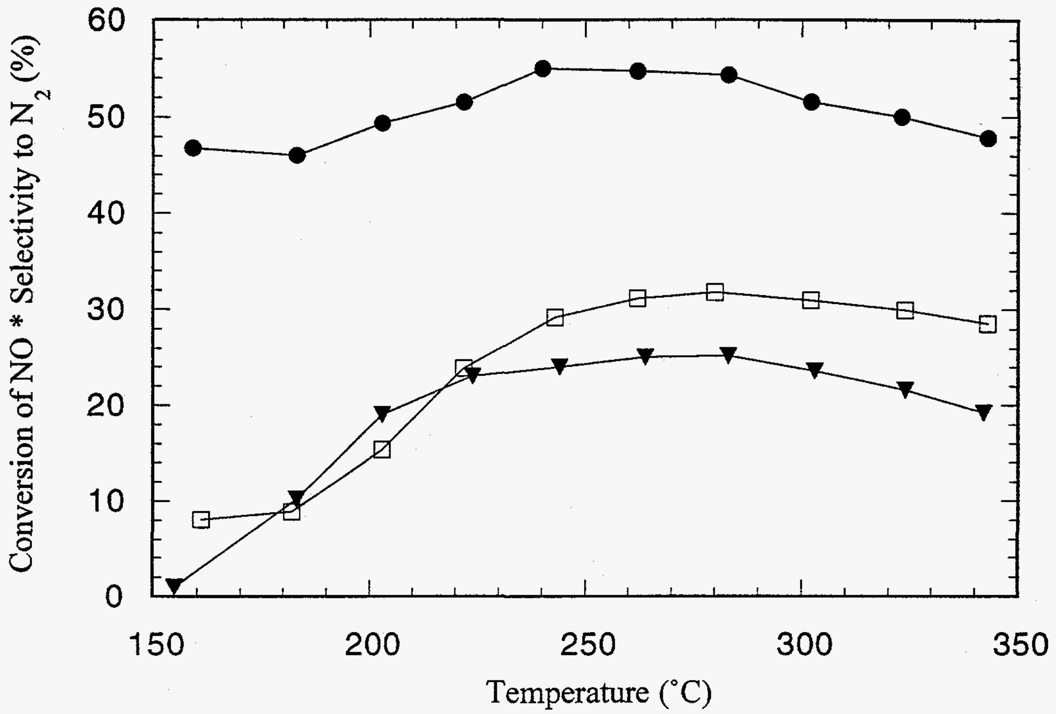


Figure 3-10. **PRODUCT OF CONVERSION OF NO AND SELECTIVITY TO N_2 VERSUS CATALYST TEMPERATURE FOR FLOWRATES OF 1.25 (●), 2.5 (☐) and 5.0 (▼) SLM.**

The sampling system consists of a glass-lined sampling probe that will be introduced into the stack or other ducting. The sample will be drawn isokinetically through a heated sample line to a quartz filter to remove the solid material. The remaining portion of the sample is drawn through a condenser, trap, and a series of chilled impingers containing solutions chosen to collect the targeted analytes. PAH sampling will be conducted in Penn State's research boiler (2 million Btu/h watertube boiler) prior to and downstream of the baghouse. Extracts from the collected materials will be concentrated and analyzed for targeted PAHs. Virgin glassware has been purchased and reserved for sole use in the PAH investigation. All chemicals purchased meet purity requirements.

3.6 Subtask 1.6 Conduct Trace Element Study

The objective of Subtask 1.6 is to characterize trace element emissions from coal-fired industrial boilers. Activities continued on this subtask during this reporting period and the activities that were conducted included working on a literature search on trace element emissions from coal-fired boilers, specifically from utility-scale boilers. In addition, the necessary sampling equipment was identified and ordered, the appropriate analytical techniques were identified, the quantity of samples to be analyzed were determined, and a laboratory was selected for analyzing the samples.

During the next reporting period, the literature review will be completed, the sampling equipment procured, and preliminary sampling will be conducted.

3.7 Subtask 1.7 Conduct Nitrogen Occurrence Study

The origin and diagenesis of fossil organic nitrogen in oil shales is still a matter of high interest. Most of the nitrogen in oil shales derives from degraded algal material, which accumulated and was chemically transformed during sediment diagenesis. It is generally believed that the organic matter of oil shales derives from the accumulation of the refractory biopolymers of algae (algaenan). In order to understand the diagenetic processes involved in the formation of fossil organic material of oil shales, algaenans of Scenedesmus and Botryococcus braunii were examined by means of 13C and 15N NMR Spectroscopy. Their NMR spectra were compared to those obtained from an algal sapropel (Mangrove Lake, Bermuda) different Torbanites and Green River shale. It was shown that aliphatic structures became enriched with increasing maturation of the sediments. The nitrogen in the algaenans and the sapropel of Mangrove Lake occurred mostly as amide functional groups. This result shows that some of the amide functional groups can survive not only sediment diagenesis, but also chemical degradation. TMAH/thermochemolysis on the algaenan of Scenedesmus and a 6N HCl hydrolyzed sediment revealed that at least some of the amide functional groups can be assigned to proteinaceous material, which may survive chemical and biological degradation by encapsulation into the macromolecular network of the refractory biopolymer.

With increasing maturation, a shift in N-functionality can be observed. The 15N NMR spectra of Torbanites and Green River shale reveal that most of the nitrogen occurs in form of pyrolic-N. Minor amounts were identified as pyridinic-N. This transformation may be due to the selective enrichment of heterocyclic structures during prolonged sediment diagenesis, but can also be explained by heat and pressure induced chemical rearrangements of proteinaceous structures (i.e., cyclization of peptides).

The chemical changes in N-functionality during combustion is examined by means of 13C and 15N NMR Spectroscopy of chars produced as a function of retention time in a combustion chamber. While the samples with short retention times could be analyzed by NMR spectroscopy, samples obtained after longer retention times showed an increase in magnetic susceptibility. This, however leads to detuning of the NMR probe and can cause major overheating of the probe. Methods have to be found to remove magnetic material from the samples, such as treatment with HF.

The preliminary results show that pyrolic-N decreases with increasing retention time, while indolic-N, carbazolic-N and pyridinic-N increases.

4.0 PHASE II, TASK 2: COAL PREPARATION/UTILIZATION

Activities in Phase II, Task 2 primarily focused on preparing the final report and initiating a study with Carnegie Mellon University to study the fundamental behavior of atomization. Results of the study are presented in Section 4.1.

4.1 Subtask 2.10 Conduct Atomization Study

The objective of this subtask is to determine the effect of MCWM stability additives (e.g., Flocon 4800 C) on the MCWM rheology, atomization characteristics, and combustion behavior. A subcontract was issued to Carnegie Mellon University (CMU) for the MCWM rheology characterization and atomization work.

A set of six samples, shown below, was sent to CMU for preliminary measurements of apparent and extensional viscosity. After the preliminary measurements are conducted, larger quantity will be prepared by Penn State and divided into two groups. One group will be shipped to CMU for the atomization characterization and another group will be fired in a down-fired combustor at Penn State to characterize combustion behavior. The test matrix for the laboratory-scale testing is currently being finalized.

5.0 PHASE II, TASK 3 ENGINEERING DESIGN AND COST; AND ECONOMIC ANALYSIS

Phase II, Task 3 has been completed except for Subtasks 3.6, regional economic impacts and 3.10, integration of analysis. Activities in Phase II, Task 3 focused on working on Subtask 3.6 and preparing the final report for the remainder of the subtasks.

5.1 Subtask 3.6 Determination of Regional Economic Impacts

Activities in Subtask 3.6 included applying a Pennsylvania Computable General Equilibrium Model to the widespread adoption of new coal-fired technologies in industrial boilers. Problems were encountered in applying the model given the numerous parameter changes involved.

5.2 Subtask 3.10 Integration of Analyses

No work was performed on this subtask during this reporting period.

6.0 PHASE II, TASK 4 FINAL REPORT/SUBMISSION OF DESIGN PACKAGE

Work in preparing the final report continued. Tasks 2 (except for Subtask 2.10) and 3 (except for Subtask 3.10) have been completed.

7.0 PHASE III, TASK 1 COAL PREPARATION/UTILIZATION

7.1 Subtask 1.1 Particle Size Control

7.1.1 Attrition Milling

Further analysis of coarse particle abrasion in attrition milling of coal is in progress. In a previous report[2], a simplified model based on an assumed linear wear rate was presented. This model was found to over-predict the size-reduction process, especially after relatively long grinding times. Studies of the abrasion of individual rock particles in conventional autogenous grinding[3] have indicated that a first-order abrasion law, referred to as the Davis wear law[4] may be more appropriate than the constant rate assumed previously. The Davis law can be expressed as

$$\frac{dx}{dt} = -kx \tag{7-1}$$

where x is the equivalent-sphere particle diameter and k is a first-order rate constant. Tangsripongkul demonstrated that the Davis law was applicable to particles of different initial size, but that the rate "constant" k was, in fact, a function of grinding time. Specifically, k was found to decrease with time according to:

$$k = k_f + (k_o - k_f)e^{-at} \tag{7-2}$$

where k_o is the initial rate, k_f is the final, long-time rate, and a is a decay-rate constant. This form for the abrasion rate factor is consistent with rapid abrasion of initially highly irregular particles followed by a slowing down of the process as the particles become increasingly rounded.

Application of the modified abrasion rate law to attrition milling of coal is currently in progress.

7.1.2 Closed-Circuit Dry Grinding

Product size distributions from fine, dry grinding of coal in an opposed-jet fluid-energy mill (Majac Mini-Grinder) operated in closed circuit with a Donaldson Acucut classifier have been obtained. Size selectivity data for the same coals in the same classifier have also been acquired. Unfortunately, because of the extremely short residence time in the fluid energy mill (< 1 sec) it is not possible to determine breakage characteristics directly. A search procedure is being developed, based on circuit simulation, which can be used for back-estimation of breakage characteristics from known (circuit) product size distributions and classifier selectivity. Such estimates can be used to predict circuit performance for different operating conditions and classifier settings. Ultimately they can form the basis of design and operation of dry, fine-grinding systems.

7.2 Subtask 1.2 Physical Separations

7.2.1 Fine Coal Classification

The baseline testing of the continuous, solid-bowl centrifuge for size separation of fine coal continued. The test variables included bowl and scroll speeds. Minus 100 mesh Upper Freeport seam coal was used for all tests. The unit was operated at a constant volumetric slurry feed rate of 11.4 L/m (3 gpm) and a solids concentration of 10% coal (by weight). For these tests, the minimum weir setting was used, which gave the shallowest pond depth. Table 7-1 summarizes the operating conditions for this series of tests.

For each test, simultaneous samples of the weir overflow (fine product) and scroll discharge (coarse product) were taken. Each sample was analyzed using a Microtrac X-100 particle size analyzer. Figure 7-1 shows the reconstituted feed (discussed below) and product size distribution curves for centrifuge tests 1 and 2. As can be seen, the product size distribution of the fine stream for test 2 was finer than that of test 1. For example, 85.8% of the material in the fine stream was less than 11 μm for test 2 compared to 53.2% for test 1.

Table 7-1. Summary of the Operating Conditions and Test Results for the Solid-Bowl Centrifuge (feed rate = 11.4 L/min, minimum weir height (shallowest pool), solids concentration = 10% by weight).

