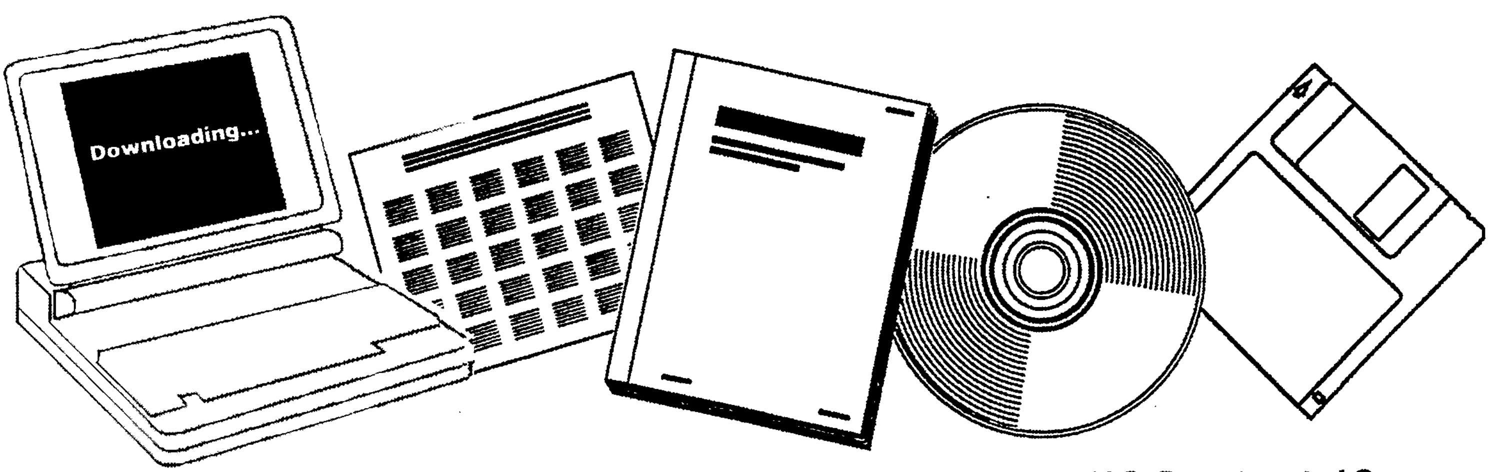
PETC1000

CLEAN ENERGY FROM COAL

DEPARTMENT OF ENERGY, PITTSBURGH, PA.
PITTSBURGH ENERGY TECHNOLOGY CENTER

JAN 1979



U.S. Department of Commerce
National Technical Information Service

PETC-1000

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PITTSBURGH, PENNSYLVANIA 15213

January 1979

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INTRODUCTION

The United States has coal resources approaching 4 trillion tons—enough to last us for several hundred years. More energy is available in the form of coal than in our combined resources of petroleum, natural gas, oil shale, and tar sands.

In view of nationwide energy shortages, the increased use of coal is vital to the nation's total supply of clean energy. However, this solid fuel can be currently applied to only a limited portion of the total national energy demand.

The primary user of coal is the electric utilities industry, where coal is pulverized and then burned in solid form in boilers. Our transportation sector depends nearly exclusively on liquid fuels, the household and commercial sectors depend almost entirely on liquid and gaseous fuels, and three-quarters of the energy used by industry is provided by liquid and gaseous fuels.

Consequently, converting coal to gaseous and liquid fuels in commercial quantities is fundamental to ensuring the availability of fuel in conventional forms for the major users as the supplies of petroleum and natural gas diminish. The ultimate objective of coal research is

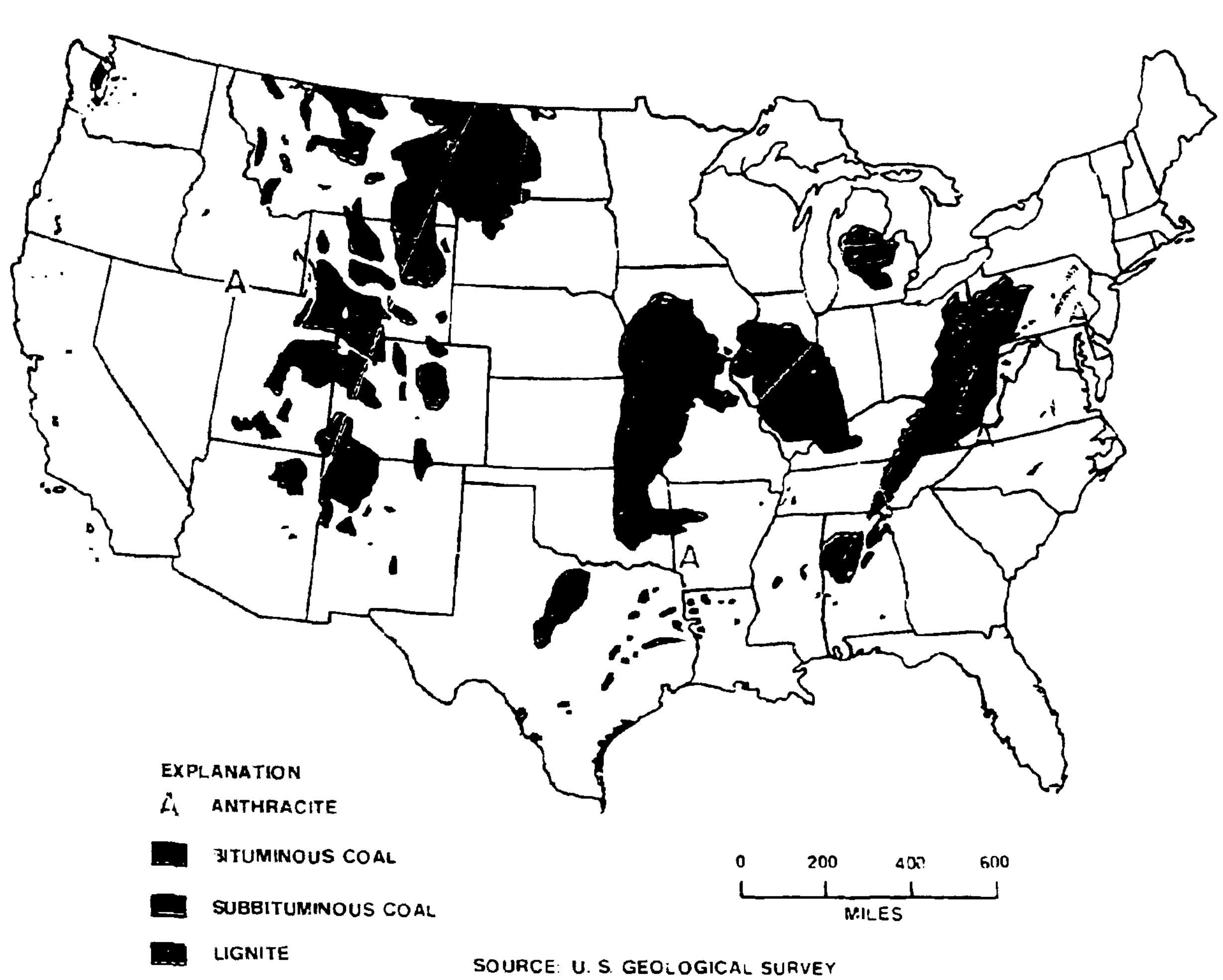
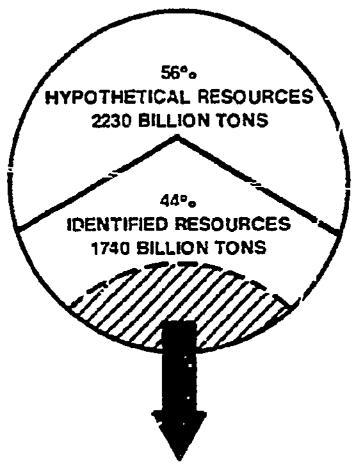


Figure 1. Coal Fields of the Conterminous United States



DEMONSTRATED RESERVE BASE (437 BILLION TONS) — 25% OF IDENTIFIED RESOURCES
ACCORDING TO RANK, SULFUR CONTENT, AND MINING METHOD

	EASTERN U. S.		WESTERN U. S.		
	ANTHRACITE	BITUMINOUS	BITUMINOUS	SUBBITUMINOUS	LIGNITE
RESERVES (BILLION TONS)	7.3	194	39	168	27
MINING POTENTIAL, %					
UNDERGROUND	59	83	79	60	0
SURFACE	1	17	21	40	100
SULFUR CONTENT					
LESS THAN 1%	87	14	29	87	38
1 to 3%	3	28	17	10	53
MORE THAN 3%	0	42	26	1	2
UNKNOWN	10	16	28	3	7

SOURCE: U. S. GEOLOGICAL SURVEY AND U. S. BUREAU OF MINES

Figure 2. Total U. S. Coal Resources and Demonstrated Reserve Base

therefore to provide the technology for improved direct combustion of coal and for rapid commercialization of processes for converting coal to clean synthetic fuels.

Figure 1 pinpoints the locations of the country's coal fields in terms of the different ranks of coal—anthracite, bituminous and subbituminous coal, and lignite. Figure 2 shows that the total of all possible coal resources in the U. S. is close to 4 trillion tons.* According to the most recent estimates by the U. S. Geological Survey, the total identified resources (known coal deposits in the ground) down to 3000 feet (900 m) are about 1200 billion tons in the states west of the Mississippi River and 500 billion in the east. An additional 2230 billion tons of undiscovered (hypothetical) resources in the U. S. probably exist.

As shown in Figure 2, only about 25 percent of our identified resources make up the demonstrated reserve base—coal readily minable by present day methods. The U. S. Bureau of Mines in 1975 summarized available data on the U. S. demonstrated reserve base. This reserve base generally includes coal to a depth of 1000 feet (300 m) in beds at least 28 inches (0.7 m) thick for bituminous coal and anthracite, and 60 inches (1.5 m) thick for subbituminous and lignite. The reserve base is also separated into portions practically minable by underground or surface methods (i.e., lying within 120 feet (36 m) of the surface).

Almost every state contains some coal or related carbonaceous deposit. Lignites and subbituminous coals are found in the western states from Canada to the Gulf of Mexico. Further east, the coals are of older origin and are classified as bituminous. The most easterly beds are anthracites. In 1975, 640 million tons of coal were mined in the U. S. If our total energy consumption had been supplied by coal, we would have used 3100 million tons of coal. The potential for increased use of coal as an energy source is obviously great. Even with increased mining, the United States contains enough coal to last at least until the 22nd century. Thus, coal is really our energy "ace in the hole."

One of today's environmental concerns is the amount of sulfur discharged into the atmosphere by the burning of coal. Most eastern coals would have to be desulfurized to be acceptable for the market. Many western coals, however, are sufficiently low in sulfur as mined so that sulfur and ash reduction are not needed to meet current air quality standards.

*The metric unit—tonne—is approximately 1.1 tons. Since all tonnage quantities in this publication are approximate, English tons are used throughout. A table of Metric Equivalents is an appendix to this publication.

The development of coal utilization and conversion processes by the U. S. Department of Energy (DOE) is oriented towards improving direct combustion of coal and towards accelerating and stimulating a synthetic fuel industry. Fossil energy research, development, and demonstration strategy is to sponsor a wide variety of technical options that are clean, more efficient, and conserve resources. Industry can then choose promising processes which will eventually be commercialized and will therefore provide the energy needed for our continued economic growth and well-being.

The Pittsburgh Energy Technology Center

The Pittsburgh Energy Technology Center (PETC) conducts research and development as part of DOE's overall program to promote production of clean energy from coal. Established in 1948 as an energy research laboratory of the Office of Synthetic Liquid Fuels, U. S. Bureau of Mines, PETC is the largest fossil energy research and development center in the U. S. PETC has a staff of about 370 scientists, engineers, technicians, and support personnel and is the major Federal laboratory for research in coal combustion and conversion of coal to clean fuels. It is located in a semi-rural area near Bruceton, in South Park Township, about 12 miles south of Pittsburgh, Pennsylvania. (The Director may be addressed at 4800 Forbes Avenue, Pittsburgh, PA 15213).

The laboratories were built in the late 1940's after the Congress passed the Synthetic Liquid Fuels Act of 1944. This law authorized the Department of the Interior to conduct laboratory research on production of synthetic liquid fuels from coal, oil shale, agricultural and forestry products, and other substances and to build and operate demonstration plants to further these efforts.

Based on earlier laboratory work at the Bureau of Mines and on technical information and expertise gleaned from Germany after World War II, researchers at PETC developed successful methods for producing liquid fuels from American coals by hydrogenation and by the Fischer-Tropsch synthesis. To continue the development, demonstration plants for both processes were operated at Louisiana, Missouri, during the period 1949-1953. These large-scale processes were successful to some degree; 1.5 million gallons of gasoline were produced by hydrogenation and 40,000 gallons by the Fischer-Tropsch process. However, the processes were expensive, increasing quantities of new oil were discovered both in the U. S. and the Middle East, and, hence, interest in synthetic fuels diminished. Laboratory and small-scale process work continued, but with emphasis on more basic research and engineering which led to the development of our present, improved coal conversion processes.

When interest in synthetic fuels renewed and expanded, this backlog of more than twenty years experience proved crucial to development of the newer, more promising versions of the earlier processes. For example, the research on the Fischer-Tropsch synthesis became the basis for development of a new

Figure 3. SYNTHANE Pilot Plant

process for making substitute natural gas, and the high-pressure coal hydrogenation work led to a new process for clean liquid fuels.

During these years of research and experience in producing synthetic fuels from coal, the energy research staff developed a number of new basic chemical and engineering concepts in these fields, in addition to engineering developments that are either presently in industrial use or on the verge of large-scale implementation. Understanding the basic chemistry and engineering of changing solid coal to liquid fuels was greatly enhanced by these studies. Much of the high pressure technology and materials used for coal conversion were developed here. The concepts of fixed-bed catalytic hydroliquefaction and dilute-phase hydrogasification of coals were results of this research. The hot carbonate process that is widely used for gas purification throughout the chemical industry was patented and is now used commercially throughout the world. Thus, the Pittsburgh Energy Technology Center has contributed knowledge for decades and still is in the forefront of research and development in the field of synthetic liquid and gaseous fuels from coal.

PETC today is in the lead in coal conversion and utilization research. Modifying conventional coal combustion equipment to permit efficient, clean firing of coal-oil mixtures and solvent-refined coal may appreciably reduce the use of petroleum to generate electric power. Progress is also extensive in developing new processes for converting coal to cleaner, more adaptable fluid fuels. These processes include an efficient method for producing low-sulfur fuel oil from coal; SYNTHANE—a second generation process to produce high-Btu, pipeline-quality gas from coal; dilute phase hydrogasification—a highly efficient and relatively simple third generation process to make pipeline gas by direct hydrogenation of coal; and COSTEAM—a coal liquefaction process using readily available and cheap synthesis gas without added catalysts. Gasoline and other light distillates can be produced by adaptations of these liquefaction and gasification processes. Research is also being performed on the chars produced in coal conversion processes to utilize them in hydrogen production and in combustion for power generation. Coal combustion research programs not only emphasize combustion of coal-oil mixtures but also development of a unique two-stage coal gasifier-combustor to supply a high temperature plasma for a combined cycle magnetohydrodynamic (MHD) power plant to produce electricity from coal more efficiently than is presently done.

