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MORGANTOWN ENERGY TECHNOLOGY CENTER

TOPICAL REPORT

ADVANCED GASIFICATION PROJECTS

By
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Coal Projects Management Division

This overview report, covering the period October 1, 1980, to September 30, 1981, prepared by Morgantown Energy Technology Center staff, describes the current status of advanced gasification projects and includes an appendix that provides summary descriptions of individual projects.

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1.0 INTRODUCTION

Research and development (R&D) programs have been conducted for many years toward the development of coal gasification processes. However, many problems are still unresolved in the establishment of a technically viable and economically competitive industry that meets today's stringent environmental standards. Analysis of current gasification technologies suggests that certain specific activities need emphasis in order to emplace efficient, environmentally acceptable technologies within a reasonable timeframe.

The maximum impact can be made by conducting research and development projects that involve novel gasification concepts, new process chemistries, and advanced gasification process reactors as well as improved technologies for the existing fixed-, fluid-, and entrained-bed configurations and catalytic gasification concepts.

The development of technically reliable, economically feasible, and environmentally acceptable means of gas-stream processing and the handling of wastewater and other effluents are of equal if not greater importance than gasification. There also should be emphasis on evolving an understanding of gas-steam characteristics and definition of optimum gas-steam treatment and processing systems such as novel and improved methods of acid-gas removal and improved hot-gas cleanup concepts and processes. Novel wastewater treatment processes are required for improved economics as well as for compliance with environmental standards.

A program for the development of advanced methods of analysis is also required to develop the necessary data base to characterize the performance of gasifiers and downstream treatment and processing units as well as to develop process models. Modeling of the physical and chemical phenomena of coal gasification and ancillary processes is critical to the development of practical systems.

2.0 TECHNOLOGY NEEDS FOR DEVELOPMENT OF COAL GASIFICATION

An analysis of the needs for coal gasification reveals the following principal categories of "information gaps" that can be filled by programs already in progress or those readily initiated. The gaps are technology base needs required for successful application of both currently available and advanced gasification processes.

The need areas are classified as follows:

- Reactor design/performance.
- Gas cleaning/cooling/separation.
- Acid-gas removal/gas shift/gas conversion.
- Wastewater treatment.
- General data base on both state-of-the-art and advanced technologies.

During the future operating and optimization phases of most of the coal gasification projects, when additional troubles will surface, the technical support program described herein will have provided the additional data base needed to correct deficiencies and/or to advance the state-of-the-art.

3.0 GASIFICATION TECHNOLOGY NEEDS

These technology needs may be referred to as target areas for advanced gasification research and development as follows:

- Novel gasification concepts, chemistries, and processes to obtain low-Btu gas used for power generation, medium-Btu gas used as a synthesis gas for indirect liquefaction and as a source of hydrogen and other industrial chemicals in addition to power generation, and high-Btu gas as a source of synthetic natural gas and other uses.

- Improved technologies for gasifiers, in particular, advanced entrained- and fluid-bed gasification approaches, as well as the currently available fixed- or moving-bed processes. Specific technical problems include the control of slagging of the mineral matter in coal either in terms of preventing slagging on the reactor walls or conversely of managing removal of intentionally produced slag and the control of entrained-bed reactor operations to prevent explosions and other hazards. Important from an economic standpoint is the assessment of problems and the generation of improved approaches for the development of systems for extracting heat from effluent gas streams. An improved understanding is required of the circulation, mixing, and agglomeration of coal particles and sintering of ash particles in fluid-bed reactor operations. The required hot- and cold-bed studies and modeling calculations would have impact and support for specific processes such as the Westinghouse agglomerating bed and IGT U-Gas processes as well as improving the general understanding of all agglomeration and sintering phenomena.
- Gas-stream treatment and processing including such diverse technologies as removal systems for acid gas, particulates, and sulfur, gas separation systems, and shift/methanation systems. Novel and improved acid-gas removal concepts and processes are required for applications that will have an impact on economics and supply reliable alternative technologies. Hot-gas cleanup is required for low- and medium-Btu gases for removal of sulfur, alkali, tar, and particulates and for nitrogen (ammonia and oxides of nitrogen) control so as to have an impact on economics and improve thermal efficiencies in combined power generation and improve fuel-cell applications. Development of combined acid-gas removal and gas separation technologies is required to have an impact on the economics of medium- and high-Btu gasification processes and indirect liquefaction processes as well as to provide for improved combinations of gasification and indirect liquefaction technologies. The development of separation technology for medium-Btu gas is required to adjust the hydrogen/carbon monoxide ratios used for various indirect liquefaction processes and for the extraction of methane from synthesis gas for use as synthetic natural gas.
- Wastewater effluent and environmental problems including the characterization of wastewater streams, definition of specific problems, development of novel wastewater treatment unit operations at the bench-scale level, and subsequent development of optimum wastewater integrated process configurations. The assessment of solid waste leaching problems and the development of concepts and strategies for solutions to these problems is also involved.