			Yield, %		Characteristic Parameters		
Test	Main Speed, rpm	Back Drive, rpm	Coarse Product	Fine Product	d_{50}, µm	k	a
1	4600	4125	77.4	22.6	18.9	0.36	0.23
2	4600	3650	91.0	9.0	8.1	0.47	0.28
3	4600	2700	92.1	7.9	4.4	0.35	0.21
4	4600	800	88.9	11.1	6.4	0.44	0.00
5	3750	1850	88.9	11.1	7.7	0.56	0.14

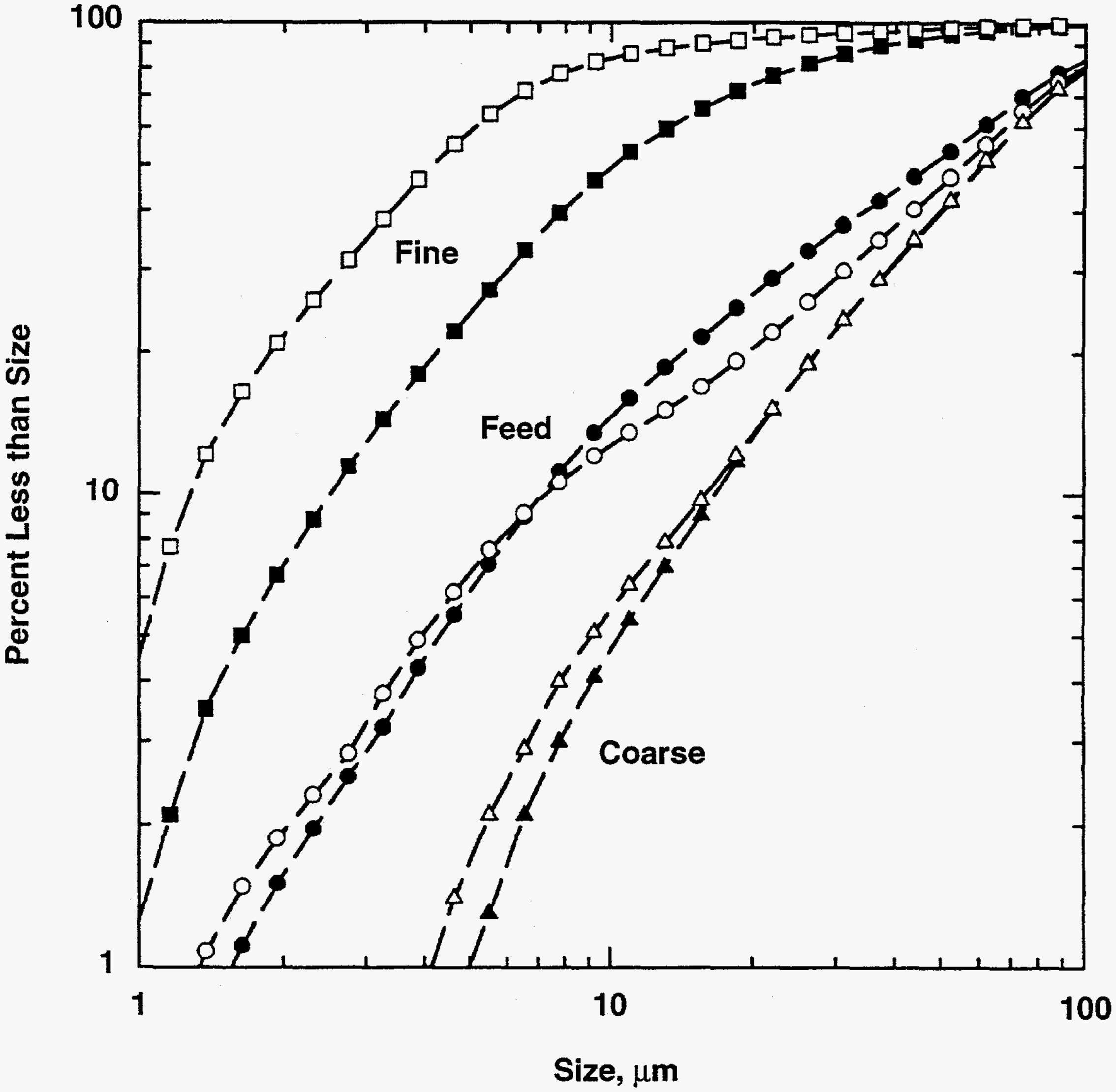


Figure 7-1. FEED AND PRODUCT SIZE DISTRIBUTIONS FOR CENTRIFUGE TESTS 1 AND 2 WHEN SEPARATING -100 MESH UPPER FREEPORT SEAM COAL
(test 1: filled symbols, test 2: open symbols)

From the size distribution data, it was possible to estimate the circulation ratio, which is defined as the solids mass flow rate of the coarse stream, T, divided by the solids mass flow rate of the fine stream, Q, by

$$C = \frac{\sum_i |p_i - q_i|}{\sum_i |t_i - p_i|} \qquad (7\text{-}3)$$

where p_i, t_i, and q_i are the fractions of material in size interval i for the feed, coarse, and fine streams, respectively. The circulation ratio is related to the yield to the fine stream, Y_Q, by

$$Y_Q = \frac{1}{1 + C} \qquad (7\text{-}4)$$

The yield to the coarse stream, Y_T, is then simply $Y_T=1-Y_Q$.

Knowing the product size distributions and the circulation ratio, the size selectivity values were calculated by

$$s_i = \frac{t_i T}{p_i' P} = \frac{t_i C}{p_i'(1 + C)} \qquad (7\text{-}5)$$

where P is the solids mass flow rate of the feed stream, and p_i' is the reconstituted feed for size interval i given by

$$p_i' = \frac{q_i + t_i C}{1 + C} \qquad (7\text{-}6)$$

The size selectivity values are related to the classification values by

$$s_i = (1 - a)c_i + a \qquad (7\text{-}7)$$

where c_i is the classification value for size interval i, i.e., corrected for apparent bypass, *a*. In order to determine the characteristic performance parameters -- the cut size, d_{50}, the sharpness index, k, and the apparent bypass, *a* -- the classification values were fitted to the log-logistic function given by

$$c_i = \frac{1}{1+\left(\frac{x_i}{d_{50}}\right)^{-\lambda}} \tag{7-8}$$

where k = exp[-2.1972/l]. The d_{50} value is the size that corresponds to c_i=0.5, and k=d_{25}/d_{75}, where d_{25} and d_{75} are the sizes that correspond to c_i values of 0.25 and 0.75, respectively. The sharpness index varies from zero for no separation to one for a perfect separation. The parameters d_{50}, k, and *a* were determined using a nonlinear optimization package. These results are also included in Table 7-1. Figure 7-2 shows the size selectivity values and fitted curves obtained for tests 1-4. Testing of the solid-bowl centrifuge is continuing.

7.3 Subtask 1.3 Surface-Based Separation Processes

7.3.1 Evaluation of Continuous Flotation Tests

The results of continuous flotation tests differed substantially from the batch flotation tests. To determine the reasons for the observed differences, the tests were analyzed using a first-order kinetics model. For this purpose, the flotation products were fractionated into several size fractions and the data were used to estimate the flotation rate constants. Large differences were observed between the flotation rates obtained from batch and continuous flotation tests. The results show that a relatively large proportion of coarse particles were lost in the continuous flotation circuit. To resolve the differences and to determine the reasons for differences in the coal recovery, another series of batch flotation tests were performed in which froth was allowed to overflow the weir. The objective of these tests was to determine the role of manual froth removal versus continuous froth overflow on the flotation response. These tests have been completed and the results are being analyzed.

7.4 Subtask 1.4 Dry Processing

7.4.1 Continuous Separation

Baseline testing of the continuous rotating plate separator continued. As discussed in a previous report, this device consisted of 2 parallel plates, 600 mm in diameter, which were spaced 100 mm apart. The plates were rotated at approximately 5 rpm and scraped continuously to facilitate product removal. The operating voltage was limited to approximately ±15 kV to minimize the potential for arcing between the plates. Separate tests were carried out using the Indiana, Pittsburgh, and Upper Freeport seam coals. The feed coal was a nominal -100 mesh, which was obtained by stage crushing in a disk

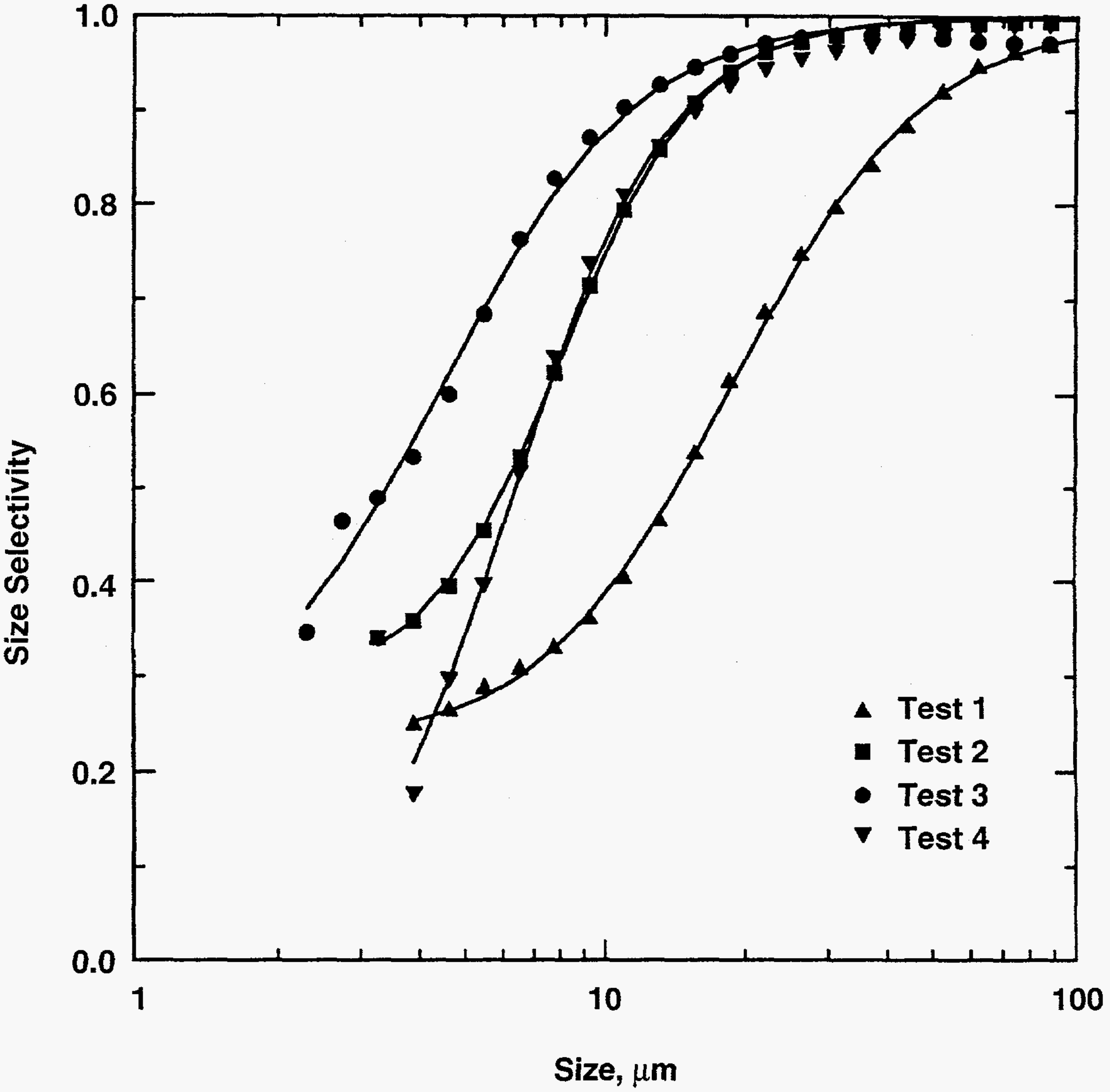


Figure 7-2. EFFECT OF BACK DRIVE SPEED ON THE SIZE SELECTIVITY CURVES IN THE SOLID-BOWL CENTRIFUGE

pulverizer and a Holmes pulverizer. The Holmes pulverizer was the same as that used to integrate the grinding and batch electrostatic separation process, as discussed in the previous report. However, in this case, the -100 mesh coal was prepared separately and stored under argon in aluminum laminated bags.

The coal was dried at approximately 105°C for two hours prior to separation. This material was then fed by a vibrating feeder into a venturi feeder and then passed through the in-line copper mixer (tribocharger) prior to electrostatic separation. Compressed nitrogen was used as the transport medium. Several hundred grams of coal were passed through the separator for a given test. Upon completion of the test, the coal and refuse were recovered from the plates, collecting troughs, and cyclones. The samples were weighed and analyzed for ash content.

Tables 7-2 to 7-4 give the weight distribution and ash values for the material collected from various parts of the separator and collection system. Ideally, the bulk of the solids would be carried into the cyclone for collection in the cyclone underflow stream. As noted in a previous report, some material will remain on the plates. For this unit, it was not possible or necessary to scrape all the material from the rotating plates after each revolution, and generally a thin layer of solids remained on each plate. This buildup had a minimal effect on the collecting ability of the plates. Furthermore, the material remaining on the plates can actually benefit the process by reducing the wear on the plates, because the scraper would not contact the plates directly.

In addition to the solids on the plates, some material settled in the airways leading to the collection cyclones. However, since any material in the airways was in the proper product stream, it could be collected and included with the appropriate product. For a long time run in continuous operation, it is likely that a steady state would be reached such that a constant amount of material would build up on the plates and throughout the collection system, allowing a steady amount of product to be collected.

As seen in Table 7-2 for the Indiana seam coal, the ash content was reduced from 9.1% in the feed to 5.0% in the clean coal at a yield of 59%. The corresponding ash content of the refuse was 15.0%. This middling material would be a candidate for regrinding followed by reprocessing to recover additional low-ash coal. In the case of the Pittsburgh seam coal (Table 7-3), a clean coal with an ash content of 3.7% was obtained at a yield of 68.5%, with a refuse ash content of 13.4%. For the Upper Freeport seam coal (Table 7-4), the ash content was reduced from 11.2% to 5.6% at a yield of 64.3%. The corresponding ash content of the refuse material was 21.4%.

In all cases, the lowest ash material was found on the negative (clean coal) collecting plate and represented over 50% of the total clean coal in some cases. Similarly,

Table 7-2. Results from the Continuous Electrostatic Separator when Processing -100 Mesh Indiana Seam Coal (calculated feed ash = 9.1%, measured feed ash = 9.2%).