Several of these processes have been scaled-up. A 700 horsepower boiler facility for coal-oil mixture firing is now operating at PETC. A SYNTHANE prototype pilot plant that could process 72 tons of coal per day into over one million cubic feet of gas was operated at PETC. Construction is almost complete on a liquefaction plant to convert 10 tons of coal per day to 30 barrels of low-sulfur oil. Design is underway for a 50 MW (120 tons of coal/day) gasifier-combustor for an MHD power generation facility to be built at Butte, Montana. These processes will help preserve the environment while meeting the nation's increasing energy needs.

As a necessary and continuing effort, extensive process and engineering research is also being conducted:

- A promising method of removing much of the sulfur from coal by pressurized air-water treatment is under development.
- Techniques for refining and upgrading coal liquids and producing valuable chemicals, such as ethanol and ethylene, are being investigated.
- Research is being conducted to develop new and improved catalysts for coal liquefaction and gasification processes.
- An important effort is devoted to development of new analytical tools and techniques to characterize coal and coal products from energy conversion processes.
- Both experimental and theoretical engineering studies are being done on reactor modeling.
- And in all research and development studies, environmental impact and conservation techniques are an integral part of each project scheme.

Because of decades of research and succesful process development, PETC has acquired a national, as well as an international, reputation. PETC researchers are called upon continually to share their expertise in coal utilization and conversion. Hundreds of visitors tour PETC each year, and numerous talks are given by the PETC staff. Many committees (both domestic and foreign) on which staff members serve and the numerous technical publications that staff members author each year represent an important aspect of DOE's RD & D effort in fossil energy.

The professional staff of PETC, having extensive industrial experience, has widespread relationships with universities, industry, domestic and foreign technical societies, advisory committees, civic organizations, state and local environmental boards, other governmental agencies, and the general public. Interaction with the community, both professional and nonprofessional, is a vital part of PETC's role as a DOE presence in a major industrial and energy oriented region.

The following pages describe the objectives and technology of the processes being developed at PETC. Descriptions of the pilot plants evolving from this research are included. The organization of the Center and the functions of each research and support group are also described.

COAL LIQUEFACTION

A major objective of the Pittsburgh Energy Technology Center is development of processes intended primarily to produce clean fuel oil

Figure 4. Removing Sample of Liquefaction Product

from coal. A 10 ton-per-day Process Development Unit (PDU) is now under construction for coal liquefaction research. Another process, using disposable catalysts, is being tested in a 1/2 ton-per-day unit. A third process, termed CO-STEAM, is aimed toward use of low rank coals without a catalyst and with cheaper reacting gases. These different liquefaction processes thus employ various materials and operating conditions to reach similar objectives.

Liquefaction Process Development

PETC engineers are developing processes to convert coal into fuel oil which has a low sulfur and a low ash content. It would permit abundant high-sulfur coals, presently barred from use in electrical power plants by sulfur-limiting air quality standards, to reenter the utility fuel market and help relieve the shortage of clean fuels. Petroleum products and natural gas now used in power plants for electrical power generation would then become available for other markets.

At present, a pilot plant is converting 1/5 ton of coal per day into clean fuel oil at a yield of three barrels of oil per ton of coal. The process works with any kind of coal; five different grades have been processed. An inexpensive Kentucky coal having 5.5 percent sulfur and 17 percent ash has been converted to clean fuel oil having only 0.17 percent sulfur and 0.7 percent ash. In these experiments, coal conversion was 98 percent, and energy conversion efficiency was 78 percent.

To accelerate process studies, a second, more advanced unit with a higher throughput, 1/2 ton of coal per day, is currently operating. These research facilities, as well as the 10 ton-per-day Process Development Unit under construction, will be employed to conduct process optimization studies, to generate oil for product utilization investigations, to gain operational experience, and to provide information for the design of larger plants.

Experimental studies in models of the reactor and in separation of residual solid matter from the product oil by types of centrifugation are other topics being investigated by engineers at PETC.

The solid residue is a heavy, sludge-like material that contains an appreciable quantity of usable product oil. Recovery by pyrolysis, using either a rotary calciner or a

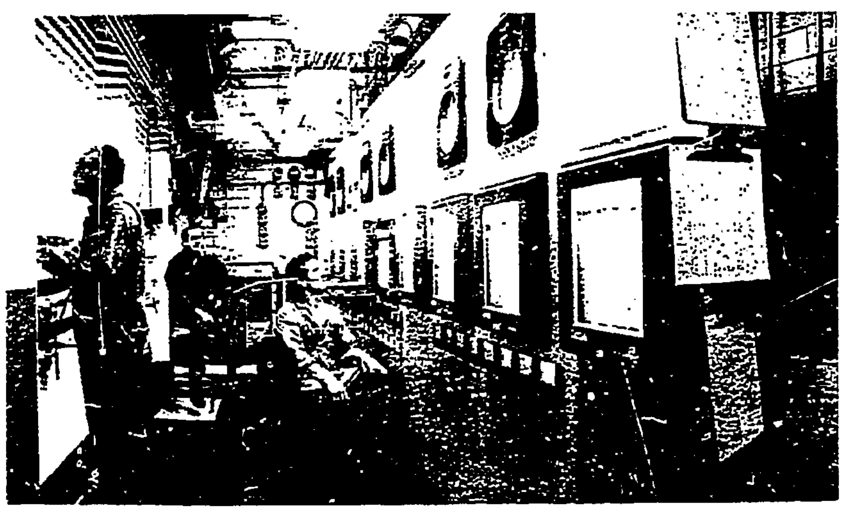


Figure 5. Control center for the 1/5 ton per day liquefaction pilot plant. Operating conditions throughout the plant are monitored on the panel at right. At left are manual controls which extend through the safety wall and allow adjustment of flows in the high pressure plant area.

fluidized-bed system, is under investigation. These pyrolysis methods use short residence times that allow high processing rates.

Figure 6. Fluid dynamic studies of two-phase flow in a liquefaction packed-bed reactor model.

10 Ton-per-day Bruceton Coal Liquefaction Process Development Unit (PDU)

In the Bruceton Coal Liquefaction Process Development Unit (Figure 8), coal containing 3 to 5 percent sulfur and 10 to 15 percent ash will be converted into a heavy fuel oil containing 0.1 to 0.6 percent sulfur and 0.5 to 1.5 percent ash. The product could be further refined to gasoline or diesel oil or employed as a chemical feedstock. The coal liquefaction is accomplished by catalytic hydrogenation of a coal-product oil slurry in a novel, turbulent upflow, packed-bed reactor. Plant design is based upon research conducted in the smaller, 1/5 ton per day pilot plant at PETC.

When completed, about sixty people will be employed to operate this larger 10 ton per day facility. Estimated total construction costs are about $27 million. Under contract with DOE, Foster Wheeler Energy Corporation designed the facility and is currently managing its construction.

In cooperation with industrial participants, the plant's purpose is to generate data and to provide operational experience. Data acquired from this project will support design and construction of a proposed 500 ton-per-day plant.

The overall process scheme (see Figure 9) includes coal handling and pulverization, slurry preparation and pumping, slurry preheating and hydrogenation, and a series of product recovery and recycle operations.

- *Slurry Preparation and Liquefaction:* Coal is ground to 70 percent through 200-mesh (74 μm) in a conventional pulverizer. It is then thoroughly mixed with recycled product oil to form a slurry consisting of approximately 35 percent coal and 65 percent oil. After being mixed with hot hydrogen and preheated by direct exchange with products from the reactor, the slurry enters the reactor where the hydrogen liquefies the coal and removes sulfur, oxygen, and nitrogen. The reactor contains a fixed bed of cobalt molybdate catalyst and operates at a temperature of about 840°F (450°C) and pressures from 2000 to 4000 psig (14-28 MPa). Turbulent flow conditions are maintained to ensure efficient contacting of slurry and catalyst while at the same time allowing a high slurry throughput.

- *Product Recovery:* Hot products from the reactor enter the first high-pressure receiver where the high-boiling-point fractions (product oil) are separated from

Figure 7. Installing a continuous centrifuge system for removal of solids from the oil produced by the 1/5 ton per day coal liquefaction pilot plant.

the gas stream. The gas is further cooled and enters the second high-pressure separator where the low boiling point liquid fractions are separated from the recycle gas. Product oil from the first receiver is centrifuged to remove unconverted coal and ash, and a portion of this oil is recycled by mixing it with fresh coal to prepare the slurry feed.

- *Gas Purification and Recycle:* Because the gases leaving the reactor contain large volumes of unreacted hydrogen, the gas is cleaned and recycled. It is scrubbed with circulating light oil to remove hydrocarbons and with diethanolamine to remove hydrogen sulfide (which is then converted to sulfur). Recovered hydrogen is then recycled via a recycle compressor. Fresh hydrogen is added between the recycle compressor and the product gas heat exchanger. Because of the size of this PDU, hydrogen will be produced by steam reforming of propane. In a commercial plant, hydrogen would be produced by the gasification of coal and/or char (process) residues.

Liquefaction of Coal Using a Disposable Catalyst

Conversion of coal into a low-sulfur liquid fuel is recognized as one of the most desirable methods of increasing our country's supply of clean energy. PETC researchers are developing a promising liquefaction process (Figure 10), employing a disposable catalyst.

Certain aspects of this liquefaction technique offer promise for reduction of costs and improved reliability of operation. Introducing the catalyst directly into the feed slurry for one-time use circumvents the operational difficulties and lost production time associated with regenerating or replacing deactivated catalysts. Production costs are further reduced if inexpensive catalytic materials or only small amounts of more expensive materials are used. Substances currently being considered for these purposes are

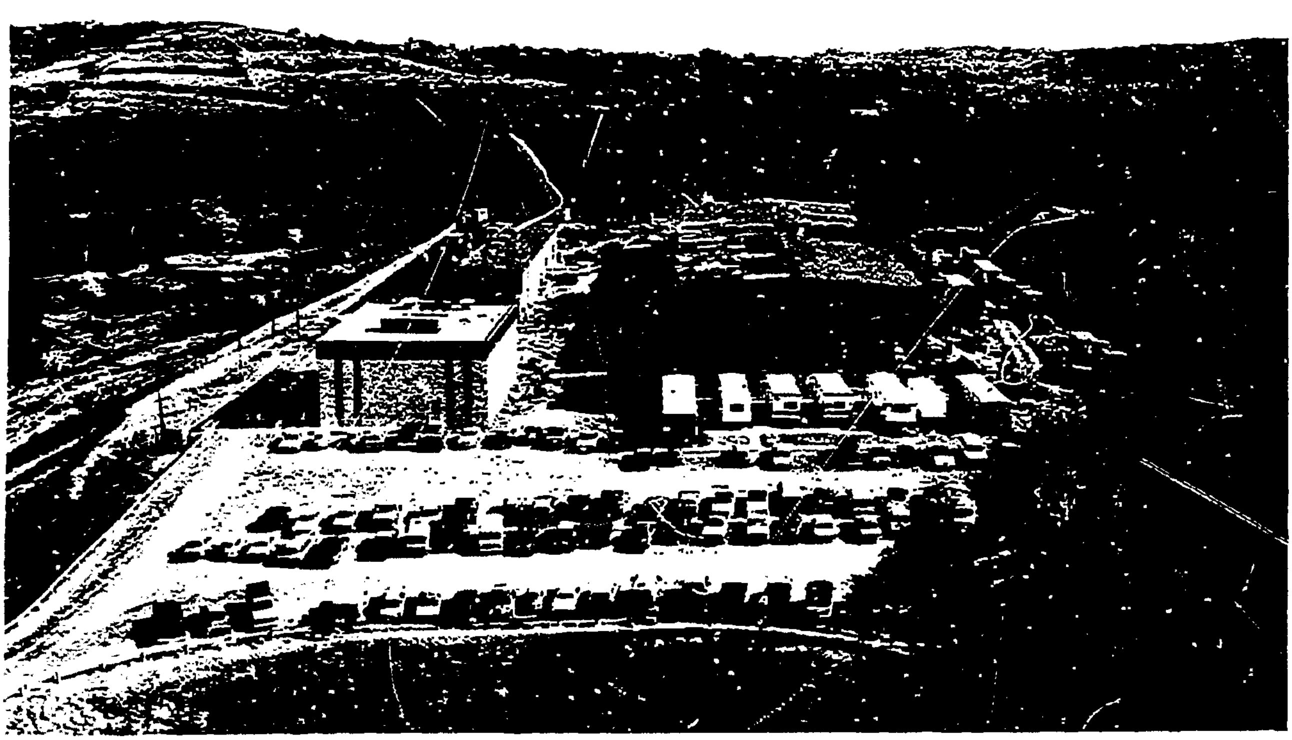


Figure 8. The Bruceton Coal-Liquefaction Process Development Unit under construction at the Pittsburgh Energy Technology Center. At right is the structural skeleton of the process building. At left is the administration building with the maintenance building behind.

traces of cobalt and molybdenum compounds or ores, iron compounds, and ash constituents from high-ash coals.

Continuous experiments needed for this study are to be conducted in a 1/2 ton-per-day unit. This unit is presently undergoing shakedown tests. Meanwhile, batch autoclave experiments are being made to guide the choice of catalysts and operating parameters to be used in the continuous unit. Development of this process is expected to provide a viable, low-risk method for producing environmentally acceptable fuel oil from coal.

COSTEAM Process for Fuel Oil from Coal

Most processes for conversion of coal to oil use hydrogen at high pressure in the presence of a catalyst. However, PETC researchers have developed a new process that does not use hydrogen directly.