4.0 SUMMARY OF PROJECTS AND RELATIONSHIPS IN GASIFICATION DATA BASE

During FY81, the Department of Energy/Fossil Energy (DOE/FE) surface gasification program included about 60 research and development type projects with industry, research institutes, national laboratories, energy technology centers, and universities. Table 4-1 summarizes these projects according to abbreviated titles and participants over the four major areas.

This comprehensive approach covers the broad technology needs of the gasification program. Additional R&D projects can be initiated and those eliminated which are completed or unsuccessful in order to address the needed targets.

Each project is summarized in Sections 4.1 through 4.4 below according to technology needs; furthermore, the project's impact on current emerging gasification programs is assessed.

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Appendix A provides more specific information on each project, such as title, contractor, objectives, results and accomplishments, applications, and any other pertinent material.

Appendix B provides a bibliography of published papers, reports, and papers presented at scientific or engineering meetings for further project details. All of these are based on work done in the specified project, or preliminary work preceding the project.

Appendix C provides a glossary of terms for the abbreviations used in Sections 4.1 through 4.4.

4.1 *Novel Gasification Concepts/Chemistries/Processes*

4.1.1 Beacon Concepts/Technology, TRW, Incorporated

The objective of this project is to develop novel medium- and high-Btu gasification processes along with power generation. These particular concepts may result in a process for medium-and high-Btu gas production with cogeneration of power through a combined power cycle operation, incorporating a significantly higher efficiency. It is expected that demonstrations on laboratory and bench scales will be made through 1982, followed by assessment of the data base and process implications and the broadening of the data base during 1983. (See also pages 15-17.)

4.1.2 Advanced Concepts, Morgantown Energy Technology Center (METC), U.S. Department of Energy (DOE)

The object of this project is to conduct an experimental effort that provides a technology data base for the development of advanced concepts in gasification. The project will make use of an in-house research facility which contains two reactor systems. An entrained-reactor system, designed to react coal through a broad range of processing conditions, will improve the fundamental understanding of gasification reactions and have an impact on the development of improved or advanced gasification concepts. A fluidized-bed reactor system will be used as a variable, reliable source of coal-derived dirty gas for downstream processing studies. These studies could lead to important contributions in advanced instrumentation and sensor testing and the development of advanced cleanup concepts. Investigators plan to have both reactor systems installed and test plans defined by the end of FY82 in preparation for a testing program beginning in FY83. (See also pages 17-18)

4.1.3 Hyrdopyrolysis, Brookhaven National Laboratories (BNL)

The objective of this project is to develop short residence time hydropyrolysis/hydrogasification processes for optimized yields of liquid hydrocarbon products (high-octane gasoline-blending stocks), along with high yields of gaseous hydrocarbons (methane and ethane for synthetic natural gas). BNL has provided reliable yield and kinetic data upon which reactors can be designed. This hydropyrolysis work may have an impact on the development of the novel concept of the simultaneous production of two high-value products in high yields. (See also pages 18-19)

4.1.4 Support Studies, Institute of Gas Technology (IGT)

The objective of this project is to develop new gasification concepts and new processing techniques. IGT examined the initial reactions in coal conversion in a gasification reactor, including the kinetics of noncaking coals devolatization and the kinetics of bituminous coals and lignite chars gasification. In addition, fluidization data were obtained in a 12-inch diameter gasifier including the effect of pressure on fluidization characteristics, sintering phenomena, and void-gas stripping from a moving bed of solids in transfer lines. This work may increase the basic understanding of coal process technology leading to new improved processes. (See also pages 19-21.)