	Clean Coal		Refuse	
Product	Wt., %	Ash, %	Wt., %	Ash, %
Electrode (Plate)	20.4	3.1	11.2	22.4
Collecting Trough	12.3	5.4	6.7	16.9
Cyclone	26.3	6.2	23.2	10.8
Total	59.0	5.0	41.0	15.0

Table 7-3. Results from the Continuous Electrostatic Separator when Processing -100 Mesh Pittsburgh Seam Coal (calculated feed ash = 6.8%, measured feed ash = 6.7%).

	Clean Coal		Refuse	
Product	Wt., %	Ash, %	Wt., %	Ash, %
Electrode (Plate)	35.2	2.0	18.2	13.9
Collecting Trough	12.1	5.3	12.9	12.9
Cyclone	21.2	5.6	0.4	9.1
Total	68.5	3.7	31.5	13.4

Table 7-4 Results from the Continuous Electrostatic Separator when Processing -100 Mesh Upper Freeport Seam Coal (calculated feed ash = 11.2%, measured feed ash = 11.3%).

	Clean Coal		Refuse	
Product	Wt., %	Ash, %	Wt., %	Ash, %
Electrode (Plate)	37.7	3.5	19.8	21.1
Collecting Trough	11.0	9.4	14.4	22.3
Cyclone	15.6	8.0	1.5	17.7
Total	64.3	5.6	35.7	21.4

the highest ash content material was typically found on the positive (refuse) collecting plate and also represented a significant portion of the respective product. Even though the splits among the plate, collecting trough, and cyclone would change depending on the total quantity of coal being fed to the unit, the overall yield and product quality should remain constant.

Some of the material for each product passed through the cyclone overflow and into the sweeper and could not be recovered. This represented between 10 and 20% of the total amount of coal that was fed to the separator. However, based of the comparison of the calculated and measured ash contents of the feed coal, it is likely that the losses were distributed in the same proportions as the product yields. Hence, the overall results would not be affected.

7.4.2 Integrated Grinding/Separation Circuit

Preliminary testing of an integrated grinding/separator circuit continued. The Holmes high-speed pulverizer was used for size reduction in combination with the continuous triboelectrostatic separator. The Holmes pulverizer was the same device used to prepare the -100 mesh coal, which was used in the previous triboelectrostatic separation tests. However, in the previous tests, the pulverized coal was stored under argon for up to several weeks prior to tribocharging and separation. For these tests, the coal was used immediately after size reduction.

Nominal -28 mesh coal was fed to the pulverizer. As the coal passed through the device, it was pulverized to approximately -100 mesh by rotating steel hammers. Contact with the hammers and the discharge screen provided the opportunity for tribocharging the coal. The pulverized coal fell into a collection funnel, which was lined with copper, and was directed into the venturi feeder of the rotating plate electrostatic separator, which had the in-line tribocharger removed. Nitrogen was again used as the transport medium. Testing of this unit is continuing.

7.5 Subtask 1.5 Stabilization of Coal-Water Mixtures

Subtask 1.5 was previously completed.

8.0 PHASE III, TASK 2 EMISSIONS REDUCTION

No work was conducted in Task 2 during this reporting period.

9.0 PHASE III, TASK 3 ECONOMIC ANALYSIS

9.1 Subtask 3.1 Cost and Market Penetration of Coal-Based Fuel Technologies

Subtask 3.1 was previously completed.

9.2 Subtask 3.2 Selection of Incentives for Commercialization of the Coal Using Technology

Subtask 3.2 was previously completed.

9.3 Subtask 3.3 Community Sensitivity to Coal Fuel Usage

Activities in this subtask focused on developing methods that integrate economic valuation with the techniques used in psychology to characterize risk perceptions to value the welfare impacts due to the presence of energy production facilities. A contingent valuation survey, designed with cognitive survey design methods, was administered to elicit quantitative information regarding individuals' perceptions of the risks associated with fossil fuel-based electric power facilities and the individuals' willingness to pay to prevent or change risk exposure levels. The quantitative measures of risk perceptions are related to the willingness to pay values using maximum likelihood estimation.

The underlying conceptual rationale for valuing changes in perceived risk combines findings from the risk perception literature with expected utility theory. Using an economic model of individual willingness to pay to avoid risks, this study identifies factors that contribute to individual willingness to prevent energy production facilities. Specific focus is placed on developing quantitative measures of perceived risk that can be utilized to derive welfare changes induced by such facilities.

An individual's *ex ante* marginal willingness to pay to prevent or change their (perceived) risk exposure level from an electric power facility, determined, in part, by the perceived risk attributes is measured. Obtaining the value of individual preferences of risk levels can assist in facility siting decisions by measuring how much individuals will pay to influence decisions or to what extent they will willingly bear the costs of a more expensive, but more desirable fuel.

9.4 Subtask 3.4 Regional/National Economic Impacts of New Coal Utilization Technologies

Subtask 3.4 was completed during this reporting period. Following is the final material prepared for this subtask which focused on estimating the effects of CO_2 emissions on the U.S. economy and its energy sectors.

9.4.1 Introduction

Energy conservation is almost universally considered a prime strategy for mitigating greenhouse gases. At present, for example, 97.9% of the CO_2 emitted from industrial countries, and 70.6% emitted from developing countries, stems from fossil fuel combustion[5]. Of course, this anthropogenic emission is only a small fraction of the carbon exchange between the atmosphere and terrestrial ecosystems. While a small change in this transfer could have a major effect on atmospheric CO_2 concentrations, it is not clear that there have been any discernible movements in this regard. Moreover, efforts to alter atmospheric concentrations through climate engineering are still only on the drawing board. With any potential major shift to renewables many years away, outright reduction in the utilization of coal, oil, and natural gas is an obvious strategy. It appears even more appealing when one considers that a good deal of conservation can be attained at a cost-savings when less energy is used outright, or at a zero net cost when, for example, energy-saving equipment must be installed. These factors have led to energy conservation being placed in the category of "no regrets" strategies, which refers to measures that do not incur added costs even if projected warming trends are not forthcoming (see, e.g., Cline, 1992[6]).

Clearly, production cost-savings and preservation of energy resources are pluses. However, to date, very few studies have focused on the potential down-side. For example, there are jobs and profits at stake in the energy industries. Moreover, declines in fossil fuel sectors will lead to declines in output in successive rounds of upstream suppliers (e.g., mining equipment, fuel service companies), as well as some downstream customers (e.g., railroads, electric utilities). It is not clear whether these negative effects will be offset by the increased efficiency of the economy, various factor substitutions, purchasing power improvements for consumers, or any multiplier effects stemming from increased production of energy-saving equipment.

The purpose of this review is to estimate the effects on the U.S. economy and its energy sectors of conservation strategies to reduce CO_2 emissions. The analysis is undertaken with a 20-sector computable general equilibrium (CGE) model by simulating various responses to command and control, carbon tax, and carbon emission permit policies.

The results indicate that the characterization of energy conservation as a "no regrets" strategy is too strong. In all of the simulations, energy sectors stand to lose, though, in some cases, not anywhere near as much as would be expected. Each of the simulations of mandated conservation also leads to a decline in output and employment for the U.S. economy. In contrast some of the price-induced conservation response strategies also simulated have a neutral impact on the overall economy.

This review is divided into five sections. In the following section, basic features of the conservation strategy and some overlooked issues are discussed. Then the model used in the simulations is summarized. Next, basic results are presented, as well as some sensitivity tests. The review is concluded with a summary and a discussion of policy implications.

9.4.2 Basic Features of the Conservation Strategy

Many proposals have been put forth to combat potential global warming. One that has received considerable attention calls for a 20% reduction in current greenhouse gas (GHG) emission levels for industrialized countries and a stabilization of developing country emissions at current levels. Several policy instruments are available to implement this reduction, the carbon tax being the most widely supported and most thoroughly analyzed (see, e.g., Manne and Richels, 1991[7]; Nordhaus, 1993[8]). In the U.S., however, strong support exists for a marketable permits approach (see, e.g., Task Force, 1991[9]).

Actually, the conservation response to a carbon tax and a marketable permit system can be modeled in the same manner. First, the optimal carbon tax rate would be equivalent to the equilibrium permit price (see, e.g., Weitzman, 1974[10]; Pezzey, 1992[11]). Second, the two instruments would result in the same efficient response, in which each polluter equates its marginal cost of abatement to the tax rate or permit price. Third, even though polluters must pay for each unit of GHG emissions under a tax regime, but these emissions are usually free (entitlements) under a permit system, this does not affect the response in the short-run. That is, the tax payments or permit revenues/expenditures affect a firm's average cost but not its marginal cost and thus only bear upon long-run considerations such as exit and entry. Moreover, these conclusions pertain to the application of these instruments at both the international level in relation to total GHG reductions and within national boundaries.

In a recent study, Rose and Stevens[12] estimated an equilibrium permit price of $38.35 that would be associated with an agreement to limit *global* CO_2 emissions at 20% below year 2000 levels. The 20% reduction stems from an oft-espoused policy pronouncement that would contribute to the stabilization of CO_2 concentrations. Emissions for the year 2000 are projected based on population and economic growth factors. The year 2000 was chosen as a base rather than, for example, 1990, since the former is likely to be closer in time to when an agreement on CO_2 mitigation might actually be reached. The optimal response of the U.S. to this price is a reduction of 12.8% of baseline emissions. Moreover, given the uniqueness of the outcome of the Coase Theorem, this abatement level is not sensitive to how the permits are initially distributed across countries. Also, internally within the U.S., there would be a unique optimal response, though, given differences in marginal abatement costs, control levels would vary across polluters (e.g., economic sectors).

The various tactics that can be applied to the mitigation of CO_2 are depicted in Figure 9-1, utilizing a step function to highlight their usual relative marginal cost positions. The

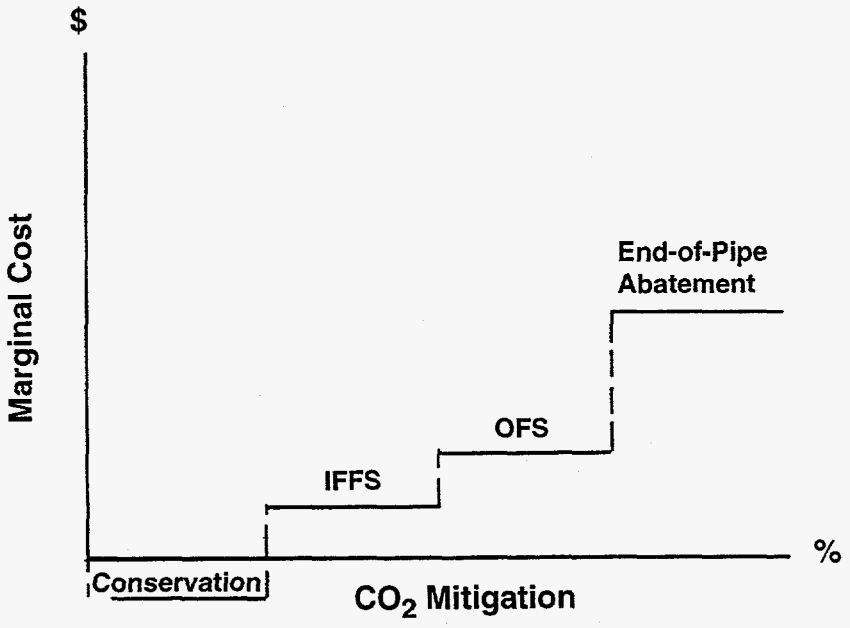


Figure 9-1. CO_2 COST FUNCTION

first step of the cost function refers to *no regrets* (costless or even cost-saving) conservation. This could stem from either a technological innovation or a move toward the efficiency frontier as a result of correcting a misallocation (e.g., eliminating energy-wasting practices). There is considerable disagreement in the literature about the extent of conservation potential. Manne and Richels[7] refer to it as *autonomous energy efficiency improvement* (AEEI), which they estimate to be on the order of 0.5% to 1.0% per year. More optimistic estimates of costless conservation—in the range of 20% to 30% total for the near term— are offered by OTA[13], NAS[13], Lovins and Lovins[14], and Jaccard et al.[15]. This holds open the possibility that the optimal U.S. CO_2 emission reduction could be met entirely by this tactic.

Another major form of conservation is *price-induced*, e.g., decreasing energy use in response to a change in the price of energy relative to the price of other inputs, as would be caused by a carbon tax or permit regime. There are several types of input substitutions that could take place and we categorize them under the headings below following Cline[6]:

OFS—Other factor substitution
IFFS—Inter-fossil fuel substitution
NFFS—Non-fossil fuel substitution
PMS—Product mix substitution

Thus, if the tax is based on carbon content of fuels, there are optimal substitution responses within the class of fossil fuels (coal emits approximately 1.26 times as much carbon per unit as oil and 1.86 times as much as natural gas) and between the class of fossil fuels and other sources (e.g., nuclear, hydro, solar). All of these responses incur some costs unless the elasticity of substitution is infinite.