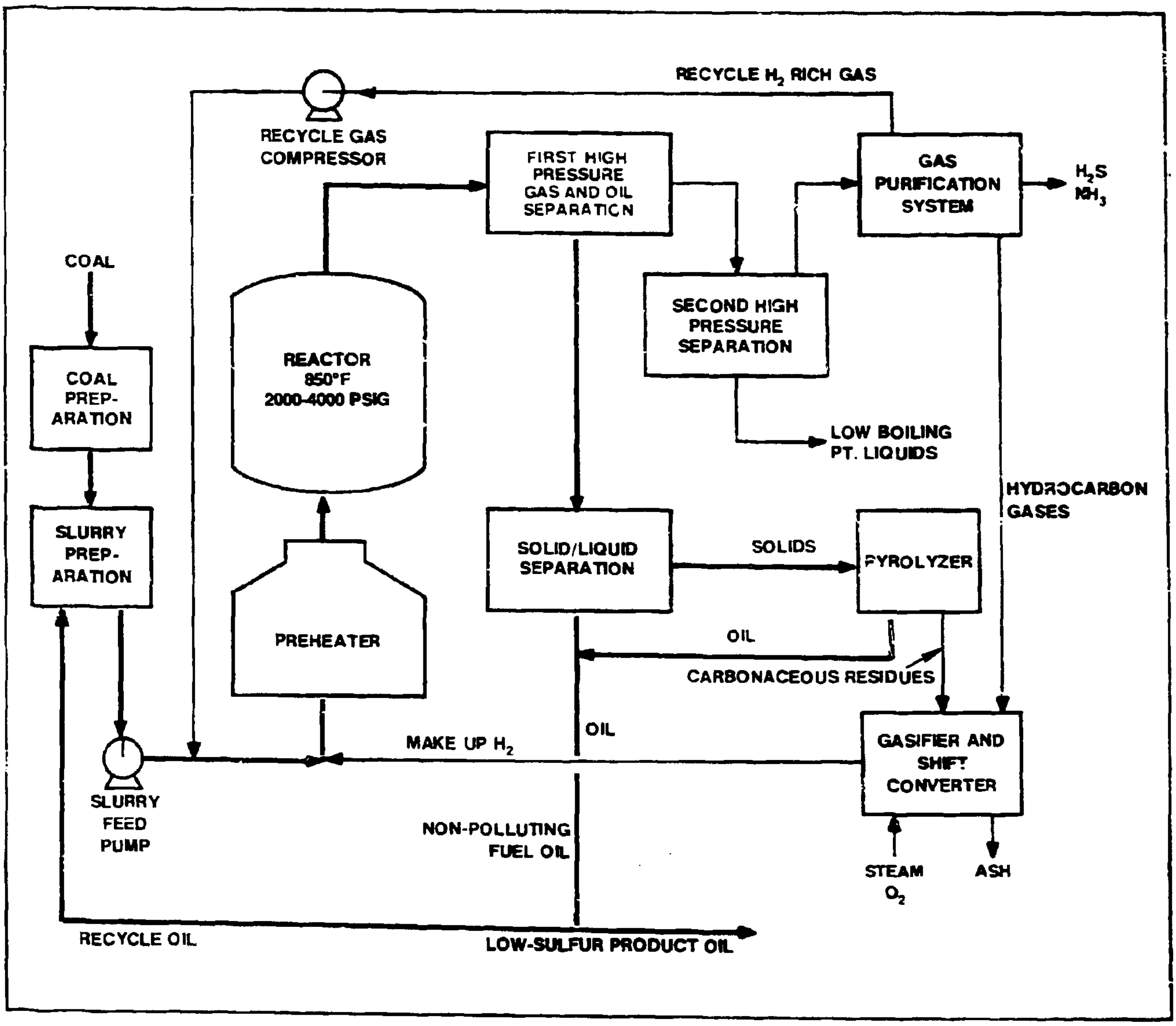


Figure 9. Coal Liquefaction Process, Flow Diagram

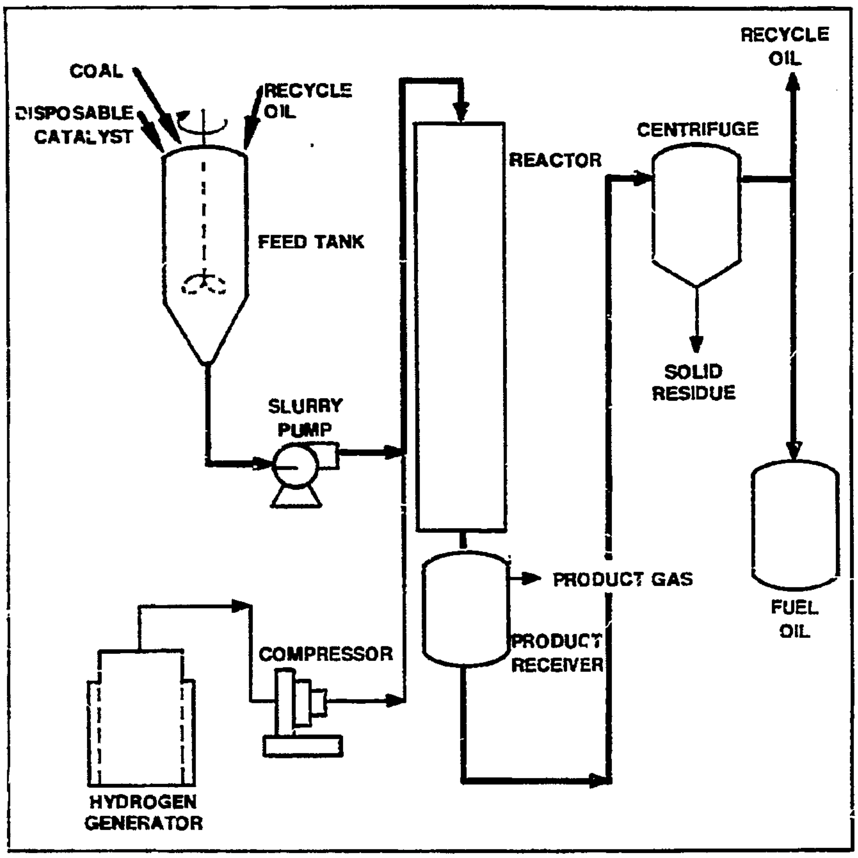


Figure 10. Liquefaction of Coal with Disposable Catalyst, Flow Diagram

This route consists of reacting coal with carbon monoxide or mixtures of carbon monoxide and hydrogen (synthesis gas) and steam. It works especially well on sub-bituminous coals and lignites and usually does not require the addition of a catalyst; the alkali salts that catalyze this reaction are present in the coals.

In the COSTEAM process (which is similar to that shown in Figure 10), a slurry of pulverized coal in some of the product oil is pumped into a reactor with synthesis gas at a pressure of 4000 psig and a temperature of 800 to 840°F (430-450°C). (In the case of lignites the naturally occurring moisture is adequate for the reaction.) The gaseous and liquid products are separated in a receiver. The liquid is then freed of ash and unreacted coal in a centrifuge or filter. The low-sulfur, low-ash product can then be used as an industrial fuel oil.

The use of low-cost coals, low-cost reducing gas, and the absence of added catalysts offer promise that the COSTEAM product will be lower in cost than oils from conventional coal processing.

COAL GASIFICATION

PETC is conducting research and development on two processes designed to produce substitute natural gas (SNG) from coal. The SYNTHANE process, tested in a 72 ton-per-day plant, will be considered, along with several other processes under development elsewhere, for recommendation by DOE to industry for ultimate commercialization. Another process under study at PETC appears to have certain advantages of even simpler, more efficient operation that will be explored for possible input into DOE's general gasification program.

SYNTHANE Process, Coal to Pipeline Gas

SYNTHANE (SYNthetic meTHANE) is one of the promising processes for producing substitute natural gas from coal. The process, shown in Figure 11, consists of coal pretreatment, coal gasification, shift conversion, gas purification, and methanation systems. SYNTHANE can operate with any coal—lignite, subbituminous, bituminous (including highly-caking coals), and anthracite.

Coal is first reacted in a pressurized, fluidized bed with a steam-oxygen mixture at 800°F (425°C) to destroy its caking properties. The coal is then gasified with steam and oxygen in an 1800°F (980°C) fluidized bed at 1000 psi. Char produced in the gasifier is used to produce steam required for the process.

Gas leaving the gasifier is scrubbed to remove fine particles, tars, and water. The cleaned gas passes through a shift converter and then goes to the hot-potassium-carbonate plant (a PETC development that is now commercial) for removal of CO_2 and sulfur compounds. Hydrogen sulfide is converted to sulfur, which is used for commercial purposes or stored for later use.

Finally, the purified gas passes to the methanator for conversion of the hydrogen plus carbon monoxide to methane, increasing the heating value to that of natural gas. This process can be modified to make gasoline, methanol, or low-Btu gas.

SYNTHANE Pilot Plant

The SYNTHANE pilot plant at Bruceton was designed and engineered for DOE by CE-Lummus Company. The plant was constructed by Rust Engineering Co., and CE-Lummus Co. operated it under a government contract. The plant was designed to convert 72 tons of coal per day into 1.2 million cubic feet (34×10^3 m^3) of gas. The installed cost was about $16 million; annual operating cost was approximately $8.2 million; and about 200 people were employed in operating the plant.

The overall process includes coal sizing and pressurization, pretreatment and gasification, and a series of clean-up and conversion operations. Coal is delivered by truck, loaded into a 240-ton raw-coal storage bin, then ground from the original minus 3/4 inch (2 cm) to minus 20 mesh (0.8 mm) in a hammer mill

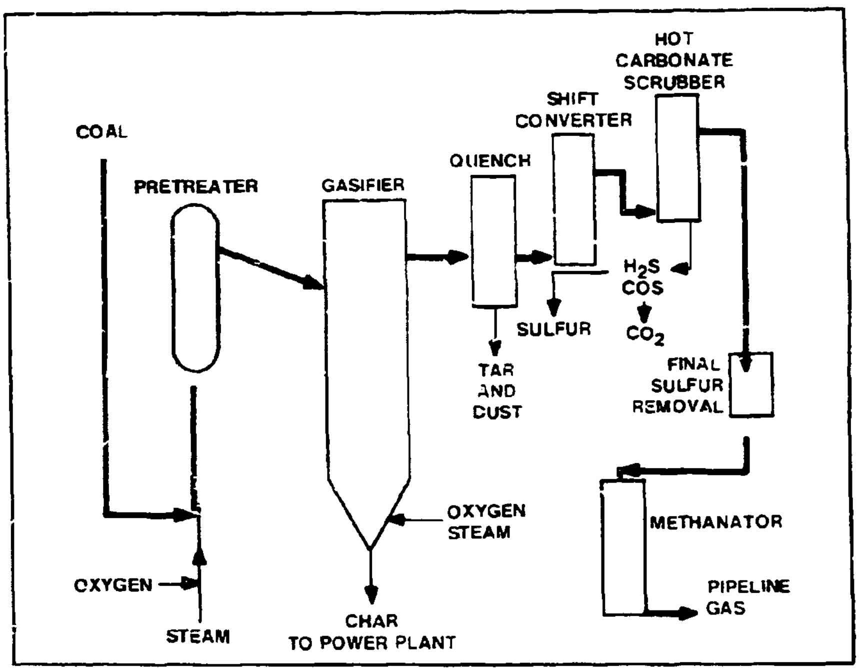


Figure 11. SYNTHANE Process, Coal-to-Pipeline Gas, Flow Diagram

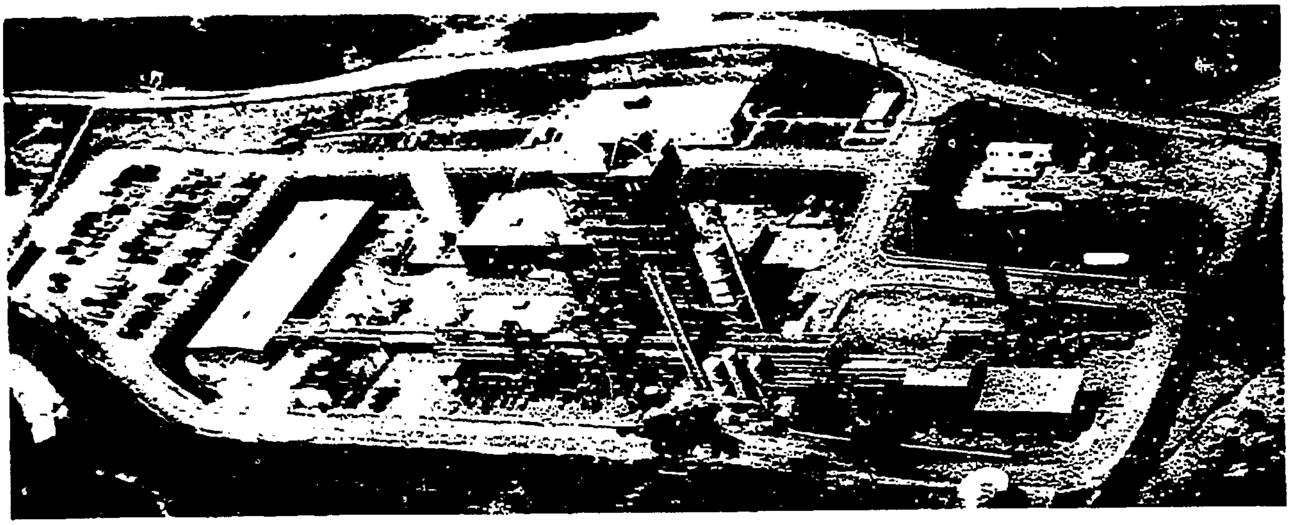


Figure 12. SYNTHANE Pilot Plant

and pneumatically transferred to a 100-ton pulverized-coal storage bin.

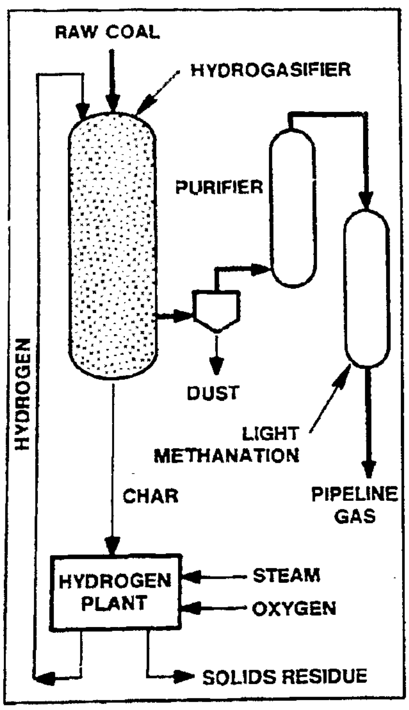


Figure 13. Dilute-Phase Free-Fall Hydrogasification Process, Flow Diagram

The pretreatment and gasification section is continuously fed from lock hoppers where the coal is pressurized to reaction pressure (600 to 1000 psig). In the fluidized-bed pretreatment, the coal particles are partially oxidized at 800°F (425°C) with steam and oxygen to prevent agglomeration; this step is not required for noncaking coals. The gasifier is a single-stage fluid-bed reactor, operating between 1400° and 1800°F (760-980°C). The bottom section is a fluid-bed char cooler from which there is a continuous char blowdown at reduced temperature (600°F) (315°C).

Raw gas from the gasifier, containing methane, hydrogen, carbon monoxide, carbon dioxide, steam, sulfur compounds (mainly H_2S), and several minor products, must be passed through a series of clean-up and conversion operations to produce clean high-Btu gas. These steps consist of water scrubbing, carbon monoxide shift conversion to adjust the hydrogen/carbon monoxide ratio to 3:1 for subsequent methanation, acid-gas removal using a Benfield unit (hot potassium carbonate), and finally methanation.

Methanation will be carried out using two methods developed at PETC. The first method utilizes a Tube Wall Reactor which consists of a shell and tube heat exchanger with the internal surface of the tubes coated with Raney nickel catalyst. Dowtherm is used to remove the heat of reaction from this methanator. The other method involves Hot-Gas Recycle through a bundle of stainless steel plates coated with Raney nickel catalyst. Temperature in this methanator is controlled by diluting the fresh feed gas with recycle gas. Offgas from the Benfield unit will contain most of the sulfur originally in the coal and will be treated in a Stretford unit which converts hydrogen sulfide to elemental sulfur.

Present plans for operation of the pilot plant cover the period from July 1976 to September 1980. During this period at least four different types of coal will be tested under a variety of operating conditions in order to demonstrate operability and reliability and to collect suffi-

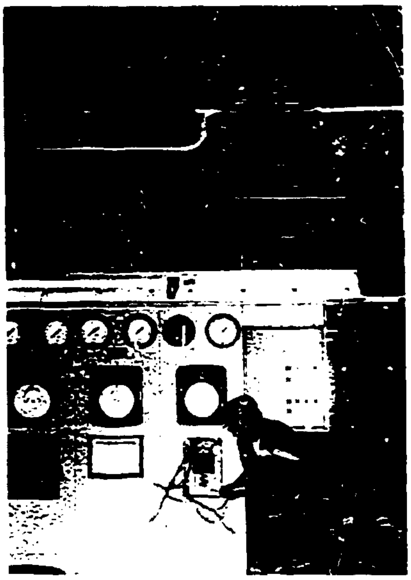


Figure 14. Assembling cold-flow model for fluid dynamic studies of the dilute-phase hydrogasification reaction.

cient data for the design of commercial plants. A western subbituminous coal, a mildly caking eastern coal, a highly caking eastern coal with high sulfur content, and a lignite will be tested. The gas purification, sulfur removal, and methanation units will be brought on line incrementally during the test program.