4.1.5 Electrolytic Hydrogen, BNL

The purpose of this project is to investigate the feasibility of electrolytic production of hydrogen from coal-water slurries flowing through a magnetic field. This novel concept is based on the production of an electrical potential by a magnetic hydrodynamic effect due to rapid flow of the slurry in the field. Development of this concept might offer an inexpensive source of hydrogen for energy or chemical use. (See also pages 21-22.)

4.1.6 Photo-Assisted Electrolysis, University of New Mexico (UNM)

The purpose of this project is to investigate the detailed mechanism and feasibility for practical applications of coal gasification by photo-assisted electrolysis. Successful results from this project could lay the groundwork for implementation of a new coal gasification technology. Such a process would use solar energy for gasification rather than the usual strongly endothermic steam-carbon reaction. (See also page 22.)

4.2 *Improved Technologies for Gasifiers*

4.2.1 Entrained-Bed Gasification

4.2.1.1 Characterization, Brigham Young University (BYU)

The objective of this project is to determine detailed gas and char particle characteristic profiles in a bench-scale, entrained-bed gasifier. Mixing and particle reaction data from local points within the reactor could significantly impact entrained-bed gasifier modeling, design, and operation. (See also pages 22-23.)

4.2.2 Fluid-Bed Gasification

4.2.2.1 Tri-Gas, Bituminous Coal Research, Incorporated (BCR)

This project plans to develop an integrated triple reactor process for fluid-bed gasification of caking coals to produce a tar-free, low-Btu gas. The problems inherent in complex fluidized-bed systems have been thoroughly investigated, and the results can impact fluid-bed reactor design and operation. (See also pages 23-24.)

4.2.2.2 Cold Model, Pittsburgh Energy Technology Center (PETC), DOE

The purpose of this project is the experimental determination of the effect of pressure on fluidization parameters of coal and char in a cold-flow mode. This project could provide information needed for the design and scale-up of fluidized-bed gasifiers. (See also pages 24-25.)

4.2.3 Modeling

4.2.3.1 Computer Model, Systems, Science, and Software (S^3)

The objective of this project is to develop fundamental computer models for fluid-bed and entrained-flow gasifiers. S^3 has developed a complex model for each type of gasifier which, after validation and calibration, will be useful for predicting gasifier behavior and scale-up effects. (See also pages 25-26.)

4.2.3.2 Computer Model, JAYCOR, Incorporated

This project plans to develop fundamental computer models for mixing, pyrolysis, and agglomeration processes in fluid-bed and entrained-flow gasifiers. JAYCOR has developed a complex, modularized model for each type of gasifier which, after validation and calibration, will be useful for predicting gasifier behavior and scale-up effects. (See also page 26.)

4.2.3.3 Riser Modeling, Environmental Research and Technology (ERT)

The purpose of this project is to develop a model from experimental data for predicting the degree of chemical reaction conversion in a riser reactor. Although the results would have been applicable to the design of fast fluid-bed reactors and the understanding of their performance, work has been halted due to operational problems and a re-directed emphasis of the gasification program. (See also pages 26-27.)

4.2.3.4 Solids Circulation, Kansas State University

The objective of this project is to determine the local properties of a jet in fluidized-bed gasifiers and development stochastic models. The results may be fundamental to the proper design, operation, and scale-up of reactant gas feed jets in fluid-bed gasifiers, including the effects on the circulation and other phenomena of the bed of coal char. (See also pages 27-28.)

4.2.3.5 Analytical Modeling, University of Houston

The purpose of this project is to develop models for single particle char burning and gasification. The results may be applicable to the design of fluid-bed reactors and the prediction of their behavior. (See also page 28.)

4.2.3.6 Entrained Gasification, BYU

The objective of this project is to validate, refine, and document a two-dimensional, steady-state computer model for prediction of entrained-bed gasifier performance. Such a model could have a significant impact on the design and operation of entrained-bed gasification systems. (See also page 28.)

4.2.3.7 Gasification Reactions, Advanced Fuel Research Incorporated (AFR)

This project plans to develop a model from experimental data for prediction, from functional group compositions of coals, of the devolitalization and gasification products from an entrained-bed gasifier. The results might have an impact on the design and/or operation of entrained-bed gasifiers for improved yields of desired products and better control of pollutants. (See also pages 28-29.)