The final category of mitigation tactics shown in Figure 9-1, though limited in the near-term, is "end-of-pipe" abatement, such as CO_2 scrubbers. Of course other measures, such as climate engineering and carbon absorption through tree planting, might be used but are beyond the scope of this paper.

The discussion above pertains only to a first set of adjustments for any decision-maker. If the price of energy inputs decreases because of improved efficiency, ironically energy then becomes more attractive, and there will be some offsetting increase through substitution of energy for other inputs. There is also the question of whether cost-savings will be passed along to industrial and/or final consumers or whether they will increase the returns to labor and/or capital. Similar possibilities arise with respect to responses that incur positive costs, though in terms of price increases and decreases in profits and wages.

The presentation thus far has been limited to partial equilibrium analysis, but a host of general equilibrium effects could potentially further enhance or offset these effects. First, if energy conservation savings are passed on to other industrial customers, there would be the possibility of further rounds of price reductions. This could potentially change the mix of material inputs in favor of those that are energy-intensive. The overall price reduction would increase the purchasing power of consumers and provide a stimulus to the entire economy. This would also take place, but to a different degree, if price decreases were foregone in favor of increasing wages or profits.

At the same time, the reduction in energy use would lower production levels in the coal, oil, gas, refined petroleum, and electric and gas utility industries. This will touch off a chain of negative multiplier effects to upstream suppliers, such as mining equipment, field service, and finance industries, as well as downstream customers, such as railroads, pipeline companies, and electric utilities. These negative impacts would be reinforced by declines in wages and profits in all of these sectors as well. Interestingly, all of these negative effects engender additional energy conservation, though through reduction in economic growth rather than an improvement in energy efficiency. On the positive side, the resources released from the energy industries would stimulate economic activity elsewhere, though it is unlikely that they would be fully employed. Also, any increased demand for energy-saving equipment will have positive multiplier effects analogous to those mentioned in the previous paragraph. At the same time, this increased economic activity will result in increased energy use, partially offsetting conservation efforts.

Obviously, there are a sizable number of expansionary and contractionary influences. It is impossible to ascertain the net outcome a priori, and hence the need for empirical analysis based on a general equilibrium model.

9.4.3 The U.S. CGE Model

An updated version of a 20-sector CGE model developed by Lin[16] similar in nature to most SAM-based CGE models (see, e.g., Dervis et al., 1982[17]; Shoven and Whalley, 1992[18]) was utilized. A brief summary of the model is presented. Domestic producers, being profit-maximizers, produce goods and services using two primary factors, labor and capital, and intermediate goods as inputs. Intermediate goods are either produced domestically or imported, and are assumed to be qualitatively different (the Armington assumption). The utilization of inputs follows a two-stage decision process, and intermediate goods are modeled as a nested function of aggregates and components. Specifically, the energy aggregate consists of individual fuels (both primary and secondary energy), while the materials aggregate consists of goods such as plastics, glass, metals, etc., and the remaining input aggregate consists of all other intermediate goods. Inter-fuel and inter-material substitutions are allowed within their respective aggregates, which is a feature that is fundamentally required in evaluating environmental quality regulations (see, e.g., Hazilla and Kopp, 1990[19]). The two-stage decision involves finding the optimum combination of components within energy and material aggregates, and then optimizing the levels of capital, labor, energy, and materials.

To take account of inter-fuel and inter-material substitution and substitution among aggregates, flexible functional form cost functions are used to represent the technology of production sectors and it is assumed that these functions are homothetically weakly separable. The relationships between aggregates, and within the energy and material aggregates with flexible functional forms, and the relationship between other intermediate inputs in terms of fixed proportions are specified. For the current application, the Generalized Leontief (GL) functional form is used for all the flexible cost functions.

The demand component of the model includes both intermediate and final demands. Intermediate demand is determined by the cost-minimizing process discussed above. Final demand includes private consumption, government expenditures, and investment.

The modeling framework is general enough to incorporate several alternative views of equilibrium. In one version of the model, total employment is exogenously given, so full employment is achieved. Furthermore, the investment level is determined by savings, with savings rates being fixed. These specifications would have the model belong to the "classical" category. However, in the analysis below, an alternative (Keynesian) formulation of the labor market is invoked, in which the wage rate is fixed and labor supply adjusts to possibly less than a full-employment equilibrium. In addition, other components of the flow-of-funds account, such as the current account balance and government deficit, are considered in conjunction with the above for policy analysis purposes.

The core of the base year equilibrium data set of the model in this study is a SAM of the U.S. economy for 1987, constructed by Hanson and Robinson[20]. This data set contains both *make* and *use* versions of the U.S. Input-Output Table to capture the production and utilization of commodities. The SAM, in addition to providing the basic data set for model calibration, also provides initial values for endogenous variables and levels for exogenous variables. In this study, a 20-sector version of the model is used, including five mining sectors and two energy utility sectors (see Appendix A).

Some key parameters of the empirical model—Allen elasticities of substitution between aggregate inputs—are presented in Table 9-1. They represent a synthesis of estimates available in the literature. Sensitivity tests are performed on these values below.

9.4.4 Simulation Results

In this section, simulation results are presented for both autonomous and price-induced conservation strategies to be implemented in the Year 2000. The first set of simulations represents best estimates of the effects of these responses on major economic indicators for the economy in general and the energy sectors in particular. Other

Table 9-1. Allen Elasticities of Substitution for Selected Sectors

Sector	σ_{KE}	σ_{KL}	σ_{KM}	σ_{LE}	σ_{LM}	σ_{EM}
Construction	.70	.20	.55	-.25	.89	.77
Petroleum Refining	.25	.90	.35	.20	.50	.05
Manufacturing	.70	.20	.55	-.25	.89	.77
Transportation	.70	.90	.35	.25	.10	.05
Utilities	.70	.90	.02	-.10	.01	.01

[a] The symmetry properties of our production function require $\sigma_{ij} = \sigma_{ji}$.

simulations examine the sensitivity of the results to key parameters and behavioral considerations.

Energy policy responses are simulated in two ways. First, to analyze *autonomous* conservation, or the *mandated* response to a command-and-control policy, we reduce the energy use parameters in our model by 12.8% across-the-board (recall the U.S. response to a global policy regime discussed above). The model then analyzes sectoral (partial equilibrium) and multi-sectoral (general equilibrium) responses. Also, sensitivity tests are performed to ascertain the possible offsetting effects of energy-saving equipment needed to implement the policy goal. Note that in actuality, abatement cost curves will vary across sectors and the least-cost no regrets level will thus vary. Due to the lack of data on sectoral conservation potential, we simulate a uniform level. Given the fact that command and control policies are typically applied across the board, this exercise may not in fact represent too much of a departure from reality.

The direct application of a carbon tax or permit trading to examine *price- induced* conservation is simulated. This is modeled as a price increase in primary energy (tax on fossil fuel production), as indicated in Table 9-2. Note that in this case the optimal response calls forth differential reductions in energy use and differential levels of interfuel substitution across sectors.

Specifically, the following four cases were simulated:

1. Simple conservation—a 12.8% cutback in purchases of all fossil fuel energy, including utilities, in all intermediate and final demand sectors;
2. Conservation, but with the entire cost-savings in each sector being assigned to increased purchases of energy-saving equipment;
3. Price-induced substitution, but with the carbon tax being imposed only on domestic use of domestically produced primary energy; and
4. Price-induced substitution, but with the carbon tax being imposed on domestic use of both domestic and imported primary energy.

Note that, in effect, the optimal response to CO_2 mitigation policies is likely to be a combination of autonomous conservation and various types of substitution, which have been separated to isolate unique features of each. The overall outcome will thus be some weighted average of the two strategies. Referring to Figure 9-1, the exact combinations would be determined by the intersection of the carbon tax level (or equilibrium permit price) and the marginal cost of abatement.

Basic Results

The prime simulations are presented in Table 9-3 in terms of their impacts on five major economic indicators. The basic conservation case (line 1 of Table 9-3) is estimated to yield an overall decrease in GDP of 1.44% and a reduction in employment of 2.05%. Economywide investment decreases by 4.41%, with exports actually increasing by 2.75%

Table 9-2. Transformation of a Carbon Tax to an Ad Valorem Tax

	Fuel		
	Coal (ton)	Oil (bbl)	Gas (tcf)
Heat Content (million Btu per unit)	21.94	5.80	1.03
Emission Rate (kg per million Btu)	26.90	21.40	14.50
Conversion Factor (tons per unit)	0.59	0.12	0.02
Carbon Tax (1990 $ per unit carbon)	38.35	38.35	38.35
Ad Valorem Tax (1990 $ per physical unit)	22.63	4.76	0.57
Fuel Price, Year 2000 (1990 $ per physical unit)	26.64	26.40	2.72
Price Increase (percentage change)	85.12	18.02	20.83

Table 9-3. Economywide Impacts of CO_2 Mitigation, Year 2000: Base Cases
(percentage change from baseline)

Case	Real GNP	Employment	Investment	Exports	Imports	Welfare[a]	Energy Use	CO_2 Emissions
1. Conservation (100% cost-saving)	-1.44	-2.05	-4.41	2.75	-3.63	-0.84	-3.32	-3.44
2. Conservation (100% equipment offset)	-3.65	-3.94	-4.11	0.84	-3.02	-2.25	-9.16	-8.96
3. Interfuel Substitution (no tax on imported oil)	-1.56	-2.02	-3.59	-1.79	-1.93	-1.39	-24.17	-26.07
4. Interfuel Substitution (tax on all oil)	-1.77	-2.28	-3.37	-2.60	-3.38	-1.64	-25.49	-27.22

[a] As measured by compensating variation.

and imports declining by 3.63%. The difference in the GDP and Employment results indicates that there is proportionally greater substitution away from labor and labor-intensive goods than is the case for other inputs. Note also that the impact of this case (and all others) in terms of a welfare measure such as compensating variation, are also negative, though by a smaller percentage than the macro indicators.

Aggregate energy use declines as do CO_2 emissions, but startlingly less than expected. As expected, coal and electric utilities suffer the largest declines. Even though direct effects are proportional, general equilibrium effects allow for substitution away from these sectors. At first pass, one would expect declines of greater than 12.8% in each energy sector given the direct response and subsequent multiplier effects. However, it appears that the price decrease for each fuel causes energy to be more attractive to the point where there is a significantly offsetting substitution effect toward it. This has been pointed out in a number of studies that warn of the unintended side-effects of autonomous or mandated conservation (see, e.g., Khazzoom, 1980[21]). Other general equilibrium effects are operative as well but are too difficult to sort out without further experimentation (see below). Overall, the downside effects are not overcome by stimuli from increased purchasing power, international competitiveness, or multiplier effects. The results for the energy sectors are presented in Table 9-4.

Note also the irony of this policy response. In effect, the initial willingness of industry to decrease energy consumption by 12.8% results in offsetting factors that would not enable the U.S. to meet its CO_2 reduction target. That is the overall average decline of energy use of 3.32% would mean that CO_2 emission reductions would only be one-fourth of those intended. This is somewhat disconcerting, and, using rough rules of thumb, indicates that energy users on the average might need to undertake several times the amount of initial energy conservation to yield the intended overall 12.8% reduction.

The results of a modified conservation response is presented in row 2 of Table 9-3. When the entire cost savings is offset by increased costs of energy-saving equipment, the negative impacts are even greater than in the base case. Table 9-3 shows that GDP declines by 3.65% and employment by 3.94%. The key to understanding the decline is the reduction in economywide investment. It would appear that the *crowding-out* effect of investment in energy-conserving equipment is substantial and has a dampening effect on the economy (see also Jorgenson and Wilcoxen, 1993[22]). However, there is some bias in the model and its application. The investment equations are specified for more general cases. The model thus views the earmarking of investment funds for energy conservation as sub-optimal (as do the vast majority of the models in the literature). On the other hand, if the rate of return on this investment specifically reflected the gains that could be brought

Table 9-4. Energy Sector Impacts of the Conservation (100% Savings) Response, Year 2000: Base Case (percentage change from baseline)

Energy Type	Gross Output	Employment	Exports	Imports
Coal	-3.85	-4.64	0.39	-6.52
Oil/Gas Extraction	-1.03	-2.75	4.36	-4.43
Petroleum Refining	-2.28	-2.84	2.61	-5.16
Electric Utility	-4.21	-5.36	1.99	-7.18
Gas Utility	-2.49	-3.07	3.37	-5.33

and imports declining by 3.63%. The difference in the GDP and Employment results indicates that there is proportionally greater substitution away from labor and labor-intensive goods than is the case for other inputs. Note also that the impact of this case (and all others) in terms of a welfare measure such as compensating variation, are also negative, though by a smaller percentage than the macro indicators.

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The effect of Case 2 on individual energy sectors is presented in Table 9-5. The reductions come close to the 12.8% due in great part to investment considerations, which represent a type of forced substitution of capital for energy, in addition to other responses. Whereas in Case 1, energy intensity declines were below 0.2% for all sectors, here several sectors wind up with declines of greater than 2.0%.