Advantages of the SYNTHANE process include: its ability to handle any type of coal; about 60 percent of the methane is formed in the gasifier, thus reducing the quantity of oxygen needed; and its good operability and reliability characteristics. Scale-up is relatively simple because a single-stage fluidized-bed gasifier is used.

Dilute-Phase Hydrogasification

The dilute-phase free-fall hydrogasification process (Figure 13), based on earlier work on the HYDRANE process, is a promising third-generation coal gasification process currently being developed at PETC. Comparative cost studies show that it could be the most economical method of producing pipeline-quality gas from coal. It differs from steam/oxygen gasification processes in several important ways. One of its unique features is that it permits coal to be fed directly to the gasifier, circumventing the problems of caking and agglomeration, and thereby eliminating the expensive pretreatment steps common to other processes. In addition, a hydrogen-rich portion of the coal sometimes lost in pretreatment is retained. Almost all of the methane in the product gas is produced in the single-stage gasifier by direct reaction of coal with hydrogen. This process scheme results in a high energy-conversion efficiency and requires only slight methanation to remove the small amount of carbon monoxide present in the gasifier product.

In the dilute-phase, free-fall hydrogasification process, crushed raw coal and hydrogen are fed into the upper section of the single-stage hydrogenation reactor, which is maintained at process conditions of 1650°F (900°C) and 1000 psig.

From the top of the reactor, the coal falls freely as a dilute cloud through the hydrogen. Volatile matter is released and the coal loses its agglomerating characteristics. About 40 percent of the carbon in the raw coal is converted directly to methane by reaction with hydrogen. Product gas is drawn off near the bottom of the reactor and is cleaned of residual solids and unwanted gases. Finally, methanation of the small amount (2 to 5 percent) of residual carbon monoxide produces a high-Btu, pipeline quality, substitute natural gas. Char formed during gasification is utilized to produce process hydrogen by reaction with steam.

Experimental studies are currently being conducted with a small-scale continuous-flow unit to optimize the reactor configuration and to acquire data applicable to the design of a larger-scale unit. Fundamental research related to the dilute-phase process is also being conducted. Fluid dynamic investigations of coal in free-fall are carried out in a cold flow model to obtain information for improved reactor designs, and studies of the process kinetics are also in progress. Construction of a large-scale Process Development Unit is being considered. This plant would be capable of processing 10-30 tons of raw coal per day and would employ coal handling and gas cleanup procedures similar to those used in other large-scale process development units developed by PETC.

As changes in process conditions can result in the formation of an appreciable amount of liquid product, dilute-phase liquefaction studies are also planned. A small-scale unit to demonstrate this novel liquefaction concept is in the design stage.

Figure 15. Making density measurements of char formed in the dilute-phase hydrogasification process.

COAL COMBUSTION

The PETC research and development program in coal combustion has as its primary near-term objective the development of equipment and procedures for efficient and clean burning of coal-oil mixtures to raise steam for use as such or for electric power generation. Also of major interest is the development of techniques for burning coal-derived fuels such as chars and solvent refined coal (SRC) in conventional power plants. Combustion of various agricultural wastes is also being studied. The goals of these projects are to obtain more efficient combusion and to determine the combustion characteristics and air pollution aspects for the various fuels studied.

Combustion of Coal-Oil Mixtures

The combustion of coal-oil mixtures in industrial boilers designed for burning oil has been identified by DOE as having a high potential for making a significant near-term impact on our national energy supply. Some sporadic investigations have been conducted over the years when petroleum supplies were threatened, but industrial applications were not developed because the shortages were short-lived, and economic advantages were precluded by the relatively low cost of petroleum. Now, with the increasingly high cost and scarcity of petroleum products, the advantages of coal-oil mixture combustion are strikingly evident.

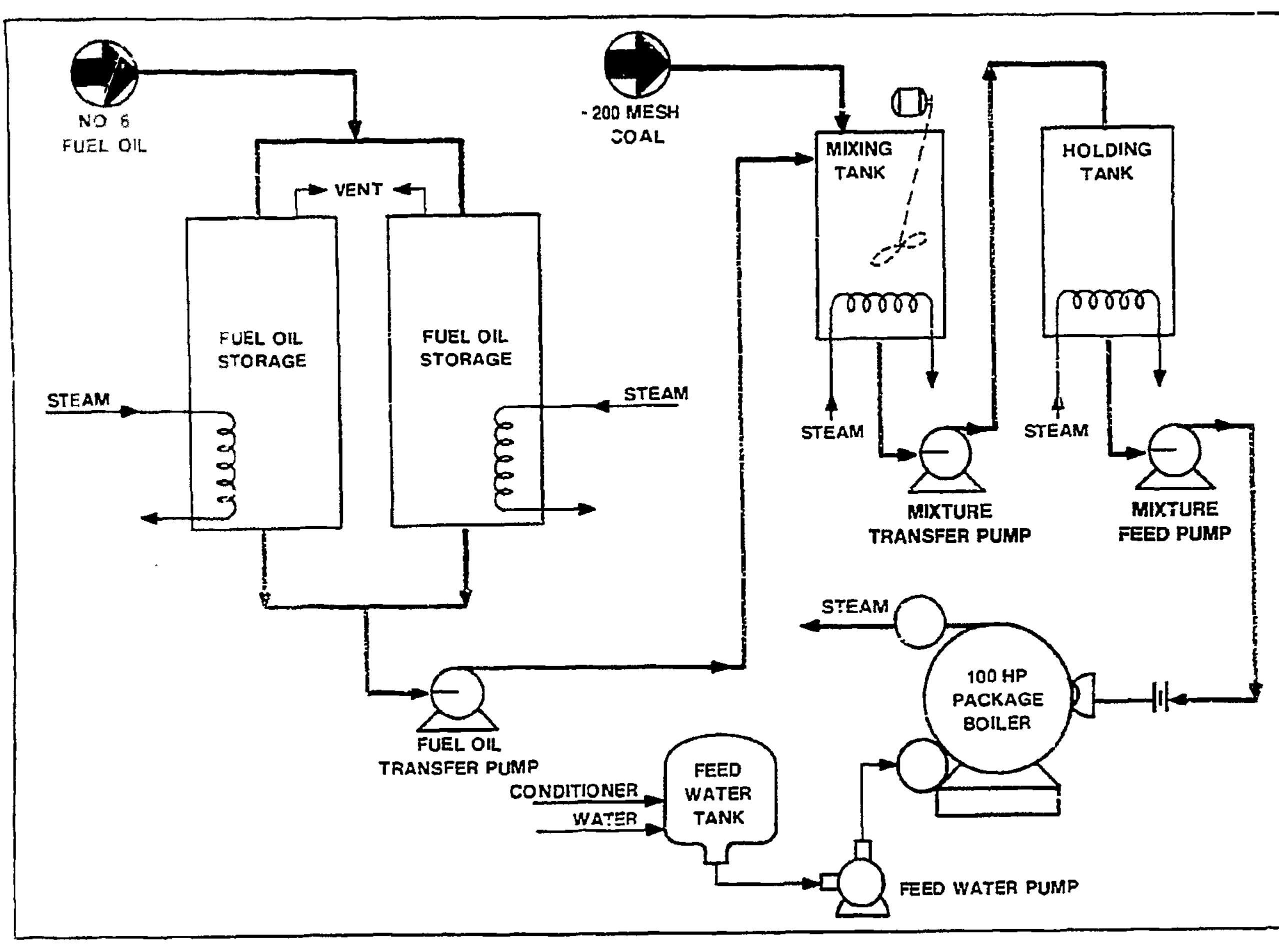


Figure 16. Coal-Oil Mixture Combustion Test Facility, Flow Diagram

Preliminary tests indicate it may be possible to replace up to 40 percent of the oil consumed by industry and utilities by relatively low-cost, indigeneous abundant, pulverized coal. Elsewhere, these coal-oil mixtures were successfully fired in short-term tests in boilers designed to burn oil or gas with little or no derating (reduction in capacity). The costs of converting oil-fired boilers to fire coal alone are very high, and the boilers would probably be derated because of the longer residence time required to burn coal alone. By comparison, the modifications required to accommodate coal-oil mixture firing are relatively simple and can be accomplished at a relatively low cost in a much shorter time. PETC will operate several test units in support of an intensive national coal-oil mixture combustion research program recently initiated.

Preliminary coal-oil mixture combustion studies were initially conducted in a 100-horsepower firetube package boiler. The principal components of the 100-horsepower facility are shown in the flow sheet, Figure 16. In addition to studying problems concerned with handling and combustion of mixtures, this facility provides information on corrosion of boiler tubes over long periods of operation.

However, a sophisticated, highly instrumented, coal-oil mixture combustion test facility, featuring a 700-horsepower watertube package boiler typical of medium and large-size oil-fired industrial boilers, is now operational. Construction was completed in 1978, and now the unit has begun an extensive test program. The highly instrumented facility will permit detailed evaluation of all aspects of mixture combustion, including flame characteristics, combustion efficiency, heat-transfer, corrosion, erosion, pollutant emissions, etc. In addition, bottom ash removal and pollutant control techniques will be developed.

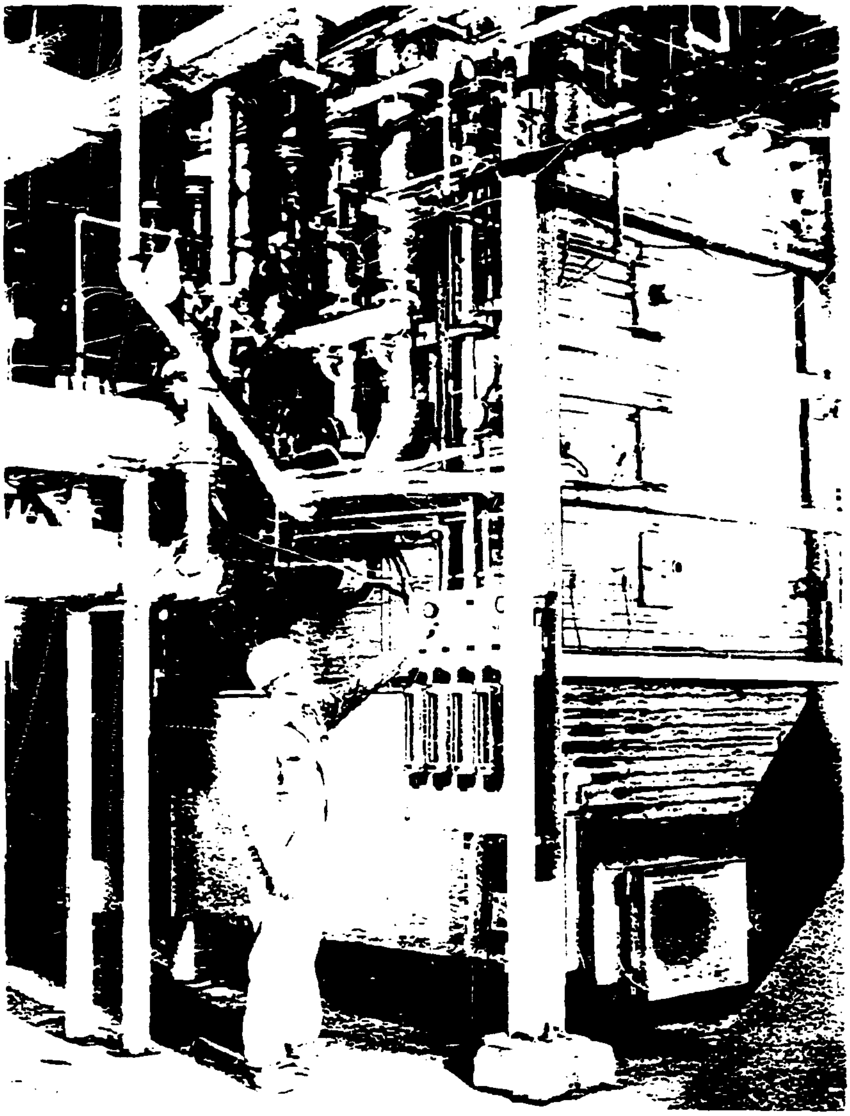


Figure 17. 500-Pound-per-Hour Coal Combustor

Combustion of Solid Fuels

A 500-pound (225 kg) per hour pulverized-coal-fired combustion test facility at PETC is being used to study pollutant emissions and other problems and to encourage the expanded use of coal in industrial steam-generating furnaces and coal-fired electric power plants. The experimental combustor closely simulates the performance of commercial plants and is the only one of its size in the country. Large industrial combustors are too unwieldy and costly to use for experimentation, while results obtained in smaller experimental furnaces are difficult to extrapolate to full scale.

The principal components of the combustion test facility are shown in the flow diagram (Figure 18). The water-cooled furnace is a wall-fired, dry-bottom unit designed to burn pulverized coal at a nominal rate of 500 pounds per hour. Fuel is pulverized in an impact mill and fed through four burners in the front wall of the rectangular furnace 12 feet high, 7 feet wide, and 5 feet deep (3.7 × 2.1 × 1.5 m). The combustion gas, exiting the combustor at 2000°F (1095°C) and cooled to about 1000°F (540°C) in the convective heat-transfer zone, flows through the recuperative air heater for preheating the secondary combustion air, then goes to a particulate collector and induced draft fan, and finally exits from the stack.

The experimental unit is principally used to devise methods for reducing the emission of pollutants from coal-fired combustors and to develop techniques for burning the unreactive char produced as a byproduct in most of the processes converting coal to substitute natural gas or oil. Economics dictate that these char byproducts be utilized, for about 50 percent of the coal ends up as char in some processes. More recently, the facility is being used to study the handling, pulverizing, combustion, and fouling characteristics of coal-derived fuels such as solvent-refined coal (SRC) and SYNTHANE char. The effects of combustion parameters such as primary and secondary air temperature, excess air, and particle size on ignition, flame stability, and combustion stability are under investigation. Pollutant emissions are monitored, and various techniques for controlling NO_x emissions are being explored.

With decreasing availability of natural gas and uncertainties surrounding fuel oil, coal will again become a prime source of fossil energy for the future. The solid fuel test facility will provide industry with operating information needed for adaptation of conventional systems for utilization of new coal-derived fuels as well as methods for improving operations with presently available solid fuels.