4.2.3.8 Jet Penetration and Mixing, University of Massachusetts

The purpose of this project is to develop nondimensional relationships describing fluidization with correlation to published data on jet penetration and mixing in fluidized-bed gasifiers. The results will provide a synthesis of fluidization data which may be useful for reactor design and scale-up. (See also pages 29-30.)

4.2.3.9 Moving-Bed Dynamic Model, Washington University

The objective of this project is to develop a dynamic model of moving-bed gasifiers with investigations into gasifier stability and controllability following load disturbances. The results will provide an improved understanding of process dynamics which can lead to increased productivity from coal conversion plants. (See also page 30.)

4.2.3.10 ASPEN Technology, Massachusetts Institute of Technology (MIT)

This project plans to transfer an Advanced System for Process Engineers (ASPEN) computer code to METC and to demonstrate the code to simulate coal conversion processes. ASPEN is a state-of-the-art code for simulation of coal conversion processes and, when validated, this simulator will be the primary process modeling tool at METC. (See also page 30.)

4.2.4 Catalytic Gasification

4.2.4.1 Catalytic Enhancement, Columbia Gas System Service Corporation (Columbia Gas)

The purpose of this project is to determine the effects of sodium carbonate catalyst in a fluidized-bed gasifier. Data are being obtained from a 3-inch diameter bench-scale unit. Use of a catalyst has the potential for improved reaction rates, reduced operating temperature, lower oxygen-to-coal ratios, reduced steam, feed, and higher methane yield. These results, if achieved, would mean lower operating costs and fewer gas treatment problems in the production of high-Btu gas from coal. (See also pages 30-31.)

4.2.4.2 Catalysis Mechanisms, General Electric Company (GE)

The objective of this project is to determine the elementary steps involved in catalytic gasification reactions, the influence of adventitious coal minerals on such reactions, and the processes by which coal/ catalyst contact is established. An understanding of the mechanisms of action of alkali and alkaline earth catalysts on several coals of differing rank may make it possible to improve gasification process efficiencies and reduce costs. (See also pages 31-33.)

4.2.4.3 Catalysis Mechanisms, SRI International (SRI)

This project hopes to determine the mechanisms involved in gasification reactions of coal char catalyzed by alkali, alkaline earth, and transition metal salts. Identification of the specific reaction steps and the parameters that control the catalytic process may provide the understanding needed to select improved catalysts and catalyst/char systems, leading to higher process efficiencies and lower costs. (See also pages 33-34.)

4.2.4.4 Catalysis Mechanisms, Rockwell International (Rockwell)

The purpose of this project is to determine the reaction mechanisms of alkali and alkaline earth catalysts in the gasification of Illinois No. 6 coal-char. The elucidation of those mechanisms and identification of the controlling parameters in catalytic gasification reactions may make possible a better understanding of the phenomena and fundamentals of catalytic reactors. This work, therefore, has the possibility of having an impact on the design and operation of catalytic gasification systems. (See also pages 34-35.)

4.2.4.5 Incorporated Catalysts, Battelle-Columbus Laboratories (BCL)

The objective of this project is the development of a coal pretreatment process involving lime and small amounts of sodium hydroxide in the presence of water. This approach has the potential for an economically favorable process for enhancing gasification while preventing agglomeration of weakly to moderately caking coals. (See also pages 35-36.)

4.2.4.6 Catalytic Effects, Sandia National Laboratories (Sandia)

This project plans to determine the catalytic effects of inherent mineral matter on the devolatilization and subsequent gasification of coal. Clarification of the role of mineral matter in gasification may make it possible to select coals and/or the degree of coal cleaning most favorable to optimum operation of coal gasifiers. (See also pages 36-37.)

4.2.4.7 Catalytic Gasification, PETC

This project hopes to determine the catalytic effects of combinations of specific cations and anions. This work may identify the catalytic trends resulting from the chemical composition of a wide variety of materials and suggest optimum choices for coal gasification catalysts. (See also pages 37-38.)