In Cases 3 and 4, the response to a carbon tax or permit trading in terms of direct inter-fossil fuel substitution (IFFS) and other factor substitution (OFS), i.e., the increased cost of the energy aggregate leads to substitution between it and other aggregate input categories is simulated. These responses are further affected by various other general equilibrium interactions that take place, including product mix substitution (PMS). The results of simulations for these responses are presented in rows 3 and 4 of Table 9-3. In Case 3, the tax applies only to domestic use of energy produced in the U.S., while in Case 4 it applies to imported energy (primarily oil) as well.

Case 3 also yields a negative impact on the economy in terms of GDP and employment. The economic impacts of this case are quantitatively and qualitatively similar to Cases 1 and 2, except that exports decrease. The negative impacts on the economy are more pronounced in Case 4 because more inputs (i.e., imported oil) suffer price increases. These impacts are not offset by relatively more favorable terms of trade in Case 4 vs. Case 3.

The effect of Case 3 on individual fuels is presented in Table 9-6. As would be expected from Table 9-2, coal bears the brunt of the carbon tax, as reflected in a reduction in the sector's gross output of over 44%. Domestic crude oil production declines by 6.77% and imports decline by 8.77%. Sectoral results for Case 4 are very similar to Case 3, except that crude oil import reductions are much greater in the latter.

Perhaps the major differences between the mandated and incentive-based conservation responses are the energy and CO_2 reductions. Referring to the last two columns of Table 9-3, under Case 3 aggregate energy use decreased by 24.17% and total CO_2 emissions decreased by 26.07% (both figures are slightly higher for Case 4). First, the nearly 2.0% differential between energy use and CO_2 emission reduction reflects a significant amount of fuel switching. The majority of the emission reduction, however, stems from a relatively much greater decrease in energy use in Cases 3/4 vs. Cases 1/2 (compare also Tables 9-4 to 9-6). Some energy intensive sectors are the hardest hit by the general equilibrium effects, e.g., steel, stone (cement), and transportation.

Apparently declines in the energy sectors do contribute to the overall negative effect on the economy in the various simulations, but there are some offsetting effects in the carbon tax/permits cases, since decreases in GDP are only slightly higher despite a 7-8 fold decrease in energy production vis-a-vis Case 1. The relatively greater labor intensity of non-energy industries is one part of the explanation (compare the economywide employment decreases between Cases 1 and 3). Other explanations include the relatively lower negative impact on investment and the spending impetus of carbon tax revenues (though only to a slight degree as will be shown below).

Sensitivity Analysis

It is acknowledged that the CGE model is based on a calibration method with less than ideal statistical properties, and that several facile assumptions have been invoked. Therefore, it is not unreasonable to question the robustness of the results. This is tested by examining the effects of utilizing alternative estimates of capital-energy substitution elasticities and by invoking alternative CGE closure rules.

Recall the K-E elasticities of substitution for major sectors are presented in Table 9-1. They range from .250 to .700, which means capital and energy are considered substitutes. It is possible that these elasticities overstate the degree of the substitutability relationship. Moreover, it is also possible that capital and energy are complements.

Note that in addition to the elasticity values in Table 9-1, a further substitution relationship between capital and energy in Cases 2 and 3 of the previous subsection has been modeled. In effect, a direct decrease in energy and an increase in capital by an equivalent amount and by half the amount, respectively, has been inserted essentially increasing the K-E elasticities by these quantities. Indirect effects are still modeled with the ordinary K-E substitution elasticities.

Two sets of sensitivity tests on elasticities were performed. The first reduced the K-E elasticity values by half. The overall results (not shown) yielded imperceptible differences for Cases 1 and 2 and only minor differences for Cases 3 and 4. The second set of sensitivity tests utilized elasticities for capital and energy that exhibit complementary relationships. This required recalibration of the production functions and mainly minor adjustments in other elasticities. The results of the application of these new parameters also had little affect on the results and are not presented here. In effect, the results are thus more

Table 9-5. Energy Sector Impacts of the Conservation (100% Equipment Offset) Response, Year 2000: Base Case (percentage change from baseline)

Energy Type	Gross Output	Employment	Exports	Imports
Coal	-8.05	-9.12	-13.01	-4.73
Oil/Gas Extraction	-9.63	-12.07	-1.34	-13.66
Petroleum Refining	-11.35	-12.10	-34.42	3.47
Electric Utility	-6.92	-9.30	-12.06	-4.24
Gas Utility	-10.05	-11.32	-30.66	2.48

Table 9-6. Energy Sector Impacts of the Interfuel Substitution Response to Tax on Demostically Produced Energy, Year 2000: Base Case (percentage change from baseline)

Energy Type	Gross Output	Employment	Exports	Imports
Coal	-44.37	-37.43	-65.44	-19.31
Oil/Gas Extraction	-6.77	-8.76	-3.35	-8.77
Petroleum Refining	-7.72	-6.39	-32.05	8.74
Electric Utility	-7.85	-10.11	-34.49	9.32
Gas Utility	-1.69	-2.90	-18.94	8.34

sensitive to substitution levels across input aggregates, than within them, even for the case of interfuel substitution.

The third set of sensitivity tests is based on alternative assumptions about the labor market, factor mobility, and fiscal balances. In order to achieve equilibrium in constructing the CGE model, one cannot over- or under-constrain any of the markets. For example, in the case of labor supply, both the labor supply and wage rate fixed cannot be held fixed, nor can both of them vary. The specification of which aspect is fixed and which is variable in this and in other markets is known as a *closure rule*.

In the simulations above, a fixed real wage rate was assumed. Next the implications of an alternative closure rule that sets labor supply fixed and allows the wage rate to adjust is examined. This forces full employment of resources directly and indirectly released by the decrease in energy production. In addition, the implications of the assumption about the perfect mobility of capital are examined. Finally, the sensitivity of the result to whether carbon tax revenues are used to expand government expenditures or used for deficit reduction (with government expenditures being fixed) are examined. The conditions underlying the various sensitivity tests are presented in Table 9-7.

The results of these sensitivity tests applied to Case 4 (Interfuel Substitution/Tax on All Oil) are presented in Table 9-8 (note that Case 4.1 is the same as Case 4 listed in Table 9-3). As in the original simulations, the impacts on real GDP are negative in all cases, though they are negligibly so in Cases 4.2 and 4.5 because of the employment forcing. In only two of the cases (4.1 and 4.4) are the negative impacts on GDP and employment greater than in Case 1, and then only marginally so. It appears that using carbon tax revenues for deficit reduction, rather than expanding government expenditures, does enhance negative impacts but only slightly. It also appears that a fixed capital stock assumption reduces the negative impact somewhat (Case 4.3). The explanation would appear to be that capital is prevented from leaving the U.S. (also compare the export and import figures for Cases 4.1 and 4.3).

Results for individual energy sectors (not shown) are reasonably similar for all cases. The only significant difference is that crude oil imports decrease slightly in Cases 4.1 and 4.6.

9.4.5 Conclusions

The general equilibrium impacts of a conservation strategy to reduce CO_2 emissions results in a negative impact on GNP, employment, and other macroeconomic indicators has been examined. Not surprisingly, it was also found the impact on the energy industries to be strongly negative. Potentially positive ramifications of conservation, such as cost savings, increased consumer purchasing power, and multiplier effects of investment in

Table 9-7. Definitions of Subcases of Simulation 5

Sub-cases	Government Expenditure	Total Labor Supply	Sectoral Labor Demand	Total Capital Stocks	Sectoral Capital Stocks	Characterization
5.1	NF	NF	M	F	M	UNEM
5.2	NF	F	M	F	M	FULEM
5.3	NF	NF	M	F	F	S-R
5.4	F	NF	M	F	M	UNEM
5.5	F	F	M	F	M	FULEM
5.6	F	NF	M	F	F	S-R

Note:
F = Fixed
NF = Not Fixed
M = Mobile

UNEM = Underemployment equilibrium
FULEM = Full employment equilibrium
S-R = Short-run case

Table 9-8. Interfuel Substitution Impacts, Year 2000: Sensitivity Tests
(percentage change from baseline)

Case	Real GNP	Employment	Investment	Exports	Imports	Welfare[a]	Energy Use	CO_2 Emissions
4.1	-1.77	-2.28	-3.37	-2.60	-3.38	-1.64	-25.49	-27.22
4.2	-0.14	—	-2.24	-1.36	-1.60	-0.65	-24.09	-25.82
4.3	-1.34	-1.75	-3.71	-1.64	-3.20	-1.39	-22.45	-23.93
4.4	-1.79	-2.34	-1.83	-2.53	-3.25	-1.66	-25.55	-27.27
4.4	-0.08	—	2.97	-1.03	-0.99	-0.63	-24.13	-25.86
4.6	-1.50	-2.00	-1.67	-1.62	-3.17	-1.48	-22.59	-24.08

energy-saving equipment, were not able to offset the partial and general equilibrium downside effects of decreased energy use. Moreover, the results were robust to alternative assumptions on the degree of cost savings associated with conservation, the ease of substitution between energy and other inputs, and various macroeconomic closure rules. Finally, the results are in the ballpark of estimates undertaken by others, such as Manne and Richels[7, 23] and Jorgenson and Wilcoxen[22], though these studies placed a lesser emphasis on conservation. Thus, it has been concluded that conservation should not be characterized as a "no regrets" strategy.

This does not, of course, mean that conservation is a poor strategy, but simply that it should not be oversold as costless. In addition, the scope of this review has been limited to one side of the ledger, and the existence of reasonable estimates of net benefits of reducing CO_2 emissions in the tens of billions of dollars per year for the U.S. alone (see, e.g., Nordhaus, 1993[8]; Boyd et al., 1995[24]) is acknowledged.

However, it should be pointed out that a 3% decline in GNP in the Year 2000 translates into nearly $200 billion per year of opportunity costs.

Finally, it must be noted that the results pertain only to the short term. This, however, is the time period for which "no regrets" strategies apply, i.e., measures that can be taken until uncertainties about global warming are resolved. If predictions about the onset of warming are verified, a strategy need not be costless to be viable. Moreover, conservation may be able to play an expanded role in the longer term. Rather than the limited range of short-term options we have analyzed, some researchers have proposed more sweeping "eco-restructuring" for both industrialized and developing economies (see, e.g., Ayres and Simonis, 1994[25]). It is likely that these strategies would not bode well for traditional energy industries. However, their goal is to integrate innovative approaches to resource utilization into the economy so as to establish a path of sustainable development. Thus, further research is warranted to examine the long-term impacts of conservation.

9.5 Subtask 3.5 Economic Analysis of the Defense Department's Fuel Mix

Subtask 3.5 was previously completed.

9.6 Subtask 3.6 Constructing a National Energy Portfolio which Minimizes Energy Price Shock Effects

9.6.1 Introduction

Investors have long sought to reduce their exposure to market ups and downs by holding a diverse mix of investment instruments, which can reduce investor risk dramatically. By examining the variance, covariance and expected return between a group of assets, Markowitz[26] constructs an efficient portfolio which maximizes expected return for a given level of risk. The dual goal of maximizing return while minimizing variance produces a set of efficient portfolios an agent can chose from according to his or her personal preferences.

Portfolio theory and diversification have proved useful in areas other than personal and corporate investing. Adegbulugbe *et al.* [27] examine the long-term optimal structure of the Nigerian energy supply mix. They use a multiperiod linear programming model of the total energy system to minimize direct fuel costs while maintaining balanced development. Bar-Lev and Katz[28] examine fuel procurement in the electric utility industry and create a Markowitz efficient frontier of fuel mixes which minimize expected fuel costs and risk. Electric utilities rely heavily on long-term contracts with price adjustment clauses for fuel supplies. The possibility of price increases (or decreases) creates an atmosphere of uncertainty which must be factored into the fuel procurement decision, not unlike the problem of selecting risky securities. Kroner and Claessens[29] show how diversifying the composition of a country's foreign debt can act as a hedge against changes in exchange rates and commodity prices. The conditional covariance matrix of exchange rates and terms of trade, which changes through time, determines the optimal portfolio.

This section uses portfolio theory to demonstrate how the energy mix consumed in the United States could be chosen if the goal is to reduce the risks to the domestic macroeconomy of unanticipated energy price shocks. An efficient portfolio frontier of U.S. energy consumption is constructed using time-varying variances and covariances estimated with generalized autoregressive conditional heteroskedastic models. This allows the efficient portfolios to shift over time in response to price changes and past volatility. A trade-off between risk and cost exists. The set of efficient portfolios developed are intended to minimize the impact of price shocks, but are not the least cost energy consumption bundles. Although linear or quadratic programming techniques could also provide estimates of a unique optimal energy mix, the portfolio methodology is superior because it creates a set of efficient energy mixes, which vary in response to market events, and leaves the final choice to policy makers.

The United States government, through national energy policy, has long attempted to decrease the domestic economy's exposure to the impact of an energy shock. Such attempts have included quotas on imported oil, greater self-sufficiency in energy, increased research into alternative fuel sources, the strategic petroleum reserve, and increased domestic coal consumption. Underlying this goal was the belief that decreasing the heavy dependence on oil, and foreign oil in particular, would limit the potential effects of a price shock from a single energy source. As recently as 1993, Secretary of Energy for the

Clinton Administration Hazel O'Leary called for further diversification of U.S. energy consumption.