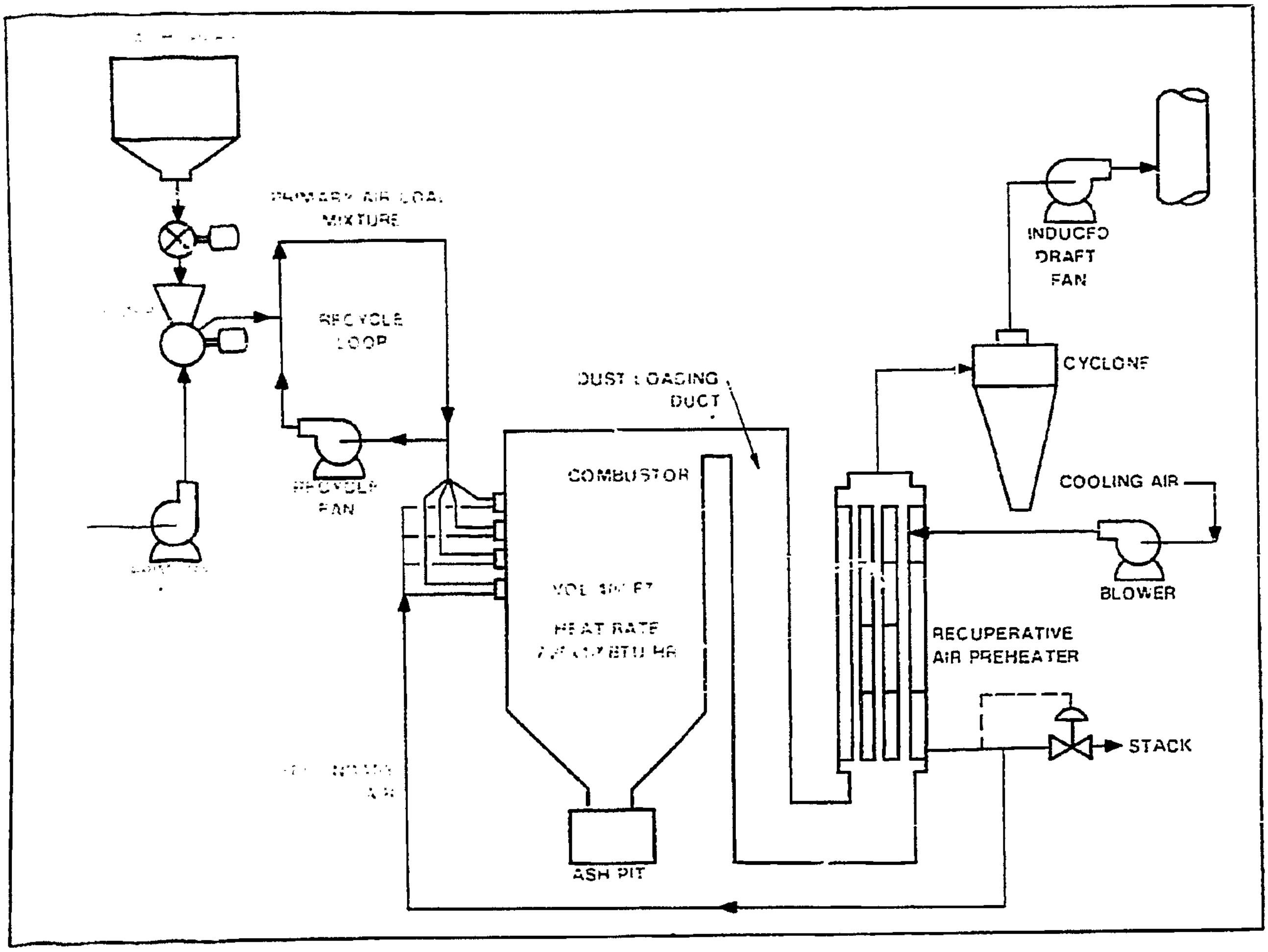


Figure 18. 500-Pound-per-Hour Coal Combustion System, Flow Diagram

MAGNETOHYDRODYNAMIC POWER GENERATION

A promising technique for improving the efficiency in converting fossil fuels into electrical energy involves the principles of magnetohydrodynamics (MHD). In an MHD power plant, electricity is generated by passing very high-temperature, electrically conductive combustion gases through a magnetic field. The gases leaving this MHD generator are still hot enough to produce additional electricity in a conventional steam power plant. The efficiency of a commercial combined MHD steam turbine plant would be 25 to 50 percent greater than that of modern coal-fired stations. Research conducted at the Pittsburgh Energy Technology Center has also shown that MHD power plants will operate with extremely low levels of pollutant emissions. Low-grade, high-sulfur coals can thus be utilized in an environmentally desirable manner

Component Development and Integration Facility

Research in MHD energy conversion is oriented toward the design, fabrication, and testing of a 50-megawatt thermal (120 tons of coal

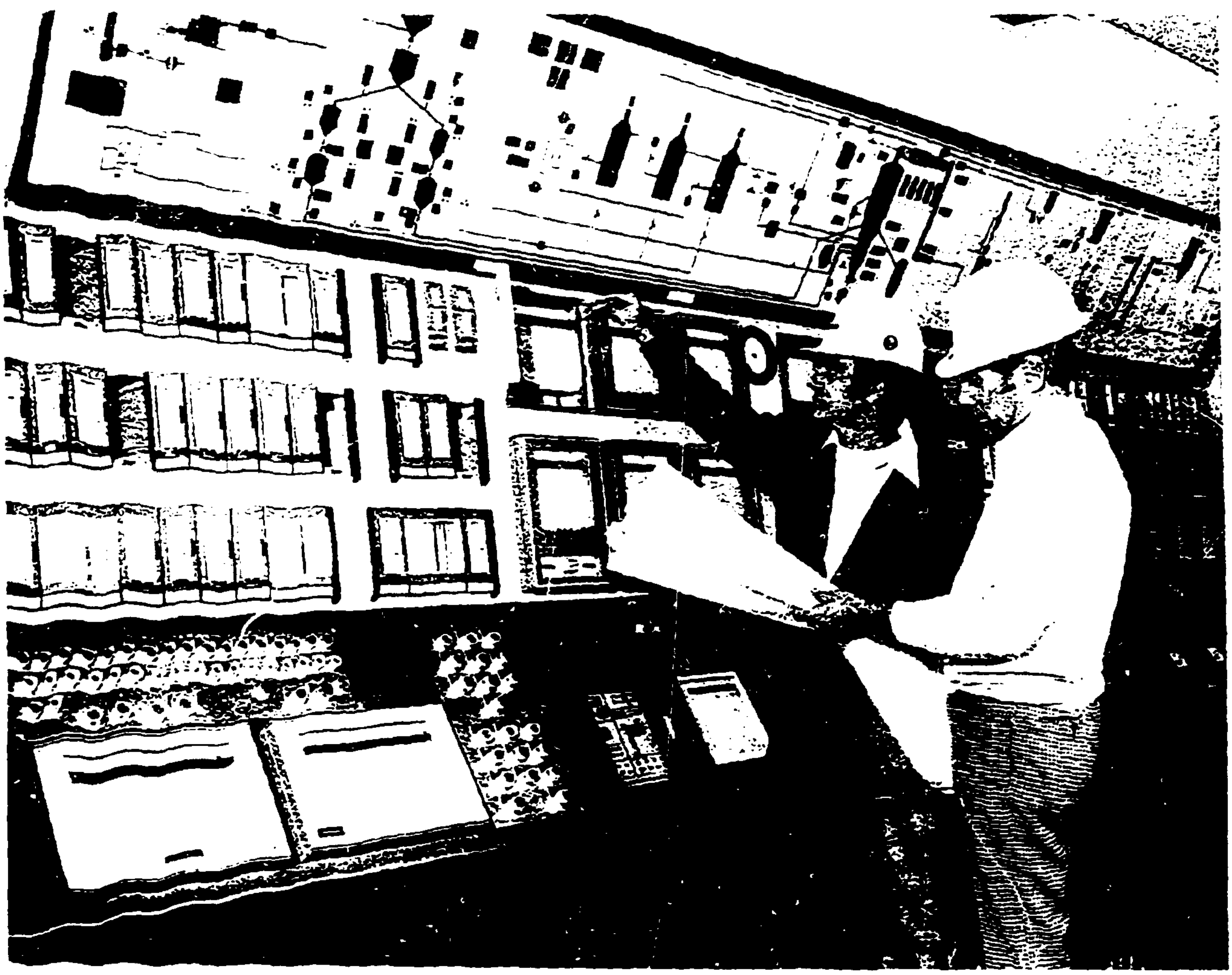


Figure 19. Control Room. Two-Stage Pressurized MHD Coal Combustor

per day) MHD gasifier-combustor. This unit will be installed in the Component Development and Integration Facility (CDIF) located in Butte, Montana. The CDIF represents a key element in the national MHD development program. Operations at the facility are expected to begin in 1980.

The CDIF combustor will consist of two stages and will operate at a pressure of 6 atmospheres. In the first stage, a cyclone gasifier, a relatively clean low-Btu fuel gas is produced. Most of the coal ash is rejected from this first stage as molten slag. Potassium carbonate "seed" is then added to the fuel gas which is burned in the second stage to produce the high-temperature plasma required to generate electricity. The seed material is recovered, regenerated, and recycled for use again.

Design data for the CDIF combustor was initially acquired through operation of smaller-scale facilities at PETC. A two-stage pressurized combustor, which will burn approximately 1000 pounds of coal per hour, began operating in 1976. This unit, except for size, is conceptually similar to that proposed for the CDIF. All data are collected automatically and are fed to a computer for detailed computations.

CHEMICALS FROM COAL

Fuel and Petrochemicals from Synthesis Gas

Projections of demand for C_2-C_4 olefins in the U. S. during the next decade indicate that a two-fold expansion in manufacturing capacity will be necessary. This new capacity will be based primarily on cracking heavier feedstocks, such as naphtha or gas oil derived from coal. Besides these olefins, which are valuable as basic chemicals for the manufacture of plastics and rubber, the paraffinic C_2-C_3 hydrocarbons are valuable as high-Btu supplements for pipeline gas. Any excess of propane or butane will find its way to market via liquefied petroleum gas. Alcohols and hydrocarbons of somewhat higher molecular weight can be used as gasoline blending stocks or cracked to gaseous hydrocarbons.

The production of C_2-C_4 hydrocarbons or other chemicals from coal could be achieved by a combination of processes with synthesis gas as the feedstock. The flow diagram, Figure 20, shows the gasification of coal in the presence of steam and oxygen to produce synthesis gas, a mixture of carbon monoxide and hydrogen. Commercial gasifiers such as Koppers-Totzek, Lurgi, or Winkler could be used. New gasifier designs, such as that used in the SYNTHANE, HYGAS, or BI-GAS processes, are being tested and will become available for this purpose.

Following the gasifier, entrained dust and condensable tars are separated from the gas product in a spray tower. Gas leaves the spray tower and enters a shift converter in which the volumetric proportion of hydrogen to carbon monoxide is adjusted to the desired ratio by the reaction of water vapor with carbon monoxide. After shifting, the gas is purified by removal of carbon dioxide, hydrogen sulfide, and carbonyl sulfide, the latter two being poisons for the catalysts used in the conversion of the synthesis gas to hydrocarbons of low molecular weight. The clean, sulfur-free gas finally is sent to the hydrocarbon catalytic converter.

The technology for achieving all the steps up to the hydrocarbon catalytic converter is already available. A considerable research effort is being devoted to development of a catalytic process for selective formation of C_2-C_8 hydrocarbons and oxygenates. Since the reaction is highly exothermic and the reaction temperature in the converter is an important variable, it is possible that the tube-wall or hot gas recycle reactor found useful in the SYNTHANE process will be used to control reaction temperatures. Another aspect of the tube wall reactor is its potential to improve the overall thermal efficiency of Fischer-Tropsch plants.

Ethanol and Ethylene from Coal

Methanol is made commercially from synthesis gas. Methanol can be further reacted with additional synthesis gas, in the presence of a homogeneous catalyst, to produce

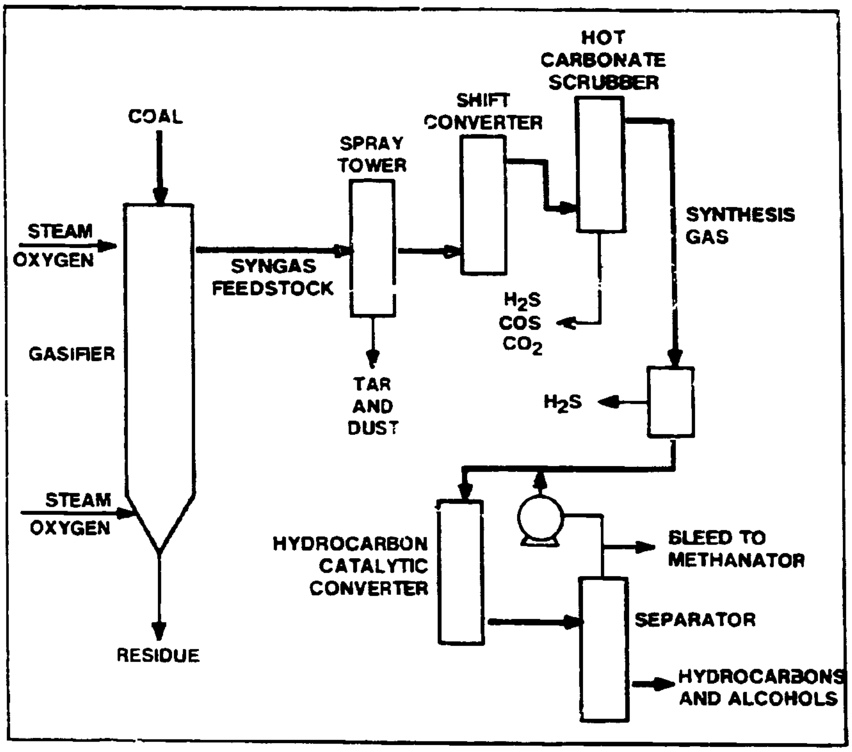


Figure 20. Hydrocarbon Synthesis, Coal to Fuels and Petrochemicals, Flow Diagram

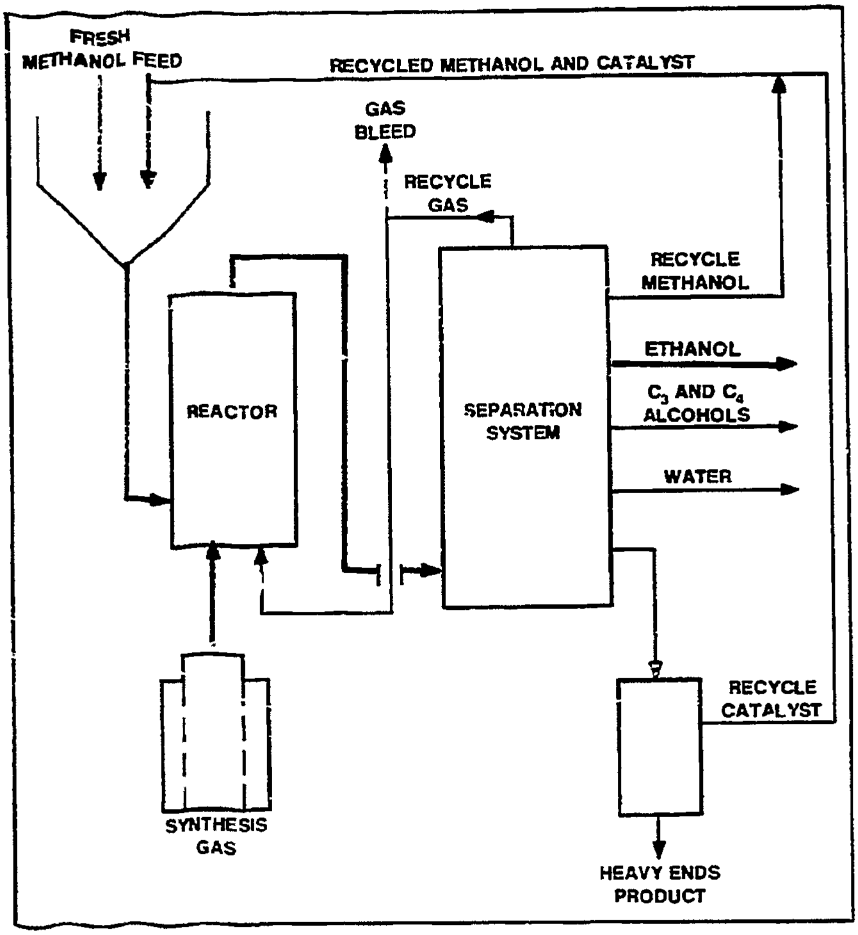


Figure 21. Homologation of Methanol to Ethanol, Flow Diagram

ethanol and small amounts of higher alcohols. This reaction, catalyzed by dicobalt octacarbonyl, was discovered in this laboratory 25 years ago. It was then regarded as not much more than a scientific curiosity. In the past few years, however, interest in the synthesis of ethanol from methanol has grown because olefins, especially ethylene, can be made by dehydrating the alcohol products. A typical flow diagram is shown in Figure 21. Investigation of various catalysts, cocatalysts, and promoters has been initiated to find the combination that will yield the most ethanol and the least byproduct.