4.2.4.8 Catalytic Conversion, Los Alamos National Laboratory (LANL)

The purpose of this project is to determine the changes in coal structure produced by heating in the presence of various catalysts and gas atmospheres. This work has the potential for elucidating the chemical changes in coal that occur upon heating in the presence of catalysts up to the onset of gasification reactions. The results might have an impact on the selection of catalysts for producing structural changes preceding gasification including devolatilization reactions and control of pollutants. (See also page 38.)

4.2.5 Gasification Support Studies

4.2.5.1 C/CO_2 Reactions, West Virginia University (WVU)

The objective of this project is to obtain kinetic information on the C/CO_2 reaction and carbon-steam reaction for various sources of coal, char, and pure carbon. Fluidization phenomena as related to coal gasification were also investigated. The results may have an impact on the design and operating conditions of gasifiers. (See also page 39.)

4.2.5.2 Char Gasification, Case Western Reserve University (CWRU)

This project plans to measure the kinetics of devolatilization and gasification under a variety of conditions: pressure, temperature, and gaseous atmosphere are being varied. The results with a novel thermobalance reactor might supply more accurate kinetics data than currently available. These results would aid in gasifier design and operation. (See also page 39.)

4.2.5.3 Improved Techniques, City College (the City University) of New York (CCNY)

The purpose of this project is to develop experimental data for flash pyrolysis (hydrolysis) of coal in steam and steam-hydrogen mixtures. This approach might show promise for the cogeneration of gaseous fuel and a high market value, light-liquid (See also pages 39-40.)

4.2.5.4 Oxidative Pretreatment, University of Pennsylvania (U. of Penn.)

The objective of this project is to determine the kinetics and modeling of mild gas phase oxidative pretreatment of coal. Highly caking coals were rendered virtually non-caking by mild (200°C, 392°F) oxidation. A better understanding of the factors for optimum pretreatment of agglomerating coals under economical conditions could make it possible to use caking coals in some fixed-bed gasifiers and other gasifiers that cannot accept caking coals. (See also page 40.)

4.2.5.5 Coal Gasification, University of Utah

This project plans to investigate single-stage catalytic hydrogenation of coal to form high-Btu gas. This work might lead to a practical process which is more thermally neutral than traditional processes. Also under investigation is the steam reforming of aromatic compounds. This could lead to a new use for coal-derived liquids. (See also page 40.)

4.2.5.6 Particle Structure, Vanderbilt University

The purpose of this project is to determine the changes in the particle structure of coal-char in the reaction with carbon dioxide. The relationships between conversion in the reaction and the particle surface area and effective diffusivity of gaseous reactant and product through the pores of the particle are being analyzed. A better understanding of the influence of changing particle structure on the rate of gas-solid gasification reactions could help in the design and operation of gasifiers. (See also page 41.)

4.2.5.7 Heterogeneous Kinetics, Brown University

The objective of this project is the determination of heterogeneous kinetics of the reactions between the gases present under coal gasification conditions and coal-char. The effects of temperature, pressure, coal-char type and preparation history, and particle size are studied experimentally and systematically to make fundamental contributions to the elucidation and quantification of coal-char gasification kinetics. (See also page 41.)

4.2.5.8 Solids Flow, PETC

The purpose of this project is the testing and evaluation of developmental and commercially available instruments for monitoring and measuring the mass flows of coal and char in pneumatic transport systems. Reliable and accurate solids flow measuring systems are critical to the success of many coal conversion processes. (See also pages 41-42.)

4.2.6 Pyrolysis

4.2.6.1 Rapid Pyrolysis, MIT

This project plans to determine the effects of various operating factors on the rapid pyrolysis and hydropyrolysis of coal. Coal type, particle size, mineral matter, temperature, hydrogen partial pressure, and reactions of volatiles have all been found to influence the choice of gasifier operating conditions for optimum results. (See also pages 42-43.)

4.2.6.2 Kinetics of Pyrolysis, Pennsylvania State Univeristy (Penn State)

The purpose of this project is the determination of the kinetics of pyrolysis and gasification of as-received and pretreated coals following their rapid heating to maximum temperature in nitrogen, steam, and syngas atmospheres. The catalytic activity of inorganic constituents in chars for the concurrent methanation and hydrogasification reactions will also be determined. Results could influence the choice of coal pretreatment and/or gasification conditions. (See also page 43.)