A negative correlation between oil prices and real output has been well established empirically. Fried and Trezise[30] find that the 1973 oil shocks increased the general rate of inflation by two percentage points, led to a terms of trade loss for oil importing countries equal to 1.5 to 2 percent of GNP, and decreased economic output by two to three percent within OECD countries. Rasche and Tatom[31] estimate a 7.0 percent average long-run reduction in U.S GNP following the 1973-1976 oil shocks, Darby[32] estimates a 2.5 percent decline, and Hamilton[33] confirms the negative relationship between oil prices and real output for the U.S. both before and after the price increases of the 1970s. Mork *et al.*[34] find this correlation extends in data through 1992, including the Persian Gulf War of 1991.

The goal of minimizing exposure to foreign oil price shocks by reducing oil imports ignores the possible covariance relationships between different energy sources. Shocks in the oil market can spill over to the coal and natural gas markets, and the relationship between domestic and foreign oil prices is strong and positive. Thus, establishing a goal of oil independence will not buffer the U.S. economy from foreign oil price shocks unless accompanied by the total isolation of the entire domestic energy market from the world market. As Heal[35] notes, a choice of isolation would create artificially high energy prices domestically and be economically inefficient. A better solution is to look for those combinations of oil, natural gas, and coal where price volatility in one fuel is offset by opposing volatility in another fuel, as portfolio diversification and management are designed to do.

9.6.2 Methodology

The primary goals of a rational investor are to maximize expected return and minimize risk. Higher risk is usually compensated for by higher expected returns. By purchasing a combination of assets, an investor can generate the highest possible return to their investment dollars at the least possible risk. The expected return of such a portfolio depends on the expected returns of the individual assets and the relative percentage of funds invested in each. The risk of the portfolio depends on the riskiness of the assets and the covariance or correlation of the assets. While the correlation has no impact on portfolio return, it plays an important role in determining the risk associated with the portfolio. The lower the correlation between two assets, the greater the risk reduction potential when combining them in a single portfolio.

The expected return for an n-asset risky portfolio is

$$E(R_p) = \sum_{i=1}^{n} w_i E(R_i) \qquad (9\text{-}1)$$

where $E(R_i)$ is the expected return from asset *i* and w_i is the weight of asset *i* held in portfolio *p*. The corresponding risk of such a portfolio, as measured by its variance, is

$$\sigma_p^2 = \sum_{i=}^{n} \sum_{j=}^{n} w_i w_j \operatorname{cov}(i,j) \qquad (9\text{-}2)$$

where *cov(i,j)* is the covariance between two risky assets *i* and *j*. By varying the weights of the assets, a set of potential portfolios can be generated. The efficient portfolio frontier is the subset of all dominant portfolios from the set of all possible portfolios. In a dominant portfolio, return can not be increased while holding variance constant and variance can not be decreased while holding return constant. Assuming risk aversion in decision makers, rational choice should lead to investment decisions only on the efficient frontier.

The return and variance of any portfolio can be calculated and the efficient frontier generated as long as the expected return of each asset and the covariance matrix is known (equations 9-1 and 9-2). In their analysis of the electric utility industry, Bar-Lev and Katz[28] use a quadratic programming approach to estimate these values. However, such a methodology requires the covariance matrix to remain constant over time, regardless of any new information which enters the market. Allowing the covariance matrix to be systematically updated over time as new events occur provides more realistic and efficient estimates. The generalized autoregressive conditional heteroskedasticy process (GARCH) introduced by Engle[36] and Bollerslev[37] allows the error variance and covariance to respond to price shocks and changes in volatility. GARCH has been used extensively for modeling financial time series. Bera and Higgins[38] and Bollerslev, Chou, and Kroner[39] provide surveys of the GARCH literature.

The GARCH(p,q) process is defined in terms of the properties of the distribution of the error terms in the model

$$Y_t = X_t'\partial + \varepsilon_t \qquad \varepsilon_t \; i.i.d., \qquad t=1,\ldots,T \qquad (9\text{-}3)$$

where X_t is a *kx1* vector of exogenous variables which can contain lagged dependent variables, δ is a *kx1* vector of regression coefficients, and ε_t is the error term. ε_t is assumed to have a traditional constant unconditional variance, but its conditional distribution depends upon the information set ψ_{t-1}, or

$$\varepsilon_t | \psi_{t-1} \sim N(0, h_t) \tag{9-4}$$

where

$$h_t = c_o + \sum_{i=1}^{q} \alpha_i \varepsilon_{t-i}^2 + \sum_{j=1}^{p} \beta_j h_{t-j}. \tag{9-5}$$

The conditions ensuring non-negativity and stationarity can be found in Nelson and Cao[40]. The conditional variance h_t is a function of the information set ψ_{t-1}, and the underlying functional form effectively models the volatility clustering commonly seen in financial time series data. The generalized GARCH(p,q) model allows the present conditional variance to depend on past conditional variances in addition to past squared innovations.

Computing time-varying covariances requires the simultaneous estimation of a multivariate system (Bollerslev, Engle, and Wooldridge,[41]). Generalizing a univariate GARCH model to a multivariate model requires allowing the entire covariance matrix to change with time, rather than just the variance. Thus, the elements of the covariance matrix would be linear functions of lagged squared errors, lagged cross-products of the errors, lagged variances, and lagged covariances. The traditional means of estimating such a system, similar to a vector autoregression, is cumbersome and sometimes impossible. Bollerslev[42] has suggested a multivariate GARCH specification which holds the correlation matrix constant over time. Using the relationship between covariance and correlation,

$$h_{ij,t} = \rho \sqrt{h_{i,t} h_{j,t}} \quad , \tag{9-6}$$

each period's covariance can be calculated. This allows the variance and covariance to change over time while the fundamental relationship between assets remains unchanged. The constant correlations model has been used successfully with foreign exchange rate data[42] and interest rate data[43]. Giovannini and Jorion[44] find the estimated variances from a constant correlation estimation are almost perfectly correlated with the estimated variances from the VAR-type estimation, and Baillie and Bollerslev[45] show that the data does not usually reject the constant correlation assumption.

The analysis of energy portfolios differs slightly from investor portfolio analysis. Since every energy investment has risk, no risk-free energy asset is available. Another difference is the inability of energy investors to hold negative weights of, or "go short on," an energy type. The equivalent to shorting stock in energy investment would be using electricity to create natural gas and then selling the natural gas, but it is impossible to efficiently create natural gas from electricity.

9.6.3 Estimation and Results

The data set consists of monthly spot energy price series of oil, natural gas, and coal. Over the next ten years, 85 percent of new non-nuclear electric generation in the U.S. is projected to be from these three sources[46]. Further investment in nuclear energy production has been stalled and much current production will be phased out over the next 20 years. The share of hydroelectricity and other nonconventional energy sources is not expected to grow over the next decade. Few new potential hydro power sites exist in the United States, and nonconventional energy sources are not currently competitive on a large scale and will likely not be so over the next ten years.

Two price series were obtained for each energy source, both nominal and not seasonally adjusted. Basic energy costs were derived from average monthly first nearby oil prices and natural gas prices from the NYMEX and average wellhead price for periods before NYMEX trading. The coal price series is the average spot price paid by electric utilities as reported to the Federal Energy Regulatory Commission. All prices are in terms of monthly million Btu/$. The second set of price series adds electric utility non-fuel costs to basic energy costs to generate a total operating cost for electricity generation from each energy source. The data extend from January 1974 to August 1995 (260 observations) and are plotted in Figure 9-2.

Each series is tested for the presence of a unit root. A series with a unit root is nonstationary with an infinite unconditional variance. The results of Dickey-Fuller and augmented Dickey-Fuller tests are reported in Table 9-9. All series fail to reject the null hypothesis of a unit root at the 95 percent confidence level. Thus, to achieve stationarity in the data, all series were differenced once.

Table 9-10 presents the historical moments of each series. The spread between the average MM Btu/$ (column 1) is smaller in the utility energy cost group than the raw energy cost group. This reflects the inverse relationship of fixed costs to variable costs. In general, oil has provided the least MM Btu/$ for an investment while natural gas has provided the most. Examining the first differenced log for each series, the mean return is

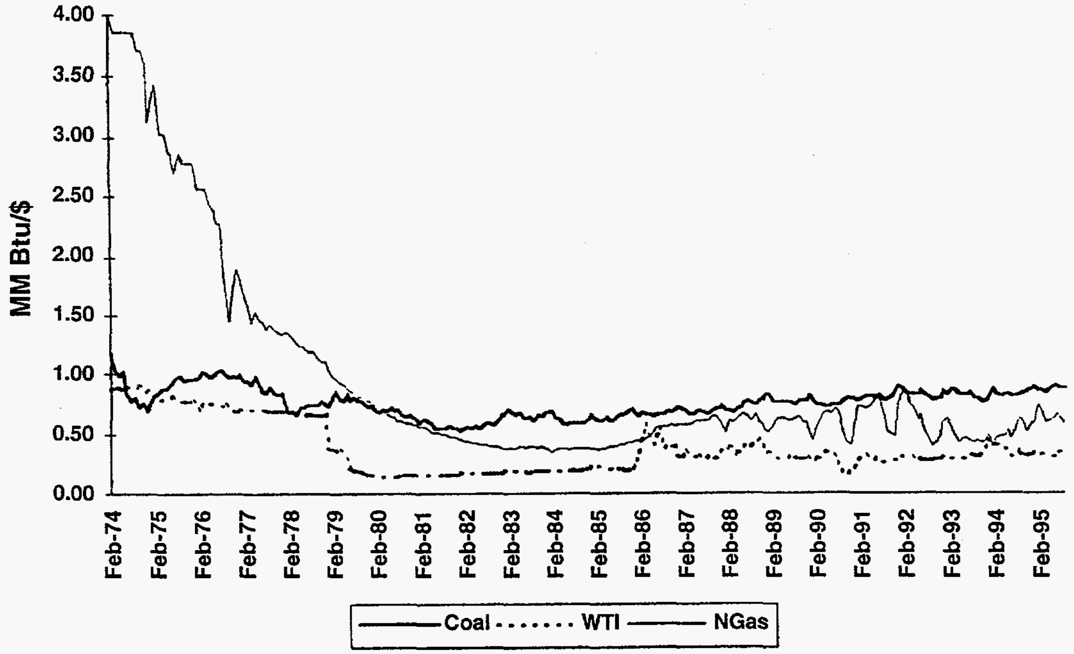

Figure 9-2. HISTORICAL ENERGY RETURN (MM Btu/$) FOR EACH ENERGY TYPE

Table 9-9. Unit Root Tests

	AR Parameter	DF Statistic	ADF Statistic	Number of Significant Lags
Coal	0.9544	-2.748	-2.748	0
Natural Gas	0.9754	-2.148	-2.120	12
Crude Oil	0.9762	-1.788	-2.269	1

The 5% and 10% critical values for Dickey-Fuller tests are -2.84 and -2.57.

Lags were considered significant at the 10% level.

Table 9-10. Moments of Price Series

	Average MM Btu/$	Differenced Log MM Btu/$				
Raw Energy Costs		Mean	Variance	Skewness	Kurtosis	Bera-Jarque
Coal	0.76	-0.0021	0.0021	-0.98	6.1	146
Oil	0.38	-0.0036	0.0068	-0.84	12.6	1016
Natural Gas	0.95	-0.0077	0.0068	0.79	8.4	336
Utility Energy Costs						
Coal	0.43	-0.0010	0.0007	-0.64	4.3	36
Oil	0.28	-0.0026	0.0043	-0.68	11.7	842
Natural Gas	0.53	-0.0040	0.0035	0.89	9.0	425

not significantly different from zero and all exhibit skewness and excess kurtosis. This is reflected in the high Bera-Jarque statistic, which rejects the null of a normal distribution at .05% in all cases.

Table 9-11 reports the correlation matrix between the price series. The correlations are generally small, with the relationship between coal and both oil and natural gas weak whether or not non-fuel costs are included. Natural gas and oil have a slightly larger though still small correlation coefficient. The relationship between natural gas and oil in the last five years of the data set (1990-1995) has become stronger, with a correlation coefficient of 0.40, probably because of the deregulation of natural gas.

The GARCH parameter estimates for equations 9-3 and 9-5 are found in Table 9-12. The significance of $\hat{\alpha}$ and $\hat{\beta}$ in the variance equation (equation 9-5) support the choice of a GARCH model in place of a homoskedastic system. Predicted volatility for each of the energy price series based on the parameter estimates is plotted in Figure 9-3. Coal prices are the most stable, with a relatively constant conditional variance and return. Oil shows significant volatility increases during each historic price shock (1979, 1986, 1991) and an overall trend to increasing volatility in the 1990s. These price shocks effect oil volatility for approximately one year. Natural gas shows the most marked change. Returns to investment have declined significantly as prices have increased over the last twenty years. Natural gas prices have also been very volatile in recent years, reflecting the deregulation of the natural gas industry and the development of active natural gas futures markets.