The experiments currently are made in small-scale, high-pressure, batch reaction vessels. High ethanol selectivity (more than 70 percent) at moderate conversion of methanol (more than 35 percent) has already been achieved. Other homogeneously catalyzed reactions of synthesis gas to produce chemicals of low molecular weight are also being sought. Methanol and formaldehyde can be produced from synthesis gas when certain organometallic reaction sequences are followed. It may be possible to hydrogenate carbon monoxide at milder temperatures than must now be used commercially with heterogeneous catalysts in the production of methanol. Reactive organometallic systems, used as homogeneous catalysts, would appear to be the most likely means of accomplishing this at lower temperatures.

A low-temperature process would be a major breakthrough in technology because methanol production becomes thermodynamically more favorable as the reaction temperature is lowered. In addition, homogeneous catalysts, unlike heterogeneous catalysts, are usually not poisoned by sulfur compounds and this would be a great advantage.

PROCESS SUPPORT RESEARCH

Coal conversion processes that are currently being developed require, due to their complex nature, incorporation of techniques and know-how in many disciplines of science and engineering. Even though both coal liquefaction and gasification processes, for example, are based on sound process concepts, their success depends heavily on the functioning of many of the key components that constitute the basic framework of overall processes.

The primary goals of Process Support Research, therefore, are to perform research in key process areas, to develop new and improved methods to ensure successful overall process development, and, at the same time, to generate basic information as well as new process concepts to develop "revolutionary" future generation technology.

In the areas of key process component research, various disciplines, such as catalysis, pyrolysis, solid-liquid separation, product upgrading, byproduct utilization, computer simulation, etc., are key areas of endeavor. Much of the state of the art in catalyst technology originated from petroleum-oriented process applications. It is vitally important, therefore, to develop catalyst technology that is suitable for new fuel sources, such as gas from coal and liquids from coal.

Important functions of DOE's Energy Technology Centers are the generation of basic information and exploratory research for the development of future generation energy technology. With this in mind, a number of projects are directed toward meeting this goal. In the past, similar effort has been put forth, and, as a result, processes such as COSTEAM and simple chemical desulfurization of coal were conceived and are being developed. These processes have potential to utilize the abundant supply of coal and other sources of carbon in the United States for the production of environmentally acceptable fuels at the lowest possible cost.

Mechanism of Coal Liquefaction

Although various processes successfully liquefy coal, the chemical changes that occur in these processes are only partially understood. Understanding what happens chemically during the liquefaction of coal may lead to further improvements in liquefaction processes. One way to find clues as to what transpires during the conversion to oil is to study the chemical composition of the products at each stage of the reaction.

In a separation scheme used for liquefaction products and solvent refined coal, the products are separated into classes defined by solubility in three solvents: pyridine, toluene, and pentane. Further characterization of the amount, elemental analysis, molecular size, and type of compounds in each of these classes helps researchers to envision the chemical steps that take place in the conversion of coal. For example, the class labeled oil in Figure 22 is typically composed of a complex mixture of aromatic and aliphatic compounds. Some of the compounds found in the oil contain "heteroatoms," such as oxygen, nitrogen, and sulfur. Oil molecules have an average molecular weight of around 250. Asphaltenes, intermediates in the conversion of coal to oil, are somewhat larger molecules, with average molecular weights ranging from 500 to 800.

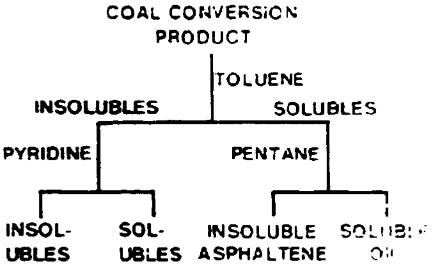


Figure 22. Separation Scheme for Coal Conversion Products

Unconverted asphaltenes increase the viscosity of the oil markedly, and asphaltenes are soluble in benzene or toluene but insoluble in pentane. Also, this class contains a somewhat greater amount of heteroatoms. The pyridine solubles are still larger molecules and have even greater amounts of heteroatoms. The pyridine insolubles are largely composed of inorganic mineral matter and a partially converted intractable organic portion of coal no more than 2% by weight of the original coal. Analyses such as these along with other evidence are the bases for the deduction that the conversion of coal to oil proceeds in a stepwise fashion. Compounds in coal are progressively reduced in molecular size as they pass through the stages: pyridine solubles to asphaltenes to oil.

Liquefaction processes use a catalyst, commonly employed in the petroleum industry, in order to remove heteroatoms, sulfur in particular, more efficiently from the liquid products. In this project, the activities of fresh and used catalyst are compared, and the mechanisms of catalyst deactivation are studied with the aid of a pulse-flow microreactor. Model compounds are selected to evaluate several catalyst

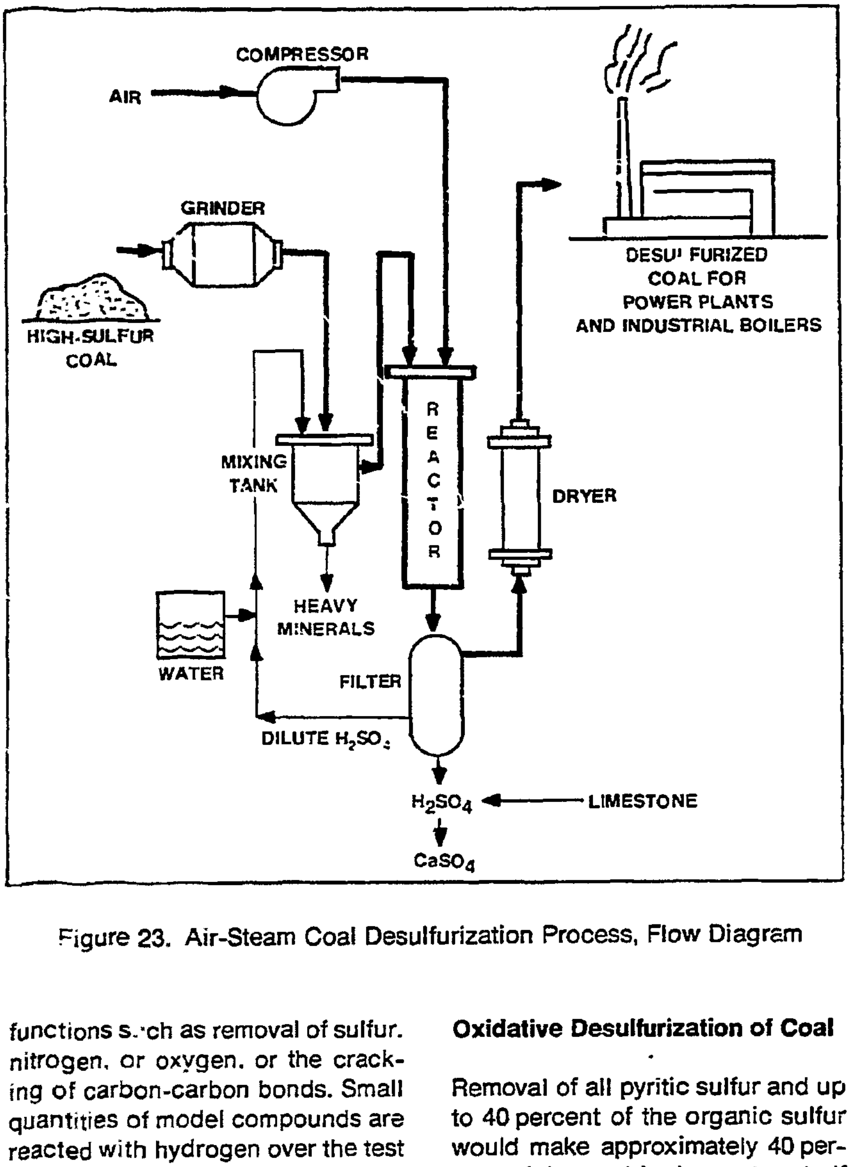


Figure 23. Air-Steam Coal Desulfurization Process, Flow Diagram

functions such as removal of sulfur, nitrogen, or oxygen, or the cracking of carbon-carbon bonds. Small quantities of model compounds are reacted with hydrogen over the test catalyst in the microreactor, and the reaction products flow directly into a gas chromatograph for immediate analysis. With such data, catalysts may be compared, the reasons for deactivation may be deduced, and various means of regeneration may be evaluated. This knowledge will be useful in preparing catalysts designed specifically for coal liquefaction processes, which would be more efficient and longer lived in this application.

Oxidative Desulfurization of Coal

Removal of all pyritic sulfur and up to 40 percent of the organic sulfur would make approximately 40 percent of the coal in the eastern half of the U. S. environmentally acceptable as fuel for electric power generation and industrial boilers. A process that does this, using only air and water, is being developed at PETC and promises to be an important near-term solution of some of our energy problems. Fuel recovery is over 90 percent, and the treated coal can be used in existing power plants without further modification. The process makes use of existing equipment technology, and, being much simpler than other coal desulfurization processes, could be developed for commercial application in the near future.

The process, diagrammed in Figure 23, uses only water, limestone, compressed air, and crushed coal. The air and coal-water slurry are continuously fed to a reactor kept at 300-390°F (150 to 200°C) and 400 to 1000 psi (3-7 MPa). Within a contact time of 5 to 30 minutes, the pyritic sulfur (FeS_2) is oxidized to sulfuric acid. As much as 40 percent of the organic sulfur in the coal may also be converted to sulfuric acid. The treated slurry, as it is continuously removed from the reactor, is filtered to separate a low-sulfur coal product from the dilute sulfuric acid. After washing and drying, the coal is suitable for direct combustion in boilers. Because the oxidative desulfurization destroys the caking properties of coal, it can be used as an effective pretreatment step for coal conversion processes where caking is a problem.

The dilute sulfuric acid formed in oxidative desulfurization could be used where acid is needed to neutralize alkaline effluents, such as ammonia (NH_3), generated in other coal conversion processes. Alternatively, the sulfuric acid can be neutralized with limestone.

At the present time, PETC is building a continuous unit to evaluate the process variables and to optimize the process prior to scale-up.

Catalysis Research

The catalysis program conducts research aimed at the development of catalytic materials for the conversion of coal to clean liquid and gaseous fuels. To carry out this task, the research program is devoted to four major areas: synthesis of new catalytic materials and their fabrication into useful catalyst shapes; characterization of their surface and bulk properties; measurement

Figure 24. Precipitation Step in Preparation of New Coal-Conversion Catalysts

of their catalytic activity and selectivity; and study of catalyst poisoning and deactivation. Also, the research program covers the development of catalysts that can be used by processes being developed at PETC as well as other laboratories. These include catalysts for converting coal to low-sulfur coal liquids, converting synthesis gas to methane or higher hydrocarbons and oxygenated products, and upgrading coal liquids to fuels and chemicals.

The various processes currently considered for the conversion of coal to liquid products, as in liquefaction and upgrading processes, require new catalysts. The catalysts now used were originally developed for refining petroleum fractions and are not well suited to coal conversion. Consequently, the properties of new catalysts have to be formulated for working with the highly aromatic molecules present in coal liquids. Resistance to poisoning by the various elements and compounds present in coals and coal liquids will also have to be developed for the catalysts to be practical.

The coal liquefaction and catalyst upgrading programs synthesize new and novel catalysts for these applications. The catalysts are tested to determine their activity, selectivity, resistance to poisoning, and effect on product composition. Phase relations, surface composition, surface area, pore structure, and other important characteristics are determined to ensure that the catalysts are stable. The correlations that are developed are used to guide the development of more effective catalysts.

The catalyst program also experiments with the variables involved in the forming of catalyst pellets, extrudates, spheres, and other forms. The forming operation and its effect on catalytic properties must be understood and controlled if metal and metal-oxide catalysts are to be successfully prepared on the commercial scale required by coal conversion processes.

Catalysis research also includes studies of the production of high-Btu gas such as in the final step in the SYNTHANE process. Methanation is the conversion of carbon monoxide and hydrogen into methane under highly exothermic conditions. To obtain high yields of methane, the temperature must be controlled, and a rugged catalyst is required. Certain metals such as nickel are very active and selective for methanation. Studies are under way to identify the factors that cause catalyst aging and loss of activity. Various catalyst modifications designed to increase resistance to deactivation are being tried, and both fresh and aged catalysts are being examined by chemical and physical techniques, including X-ray photoelectron spectroscopy, in which measurement of energies of photoelectrons, ejected by "soft" X-rays from near the catalyst surface, gives a semi-quantitative elemental analysis of the surface.

New Catalytic Processes for Chemicals

Over the past 30 years, most new processes for large-scale manufacture of organic chemicals have been based on petroleum feedstocks. As our nation shifts from petroleum and natural gas back to coal as the major source of fossil energy, great quantities of coal liquids will be produced which could, in the future, be an important source of chemicals.

Coal liquids differ from petroleum crude oil in several important ways. Coal liquefaction processes usually do not yield the sizable low-boiling fraction found in crude oil nor do coal liquids have the favorable high H/C ratio of petroleum. As a consequence, coal liquids are more aromatic and may become a preferred source of BTX (benzene, toluene, and xylene) and other aromatic chemicals. Catalytic systems capable of converting fractions of moderately high molecular weight into low molecular weight aromatics will be needed. This will require catalysts tailored for hydrocracking or hydrodealkylating without excessive hydrogenation of the aromatic ring structure. Fractions from PETC coal liquefaction processes, as well as H-Coal and Solvent Refined Coal (SRC), will be utilized as standard feedstocks in a testing program. Also, a few "simple" materials, such as anthracene oil or even specific compounds, will serve as model feedstocks in a preliminary screening test to identify catalysts with greatly different activities or to examine different reaction routes occurring over new catalytic systems. The reactions that appear to offer the greatest change of success are mild hydrocracking and hydrodealkylation. Initial work therefore will concentrate on developing short, easily reproduced screening tests.

Upgrading Coal Liquids

Coal liquids produced from processes under development by private industry, such as H-Coal, SRC, and others, generally have relatively high contents of particulates, asphaltenes, organic sulfur, nitrogen, and oxygen. The Pittsburgh Energy Technology Center is currently developing technical capabilities for upgrading coal-derived liquids in order to produce environmentally acceptable liquid fuels for engines, furnaces, and other facilities.