Combining the parameter estimates and the correlation coefficient estimates according to equation 9-6 yields estimates of the time-varying covariances of the system. Energy portfolios are constructed using these covariances and expected returns in equations 9-1 and 9-2. Figure 9-4 depicts the efficient portfolio frontier in 1990 for both basic energy costs and electric utility operating costs. The addition of fixed costs to energy costs lowers returns to electric utilities and results in a lower curve. The additional fixed charges also mean that the annual volatility becomes smaller relative to the absolute size of the costs, shifting the curve to the left.

When viewing the actual energy portfolios of U.S. consumption for 1980, 1990, and 1995 along with an example of an efficient portfolio from the estimated portfolio frontier for each year, it is noted that the actual energy consumption portfolio is far from efficient. The efficient portfolio Sharpe ratio is two to three times the size of the actual portfolio ratio. In general, a more efficient consumption bundle would include a higher percentage of coal and less oil and natural gas in the overall economy. Increasing coal consumption would both decrease volatility and increase energy return, a movement to a

Table 9-11. Correlation of Changes in Monthly Energy Return (MM Btu/$) Series 1973-1995

	Basic Energy Costs			Electric Utility Operating Costs		
	Coal	Natural Gas	Oil	Coal	Natural Gas	Oil
Coal	1			1		
Natural Gas	0.02 (0.46)	1		0.02 (0.46)	1	
Oil	-0.01 (-0.16)	0.13 (3.61)	1	-0.01 (-0.18)	0.12 (3.47)	1

Table 9-12. GARCH Estimation of Energy Return Series
(T-statistics in parenthesis)

	Mean Equation Eqn. 9-3		Variance Equation Eqn. 9-5	
	δ	c	α	β
<u>Raw Energy Costs</u>				
Coal	0.001 (0.61)	0.0001 (2.81)	0.068 (2.94)	0.72 (9.58)
Natural Gas	-0.014 (-6.22)	0.00002 (2.40)	0.096 (4.57)	0.83 (26.87)
Oil	-0.005 (-1.75)	0.0008 (5.86)	0.183 (4.47)	0.40 (4.65)
<u>Electric Utility Operating Costs</u>				
Coal	0.001 (0.70)	0.00003 (2.42)	0.077 (3.02)	0.72 (9.41)
Natural Gas	-0.010 (-6.49)	0.00005 (4.17)	0.208 (5.08)	0.62 (11.70)
Oil	-0.004 (-1.63)	0.00047 (6.02)	0.194 (4.78)	0.41 (5.15)

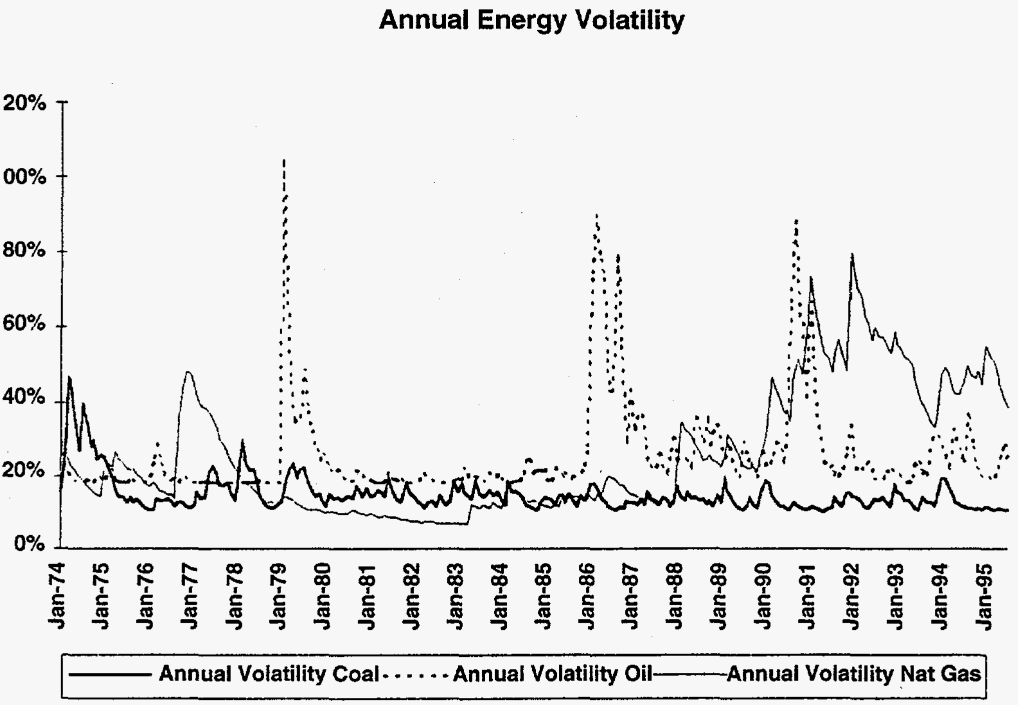

Figure 9-3. GARCH ESTIMATES OF ENERGY RETURN VOLATILITY

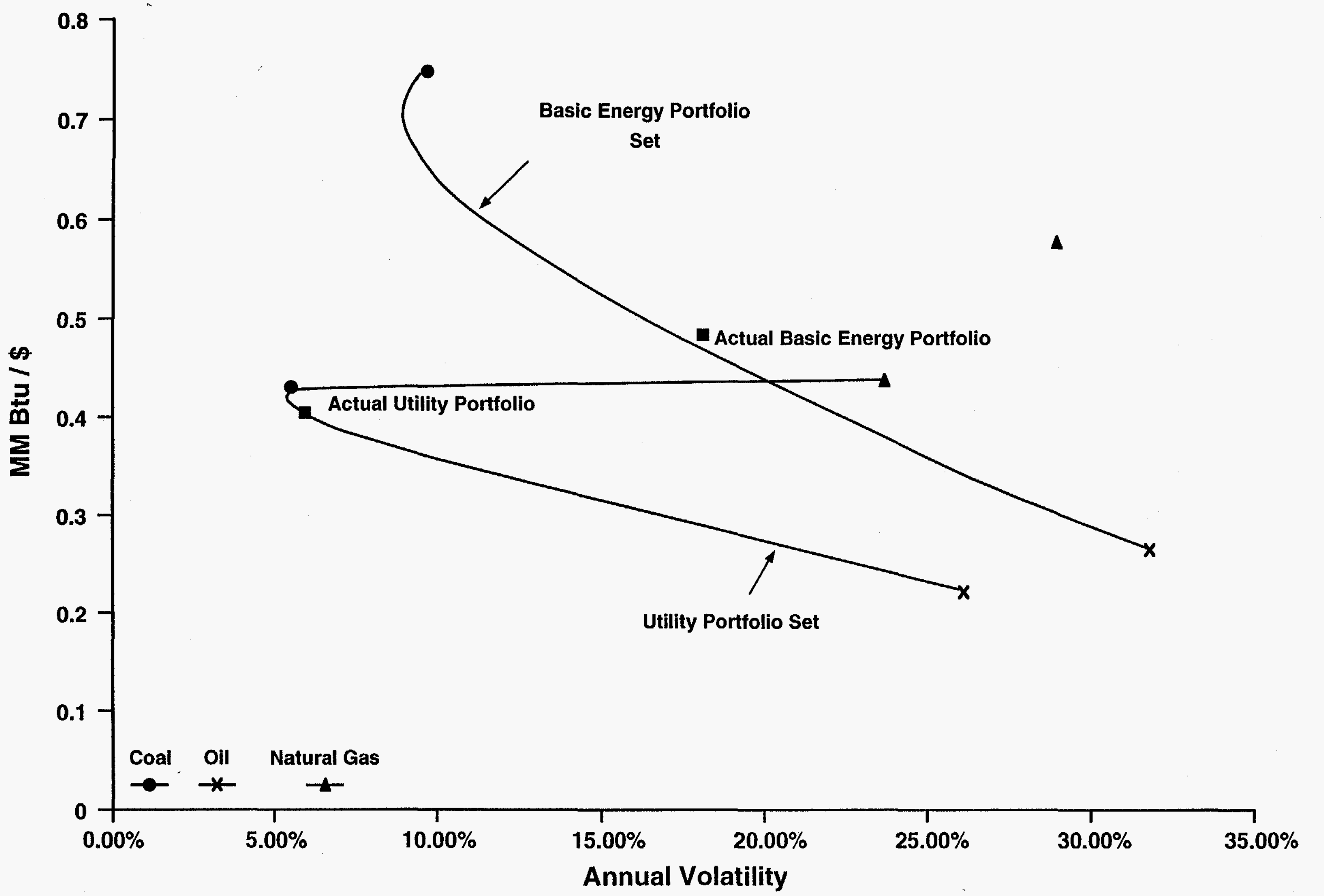

Figure 9-4. 1990 EFFICIENT PORTFOLIO FRONTIERS FOR THE UTILITY INDUSTRY AND GENERAL U.S. CONSUMPTION

dominant portfolio. It is acknowledged that the effective price of utilizing fuels differs from the market price somewhat. Given market imperfections, relatively higher costs of pollution mitigation associated with coal may not have properly been reflected, and similarly for uncertainties related to deregulation of natural gas.

For the total costs faced by the electric utility industry (energy costs plus nonfuel costs), operation has moved towards more efficient portfolios since 1980. In 1990 and 1995 the industry operated very close to the efficient frontier. The industry also operated at a position of very low volatility. The high level of coal consumption by utilities suggests a relatively high level of risk aversion, in contrast to the results of Bar-Lev and Katz[28], who found electric utilities pursuing high-risk consumption strategies. They argued that this was the result of regulatory policy that allowed electric producers to pass cost through to the consumer. However, the price shocks and volatility in the oil market since their study might have shown the limit of such regulatory largesse and have led to the observed increase in risk aversion seen by the utility consumer.

As the variance and covariance changes over time in response to price shocks and past volatility, the efficient portfolio set also changes. Some general observations can be made. Certain relationships remain unchanged. Coal is more stable than either oil or natural gas. Natural gas tends to be more volatile than either coal or oil, with superior returns to the electric utility industry and lower returns in the overall energy portfolio.

9.6.4 Policy Recommendations

The actual energy portfolio selected should be determined by the tangency of the efficient portfolio frontier and the utility curve which reflects the country's preferences regarding risk and return. Some general recommendations can be offered. The volatility (but almost certainly not the level) of overall U.S. energy consumption costs could be lowered (and expected returns raised) by increasing the percentage of coal within the overall consumption mix. Lower volatility should lead to fewer disruptions in the domestic macroeconomy. The actual level of each energy source should be determined by feasibility and the utility curves of the country. Shifting as far as 70 percent coal consumption (Table 9-12, 1990) would be physically impossible since coal is best used in boilers, which account for far less than 70 percent of U.S. energy consumption. Choice is valuable because the ability to easily switch between fuels to adjust the consumption mix allows the fuel mix to move with the efficient frontier in response to market events. Discovering ways to move cheaply from one fuel to another would be desirable.

The recommendation to shift energy consumption towards coal rests on the premise that future coal price movements are similar to historic prices. This may not be the case. The deregulation of the electric utility industry and potential introduction of coal futures contracts may lead to an increase in coal price volatility similar to that seen in the natural gas industry. However, for the near future, coal prices should remain relatively constant.

Although transparent future markets exist in oil and natural gas and there exists an active coal market, the market price of energy does not reflect the true cost of energy consumption due to the presence of externalities. Environmental, national security, monopoly, and depletion costs may not be adequately included in the market price. These costs can be incorporated into the analysis by including an estimated externality cost in the total cost of an energy source. This creates a new set of variances, covariances, and expected returns, and thus a new set of efficient portfolios from which to choose an efficient portfolio. The portfolio framework also allows selection of portfolios for sectors that may face different externality costs. The sector would construct an efficient portfolio frontier using their own externality costs and then choose from this frontier. Even with the use of portfolio analysis to select a consumption bundle, a remaining inefficiency may arise due to over-consumption of energy in general. Substitution away from energy should take place as its costs rise.

As an illustration, consider the environmental costs associated with energy consumption. Many estimates have been made of the environmental costs of energy consumption, optimal tax rates, and carbon taxes (e.g., Viscusi 1990[47], Verleger 1993[48]). Barbir and Veziroglu[49] estimate that the total costs of energy consumption in 1990 were $2.36 trillion dollars with estimated externality costs of $9.31/MM Btu for coal, $8.03/MM Btu for oil, and $5.31/MM Btu for natural gas. Adding these cost estimates to the energy cost data creates a new set of efficient portfolios, illustrated in Figure 9-5 for 1990. Including environmental costs greatly decreases energy returns and gives natural gas a higher return than coal. Although the minimum variance portfolio is the same in both this and the previous analysis (64% coal, 19% oil, and 17% natural gas), every other point on the frontier is different. Ignoring environmental costs leads to a decision to increase coal consumption to reduce volatility. Including environmental costs shifts consumption away from coal towards natural gas in order to increase the portfolio's return. Because the analysis is highly sensitive to the estimates of externality costs used, reliable estimates are essential.