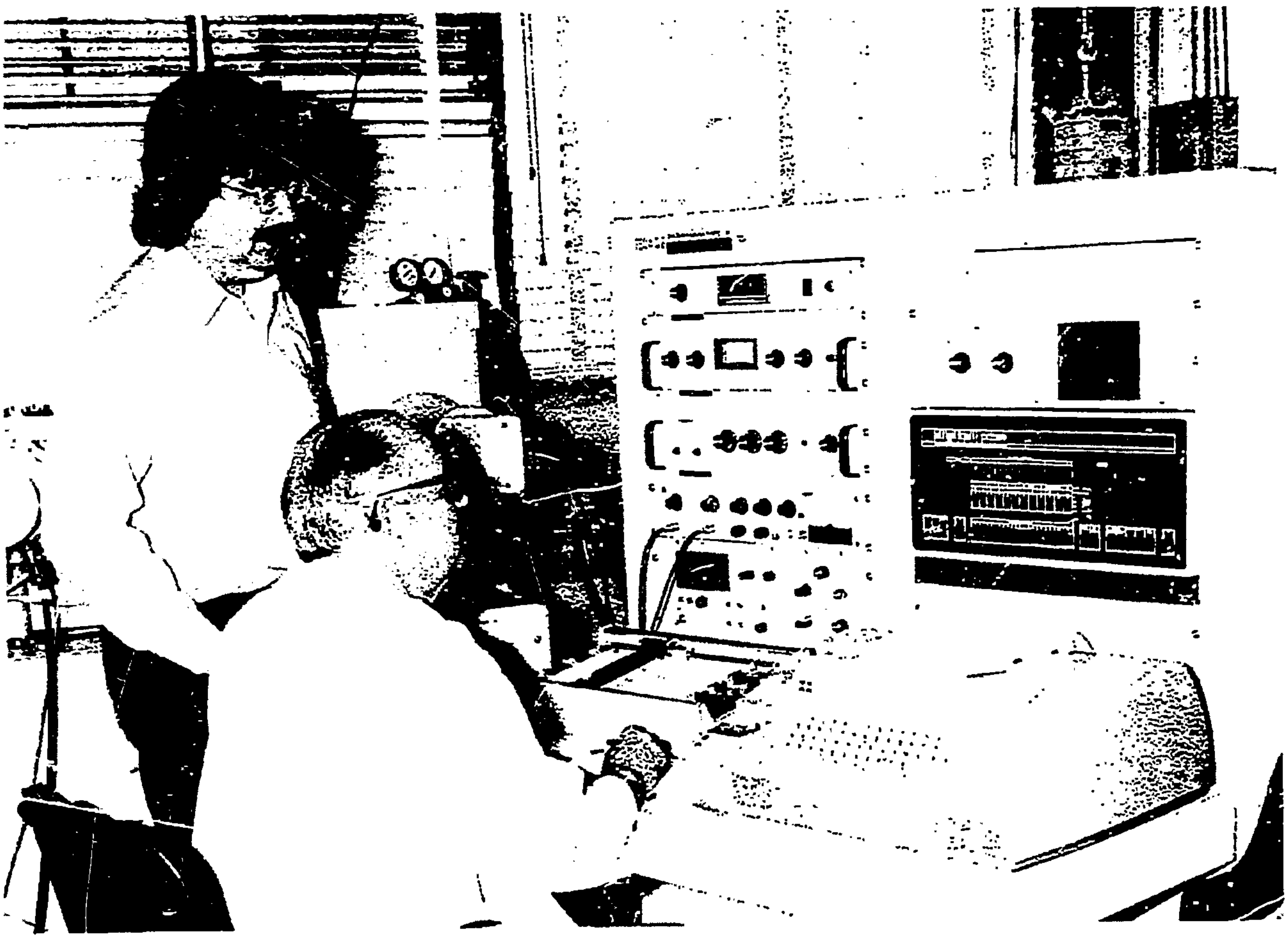


Figure 25. ESCA Unit for Surface Characterization of Catalysts

CHEMICAL AND INSTRUMENTAL ANALYSIS

Analytical support groups at PETC make use of a variety of modern instrumental techniques to study the physical and chemical structure of coal and coal products and properties of air, water, and waste pollutants. These techniques and their major applications are shown in the following list:

High-Resolution Mass Spectrometry—Characterization of liquid and solid products of coal conversion.

Low-Resolution Mass Spectrometry—Analysis of gases from SYNTHANE and other processes.

Gas Chromatography-Mass Spectrometry—Analysis of light oil products and other liquid streams.

Spark Source Mass Spectrometry—Characterization of minor and trace elements in liquefaction, SYNTHANE, and other coal conversion process streams.

Secondary Ion Mass Spectrometry—Depth profiles of elemental composition of conversion catalysts.

High Pressure Liquid Chromatography—Separation and analysis of coal liquefaction liquids.

Flame Photometric Gas Chromatography—Sulfur analysis of gases from coal conversion processes.

Infrared Spectrometry—Determination of organic functional groups in coal liquids and composition of coal minerals. Studies of adsorbed species on catalysts.

Laser-Raman Spectrometry—Investigation of deactivation of coal conversion catalysts.

Ultraviolet Spectrometry—Analysis of aromatics in coals and products, phenols in waste waters, and organic groups and compounds.

Fluorescence Spectrometry—Detection of polynuclear aromatics in coal liquids.

Nuclear Magnetic Resonance—Determination of chemical and molecular structure of coal liquids.

Electron Spin Resonance—Determination of paramagnetic species (free radicals, charge carriers, transition metal ions) in coals and products.

Low-Temperature Ashing—Preparation of nearly undisturbed minerals from coals and products for more authentic analysis than possible with conventional analyses.

Scanning Electron Microscopy and X-Ray Analysis—Observation, photography, and micro-analysis of small areas on catalysts, fly ash, and coal minerals.

Gas Chromatography—Routine gas analysis of products of coal combustion and conversion processes. Controlled by a data processing system that collects, computes, and reports data from as many as 30 gas chromatographs.

Atomic Absorption Spectrophotometry and Specific Ion Electrode Analysis—Analysis of metals in catalysts, seed materials in MHD, and trace elements in coals and conversion products.

X-Ray Diffraction and Fluorescence Analysis—Analysis of compounds and elements in catalyst materials, deposits, and effluents of coal combustion and conversion.

Automated Surface Area-Pore Volume Analysis—Determination of internal structure and external surface in catalysts and fine particulate materials.

Micro C-H-N-O-S Analysis—Elemental analysis of less than 10 mg samples of coal and coal products.

Rapid Sulfur Analysis—Determination of sulfur content of fuels in 50 mg samples in 15 minutes.

Figure 26. Laser-Raman Spectrometer for Investigating Deactivation of Coal-Conversion Catalysts

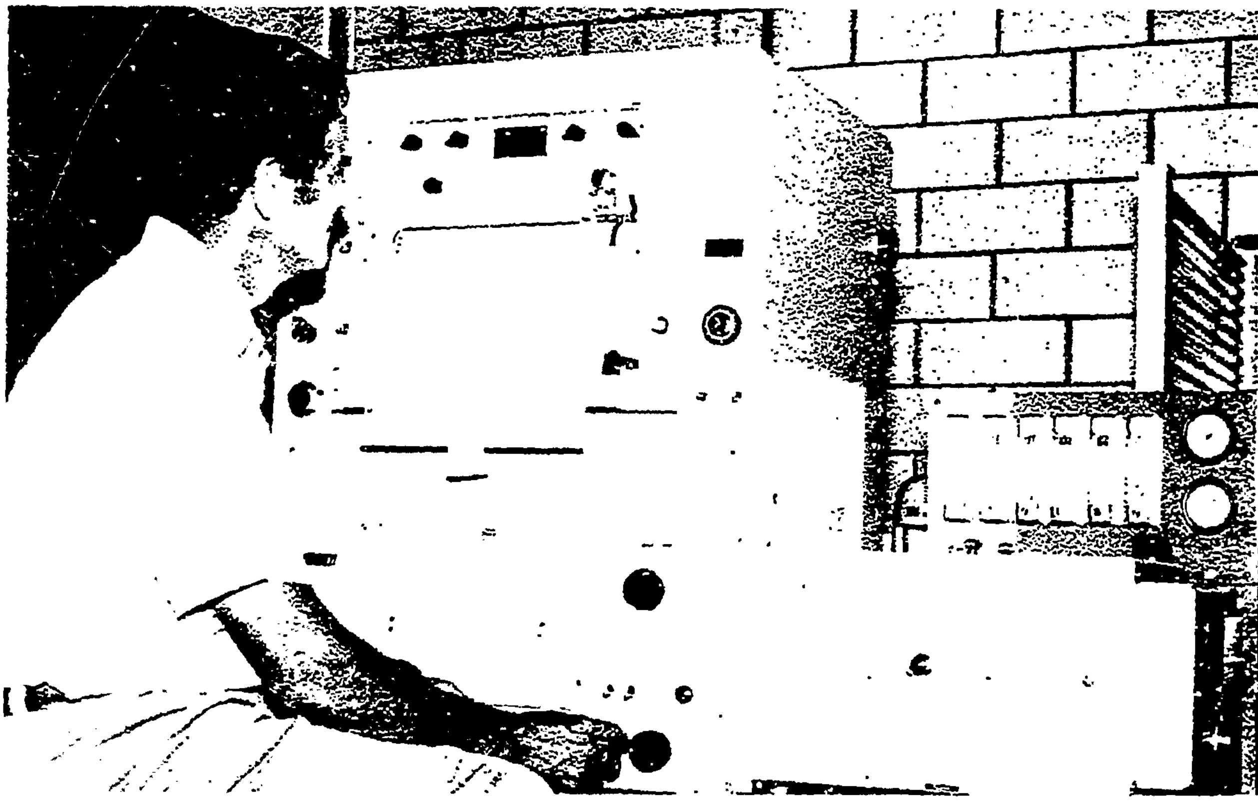


Figure 27. Ultraviolet Spectrometer Used in Analysis of Aromatics in Coal. Phenols in Waste Waters. and Organic Groups and Compounds

ASTM Elemental Analysis—Measurement of C-H-N-O-S and ash contents by standard methods.

Solvent Analysis—Determination of benzene and pentane solubles and insolubles in coal liquids.

Viscosity Determination—Measurement of viscosity of coal liquids.

Water Analysis—Determination of biological and chemical oxygen demands (BOD. COD). as well as many other parameters. in waste waters.

Recent and current applications of these instruments and techniques to development of coal conversion and combustion processes have in-

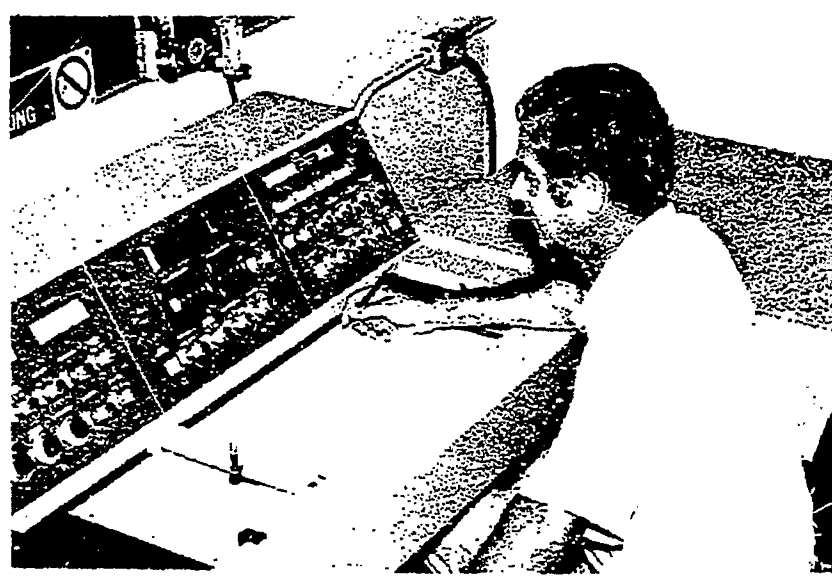


Figure 28. Infrared Spectrometer for Determining Organic Functional Groups in Coal Liquids and Composition of Coal Minerals

volved investigations such as the following:

- Mechanism of viscosity increase with age in coal-derived oils and development of inhibitors for this behavior.
- Causes of deactivation of catalysts in liquefaction and gasification processes.
- Nature and content of heterocyclic compounds containing oxygen, nitrogen, and sulfur in coal liquids.
- Presence of possible hazardous elements and compounds in process streams.
- Changes in chemical structure during coal liquefaction.

Most of these studies concern problems that have arisen in the development of coal conversion and utilization processes. Contributions to better understanding of these problems and possible solutions for them would be of great value in speeding the successful commercialization of these processes.

Figure 29. Spark-Source Mass Spectrometer

Figure 30. Nuclear Magnetic-Resonance Spectrometer

ENVIRONMENT AND ENERGY CONSERVATION DIVISION

Environmental Research

The environmental team at PETC evaluates and assesses the environmental implications of PETC operations and research developments. The two main objectives are to provide short-term environmental support in operation and research areas at PETC and to conduct long-term research to identify and resolve potential environmental problems in demonstration and commercialization of coal conversion processes. Major specific activities are diagrammed in Figure 31.

The scope of the effort includes detailed examination of the environmental parameters that relate to siting, development, and operation of coal conversion processes. These include:

- air pollution control—ambient air monitoring, stack testing, air pollution control technology, and air diffusion modeling;
- environmental impact assessment, and statement preparation and evaluation—to provide for public involvement and review of DOE's anticipated activities;
- noise pollution control—in-plant noise transmission, monitoring, and control;
- solid waste—recycling, reuse, disposal techniques, and assessments;
- occupational-environmental health—the development of guidelines for worker and consumer safety in production, distribution, and product use and disposal;
- and lastly, water pollution control—National Pollutant Discharge Elimination System (NPDES) water monitoring, water pollution control technology, waste stream characterization, and water conservation and reuse.

The results of these environmental studies are then integrated and fed back into the coal conversion development process to provide for cleaner, safer, environmentally sound, and more energy efficient processes.

This comprehensive environmental approach is being applied to the SYNTHANE and liquefaction plants at PETC. Assistance has also been provided to other pilot and demonstration plants throughout DOE and industry. Conservation and environment go hand-in-hand, and each complements and supports the other.

Conservation Research

PETC personnel also conduct net-energy efficiency studies of existing and new facilities, review designs for energy utilization in new construction, and conduct the Federal Energy Management Program at PETC. Reseachers also initiate, evaluate, and monitor projects in the areas of thermal efficiency and the potential for energy recovery associated with coal conversion/utilization programs at PETC, and advise Fossil Energy, DOE Headquarters, on energy conservation opportunities in the DOE coal conversion/utilization commercialization programs.

In general, PETC personnel contribute to:

- Development of a uniform energy-audit methodology.
- Analysis of energy conservation technologies.
- Establishment of a data base for costs and energy savings.
- Implementation of a program designed to reflect a higher priority on energy efficiency.

Specific research activities include analysis of the potential for energy conservation in coal conversion processes. This project identifies energy conservation opportunities in coal conversion and provides guidelines for their selection, analysis, and implementation. The overall objective is to attain a marketable technology attuned to the DOE national priority of optimum energy utilization in industrial processes. A significant portion of the work concentrates on what is actually being done by design firms to optimize energy utilization in large plants.