Of frequent political interest is the potential security premium representing the benefit of self-sufficiency in energy needs. Like the disagreement which exists over the size and actual impact of energy price shocks on the domestic economy, discrepancies also exist in the size and even existence of a security premium. Bohi and Toman[50] provide an overview of security premia estimates from the Department of Energy which range from $0.17/bbl of oil to $10/bbl of oil. Heal[35] estimates that between additional defense and

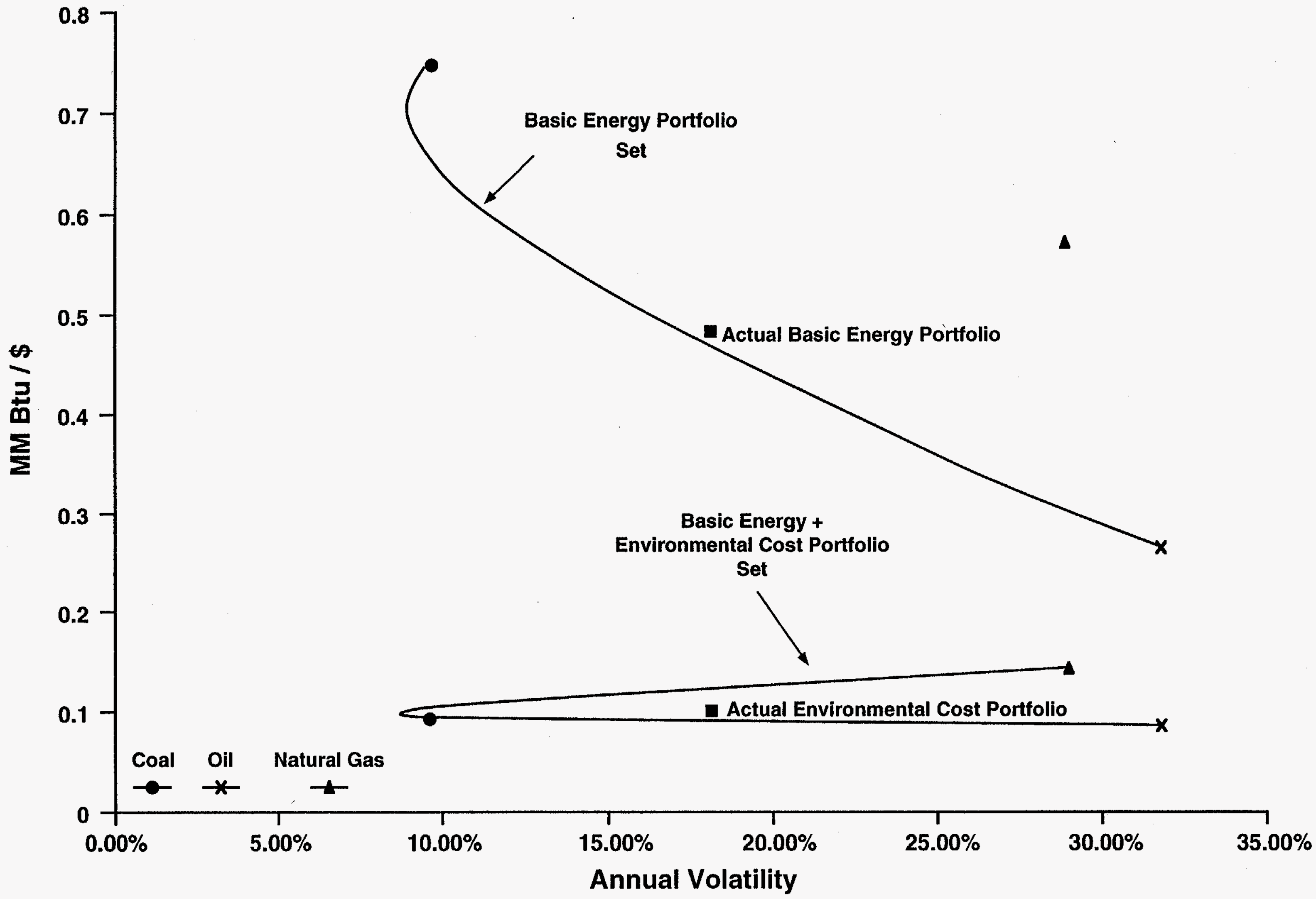

Figure 9-5. 1990 EFFICIENT PORTFOLIO AND EFFICIENT ENVIRONMENTAL PORTFOLIO

strategic petroleum reserve spending, the national security expenditure in 1985 was approximately $9/bb of imported oil.

To illustrate the effect of a security premium on portfolio choice, $10/bbl is added to the total oil price. Figure 9-6 illustrates the resulting efficient frontier. Again, the minimum variance portfolio remains unchanged, but for the same expected return a different portfolio composition arises. On average, the portfolios including a security premium include 5% less oil than the portfolios based solely on market costs. Groups such as the U.S. military, who may place a higher premium on the use of imported oil, would want to shift even more of their oil consumption towards coal.

9.6.5 Conclusions

This section has introduced a method for choosing efficient energy mixes which would reduce the risk to the domestic economy of energy price shocks. A frontier (range) of possible portfolios are generated from which policymakers must choose a desired portfolio based on their risk and expected returns preferences. The results indicate that the electric utility industry is operating very close to the minimum variance position with a risk aversion strategy. In contrast, overall energy consumption in the United States is far from an efficient mix. A shift towards coal consumption would reduce price volatility. With the inclusion of potential externality costs, the shift remains away from oil but towards natural gas instead of coal. To achieve such shifts, policymakers could use regulation or tax incentives to industries to encourage the use of certain fuels. Of course, a minimum risk portfolio does not imply a minimum cost portfolio, and selecting a low-risk portfolio may lead to higher energy costs overall. The costs associated with an occasional energy price shock may be far less than the cost associated with energy independence or a dramatic shift towards coal, synfuels, and other alternative energy sources.

9.7 Subtask 3.7 Proposed Research on the Coal Markets and their Impact on Coal-Based Fuel Technologies

Subtask 3.7 was previously completed.

9.8 Subtask 3.8 Integrate the Analysis

No work was conducted on Subtask 3.8 during this reporting period.

10.0 PHASE III, TASK 4 FINAL REPORT/SUBMISSION OF DESIGN PACKAGE

No work was conducted on this task.

11.0 MISCELLANEOUS ACTIVITIES

A paper was prepared and presented at the First Joint Power and Fuel Systems Contractors Conference in Pittsburgh, Pennsylvania on July 9-11, 1996. The paper was

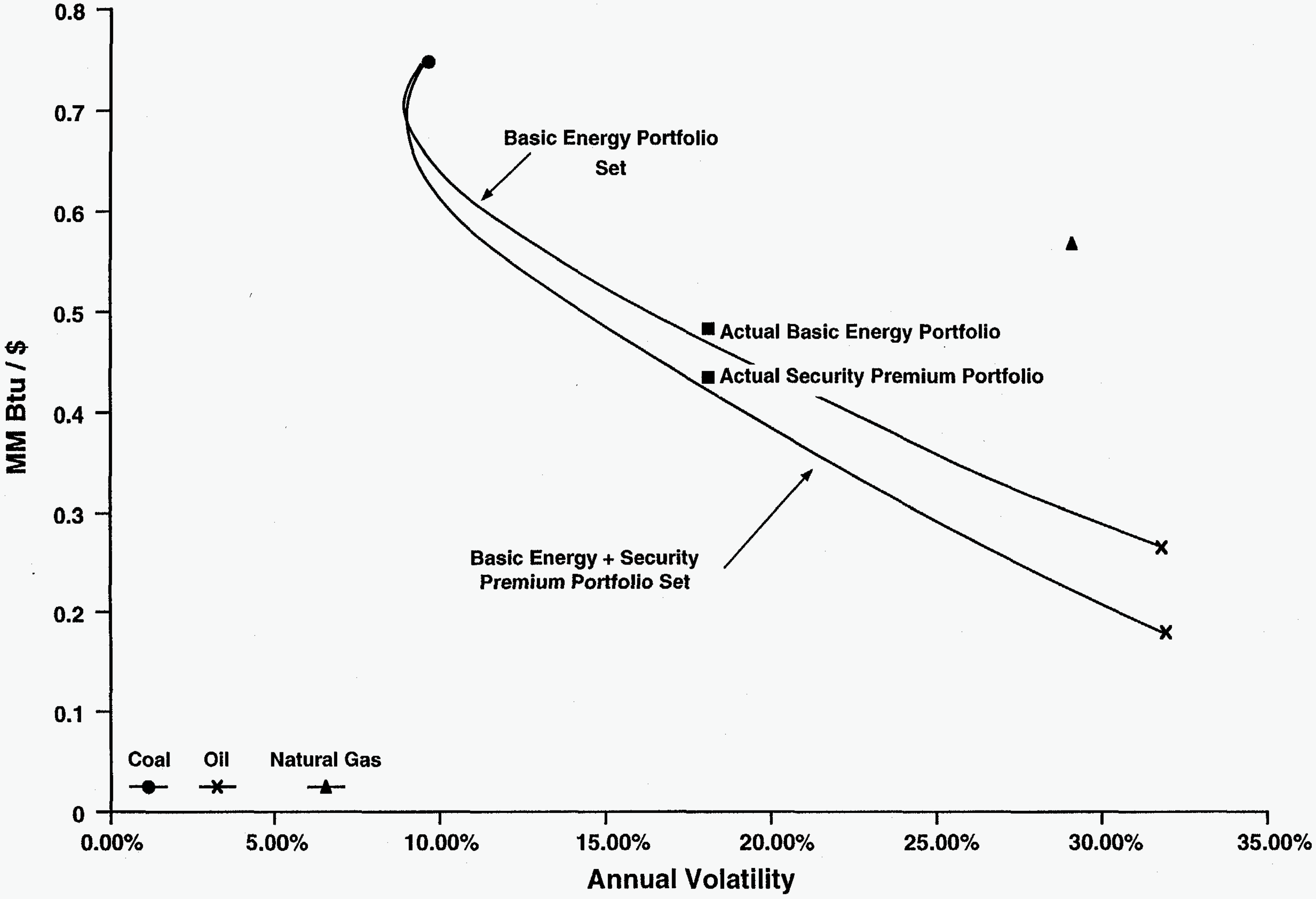

Figure 9-6. 1990 EFFICIENT PORTFOLIO WITH AND WITHOUT A $9.00/bbl SECURITY PREMIUM

titled "Characterizing and Reducing Emissions from Oil-Designed Industrial Boilers Retrofitted to Fire Coal-Based Fuels," coauthored by Bruce G. Miller and Alan W. Scaroni.

A program review meeting and tour of facilities was held at Penn State on September 19, 1996. The meeting primarily focused on discussing the Phase I conclusions, with status reports of Phases II and III given.

12.0 NEXT SEMIANNUAL ACTIVITIES

During the next reporting period, the following will be done:

- Install the ceramic filter system and auxiliary components;
- Install the sodium bicarbonate duct injection system;
- Conduct NO_X catalyst tests;
- Procure Method 5 apparatus and auxiliaries;
- Begin VOC and trace elements studies;
- Prepare the final report for Phase II, Task 2, Coal Preparation/Utilization; (except for the atomization testing in Subtask 2.10);
- Prepare coal-water mixtures for Carnegie Mellon University;
- Prepare the final report for Phase II, Task 3, Economic Analysis;
- Complete Phase III, Task 1, Coal Preparation/Utilization; and
- Complete Phase III, Task 5, Economic Analysis.

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14.0 ACKNOWLEDGMENTS

Funding for the work was provided by the U.S. Department of Defense (via an interagency agreement with the U.S. Department of Energy) and the Commonwealth of Pennsylvania under Cooperative Agreement No. DE-FC22-92PC92162. The project is being managed by the U.S. Department of Energy, Pittsburgh Energy Technology Center (PETC). Anthony Mayne of PETC is the project manager.

The following Penn State staff were actively involved in the program: Michael Anna, David Bartley, Glenn Decker, Howard R. Glunt, Bradley Maben, and Ronald T. Wincek.

APPENDIX A. SECTOR DEFINITION

Sector	Name	BEA Code
1	Agriculture	1-4
2	Iron Mining	5
3	Non-Iron Mining	6
4	Other Mining	9,10
5	Coal Mining	7
6	Petroleum Mining	8
7	Construction	11,12
8	Manufacturing	13-30,33,34,39-64
9	Petroleum Refining	31
10	Plastics	32
11	Glass	35
12	Stone	36
13	Steel	37
14	Metal Manufacturing	38
15	Transportation	65
16	Communication	66,67
17	Electric Utilities	68.01
18	Gas Utilities	68.02
19	Trade & Finance	69,70
20	Services (including Water & Sanitary Services)	71-79,68.03

Notes: Sectors 5, 6, 9, 17, and 18 form the energy aggregate.