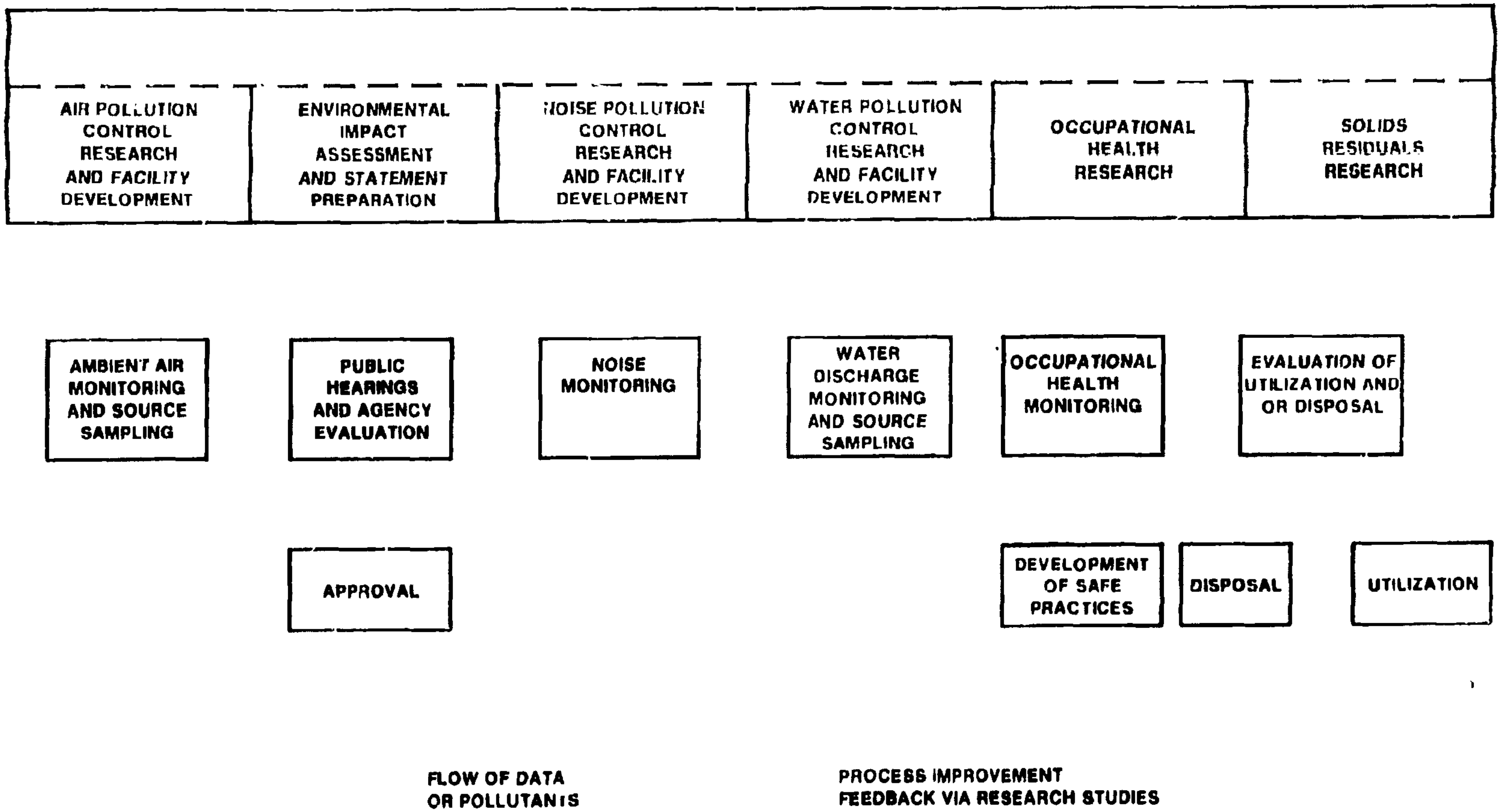


Figure 31. Coal Conversion Processes and Related Environmental Research

ORGANIZATION OF THE PITTSBURGH ENERGY TECHNOLOGY CENTER

Figure 32 shows an organization chart of PETC. The Center is composed of three engineering groups, three science and support groups, and an administrative section. These are coordinated by the Office of the Director which provides program planning and managerial support and serves as a liaison with DOE headquarters officials in Washington, D. C.

Direct Conversion Processes

The Direct Conversion Processes division conducts research and development to advance the state of the art of converting coal directly into clean liquid and gaseous fuels, via liquefaction, dilute phase hydrogasification, and other processes. Such fuels can be transported more economically than raw coal and can be utilized with minimal effects on the environment. A broad spectrum of activities is in progress, ranging from applied research on new conversion processes to development of the more mature technologies. Emphasis is placed on the development of processes which are technically and economically viable.

The responsibilities of the Direct Conversion Processes division are basically two-fold. First, new processes and modifications of existing processes are critically evaluated with respect to both engineering and economic feasibility. Then, if these evaluations prove promising, programs are initiated, as for example, the 10 ton-per-day Bruceton Coal Liquefaction PDU, to provide design data for larger-scale units. The ultimate objective is to develop the technology necessary for construction of commercial coal conversion plants and to promote the transfer of this technology to the private sector.

Process Engineering

The Process Engineering division conducts bench-scale and pilot-plant development work mainly on coal gasification processes to produce substitute natural gas (SNG). Research is also being conducted on new process concepts to improve the conversion of coal to SNG.

Currently, a 1/2 ton-per-day PDU gasifier is being used for support studies for the 72 ton-per-day SYNTHANE pilot plant, development of new gasification concepts, and to gather environmental data about gasification effluents. Treatment of the gasifier condensate water is being investigated to develop a system capable of purifying the water and reusing it in the plant. Several catalytic methanation reactor systems using Raney nickel catalyst are being tested for capacity, selectivity, and catalyst life. New catalyst forms are being developed.

Another process under investigation is the conversion of coal to automotive fuels by means of the Fischer-Tropsch synthesis reaction (H_2 + CO — liquid hydrocarbon). Fischer-Tropsch synthesis is also being investigated for possible use in a plant that produces both high-Btu gas and liquid products.

Combustion

The Combustion division is involved in research and development related to the combustion of coal, coal-oil slurries, and coal-derived fuels and to magnetohydrodynamic (MHD) power generation. A parallel concem is the control of atmospheric pollution resulting from direct utilization of coal.

Of major interest is research on using coal-oil mixtures in commercially available steam generators to extend our limited resources of oil. Present efforts include operation of a 100-horsepower (75 kW) firetube boiler for long periods to evaluate potential erosion and corrosion of equipment components, as well as to study combustion characteristics of mixtures. A larger (700-hp or 520 kW), mixture-fired, watertube boiler began operation in 1978.

Problems related to combustion of coal-derived liquid and solid fuels in conventional steam generation equipment are also being investigated. The coal-derived fuels include chars from gasification processes, solvent-refined coal, and liquid fuels.

The MHD studies focus on development of coal combustors capable of producing clean, electrically conductive plasmas at temperatures in excess of 4500°F (2500°C). Two high-temperature combustion facilities are being operated to obtain data required to design MHD combustors for power plants of the future.

A concern for utilizing coal in an environmentally acceptable manner underlies all combustion research at PETC. Integral with each of the current research programs are studies of techniques for controlling or reducing emissions of nitrogen oxides, sulfur oxides, and particulates to the atmosphere.

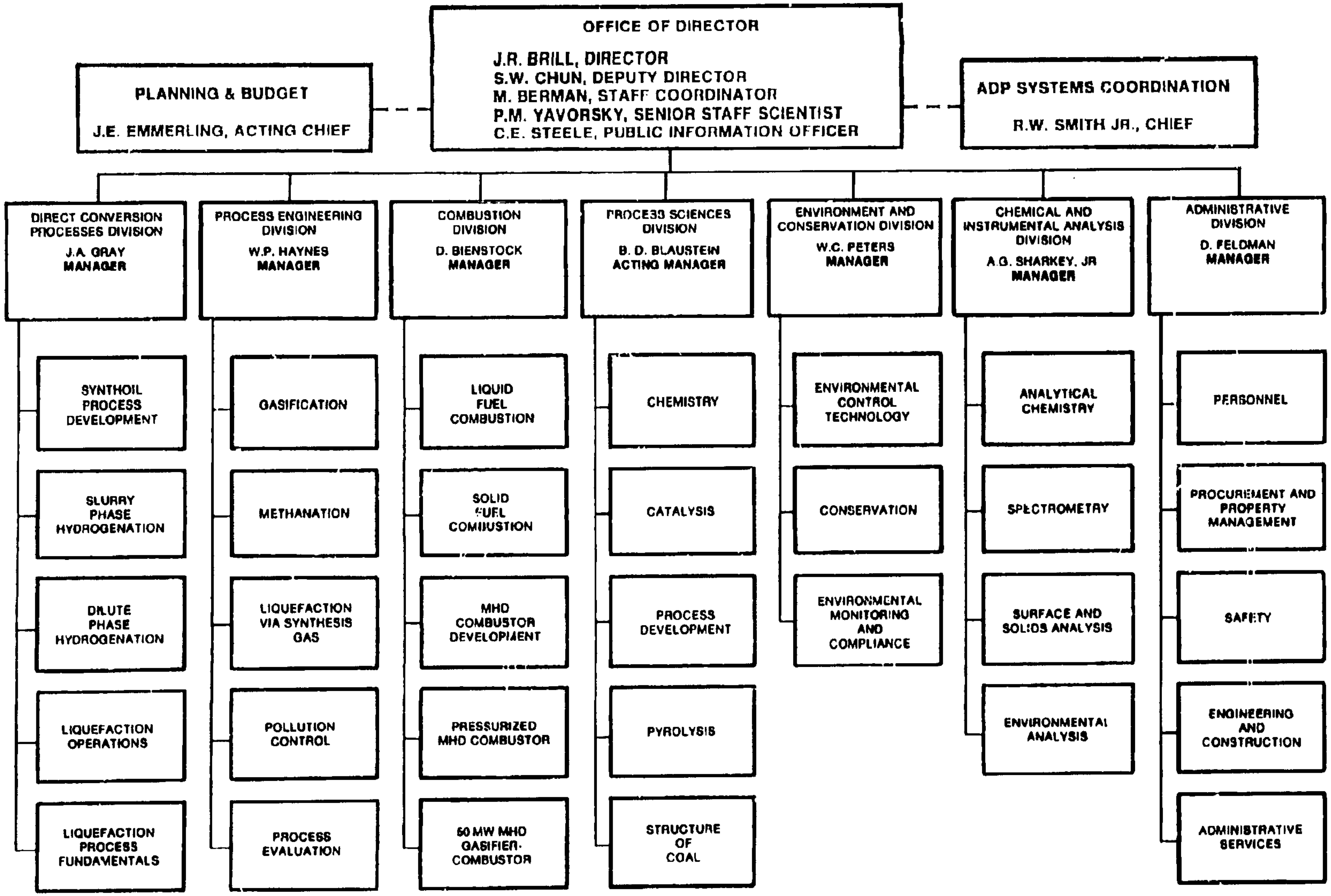


Figure 32. Pittsburgh Energy Technology Center, Organization Chart

Process Sciences

The Process Sciences division is responsible for PETC research and development functions in chemistry, catalysis, pyrolysis, and coal structure characterization. Accomplishments of the division include the COSTEAM process and a process to remove sulfur from coal via air-water treatment under pressure. The two processes have the potential for economically utilizing much of our nation's vast reserves of coal in an environmentally acceptable manner.

While research projects are selected to generate ideas to develop significantly improved coal conversion and utilization processes, substantial R & D efforts are currently focused on the development of support technology that is needed in the near term. Examples of such technology are catalyst development for both coal liquefaction and gasification, development of a solid separation technique in coal liquefaction, and coal liquids upgrading to produce coal-derived fuels that will meet both today's and future fuel specifications.

Environment and Conservation

This division plans, directs, and coordinates the environmental impact studies of PETC's coal conversion processes and participates in the review and development of demonstration plant impact studies. This division is responsible for developing methods for prevention, control, and treatment of effluents from coal conversion processes as well as promoting and monitoring analytical techniques that identify potentially hazardous components and effluents from these processes.

The division assists in the development of techniques to improve the net energy efficiency of these coal conversion processes. The division further supports energy conservation studies through process identification, optimization, and thermal conservation. The division promotes and monitors energy conservation studies for proposed buildings and facilities as well as existing operations at PETC, plus directing retrofit efforts on these facilities.

Chemical and Instrumental Analysis

The Chemical and Instrumental Analysis division is principally engaged in analysis and characterization of the feed materials and the products of coal liquefaction, gasification, and combustion processes. All data generated are tabulated and accumulated for storage in computer data bases for immediate or later correlation and comparison. The process materials of major analytical interest are the varieties of coal used and the catalysts that contribute significantly to the technologic and economic efficiencies of the processes. Characterization of coal conversion products is necessary to ensure their most effective utilization and to guard against possible deleterious environmental effects.

Office of the Director

The Office of the Director provides administrative and technical supervision for all PETC divisions. This office exercises full administrative and technical management support of all phases of the research and development programs of PETC. The selection, training, and direction of the staff of over 370 people and budget preparation are coordinated by this office. The Office of the Director also maintains liaison between PETC and the rest of DOE, as well as other government and non-government agencies and organizations.

The ADP Systems Coordination Branch analyzes, evaluates, and coordinates engineering data and acquisition systems for various PETC processes and projects. The Planning and Budget Branch coordinates program planning and reviews program accomplishments of PETC, prepares budget schedules for the Controller, and monitors industry and university needs and programs.

PETC receives administrative and contractual support from DOE's Chicago Operations Office.

The public information and public relations programs respond to individual requests and initiate contacts for general and technical information exchange. A Public Documents Center and a Speakers Bureau are also maintained at PETC.

Administrative

The Personnel Branch conducts personnel and various labor relations functions. These include organization and position management, employee benefits and services, organization and delegation of authority, employee development, and equal opportunity employment.

The Procurement and Property Management Branch obtains supplies and services for PETC. The staff prepares invitations for bids and administers supply and construction contracts. This branch also coordinates utilization, reporting, and disposal of property.

The Safety Branch not only directs safety inspections and control procedures but also organizes safety courses for employees. Programs include: first aid instruction, cardio-pulmonary resuscitation courses, and fire prevention training. The staff has recently published an in-house safety manual, and organized safety steering, and safety inspection committees. The branch contains a high-pressure cylinder control section. The medical program monitors the health of all personnel.

Buildings, laboratories, and all other physical facilities needed for research activities at PETC are overseen by the Engineering and Construction Branch. Engineering drafting personnel prepare illustrations, graphs, charts, and structural and mechanical drawings. The instrument design staff develops equipment for laboratory and bench-scale research. Construction personnel plan, monitor, and coordinate PETC's construction projects. They also act as a liaison between PETC and other DOE construction and contracting divisions.

The Administrative Services Branch is responsible for management of records, forms, publications, correspondence, mail, printing, library service, travel service, and security.

METRIC EQUIVALENTS

1 pound (lb)	= 0.454 kilograms (kg)
1 ton (t)	= 0.907 tonne = 907 kilograms (kg)
1 foot (ft)	= 0.3048 meters (m)
1 cubic foot (ft^3)	= 0.0283 cubic meters (m^3)
1 pound per square inch (psi)	= 6895 pascals (Pa)
Degrees F	= 9/5 degrees C + 32
1 horsepower (HP)	= 0.746 kilowatts (kW)
1 barrel	= 0.159 cubic meters (m^3)

☆U.S. GOVERNMENT PRINTING OFFICE: 1979-640-092/488

U.S. DEPARTMENT OF COMMERCE
Technology Administration
National Technical Information Service
Springfield, VA 22161 (703) 605-6000