4.2.6.3 Hydropyrolysis, Princeton University

The objective of this project is to determine the kinetics of coal devolatilization under closely controlled heating rates, temperature, and ambient pressures over a wide range of solids' reaction time. Successful completion might provide an experimental basis for the understanding of rapid hydropyrolysis of coal and complete the development of kinetic models which describe rate phenomena. (See also page 43.)

4.2.6.4 Fluid-Bed Pyrolysis, MIT

This project plans to determine the effects of dolomite and calcium carbonate stones on the products of coal and oil shale pyrolysis. The economic feasibility of a proposed process looks promising. (See also pages 43-44.)

4.3 *Gas-Steam Treatment and Processing*

4.3.1 Novel Acid-Gas Removal

4.3.1.1 CNG Process, Consolidated Natural Gas Research Company (CNG)

The purpose of this project is to develop proprietary concepts for low-temperature cryogenic processes for the removal of acid gases from high- and medium-CO_2 content, medium-Btu gases. The development of concepts is expected to progress to the acquisition of bench-scale data on various CO_2-content synthesis gases by about September 1982, with assessment of the economic and technical feasibilities. These novel concepts have the potential to develop more efficient and less capital-intensive acid-gas removal processes required for the manufacture of high-Btu gas and the production of acceptable gas feedstocks for indirect liquefaction or chemical synthesis. (See also pages 44-45.)

4.3.2 Alkali/Particulate Removal

4.3.2.1 Spray Scrubbers, Air Pollution Technology Incorporated (APT)

The purpose of this project is to determine the collection efficiency and power consumption of venturi scrubbers for removing particulates from high-pressure gas streams. This project might supply the data base for assessment of available spray scrubbers for use on the high-pressure product gases generated by the more advanced gasifiers. (See also page 45.)

4.3.2.2 Laminar Flow Cyclone, GE

This project plans to develop a concept for a laminar flow cyclone with high-inlet velocity. A large-scale instability, which could not be resolved, was encountered in turning the swirling flow into the axial direction; however, if this problem could be solved, it would be feasible to increase gas throughput per unit volume and greatly reduce the size of the particulate containing gas fractions while improving collection efficiency and, thereby, reducing costs. (See also pages 45-46.)

4.3.2.3 High-Temperature Alkali Removal, Westinghouse Electric Company

The objective of this project is to develop the alkali gettering concepts into a process for the removal of alkali from hot-gas streams in pressurized gasification systems. Removal of alkali from hot medium- or low-Btu gas streams intended for use in turbines in combined-cycle power generation plants is necessary to prevent serious damage to the turbine materials. This project might fill one of the major technology gaps in this advanced power generation method. (See also pages 46-47.)

4.3.3 Sulfur Removal

4.3.3.1 Solid Absorption Process, Battelle Northwest Laboratories (Battelle NW)

The purpose of this project is to develop a process concept through bench-scale experiments for removal of sulfur from hot reducing gas streams by the use of molten alkali and alkali earth eutectic mixtures held in the pores of selected stable refractory materials. Removal of sulfur from medium- or low-Btu gas streams intended for combustion in power generation plants is necessary to meet environmental standards for sulfur-oxide emissions. Successful completion could provide an experimental basis for the development of a sulfur removal process that will enhance the overall coal gasification efficiency and might have an impact on the emplacement of gasifier/combined-cycle power generation applications. (See also page 47.)

4.3.3.2 Improved Methods, IGT

This project plans to develop a concept for the desulfurization of high-temperature synthesis gases with regenerable solid sorbents having a zinc oxide/zinc chromite base. Acquisition of sulfur removal and solid sorbent regeneration data is expected to be completed in 1982. This process concept, if successfully developed, has the possibility of recovering the sulfur entirely in the elemental state with technical, economic, and environmental advantages over recovery as sulfur oxides. (See also pages 47-48.)

4.3.4 Tar Conversion

4.3.4.1 Catalysts for Reforming, Ralph M. Parsons Company (RMP)

The objective of this project is to develop a catalyst for conversion of tars or heavy oils to synthesis gas and light liquids by high-temperature steam reforming. The catalyst in shift/methanation reactors are subject to deactivation by coke deposits if tars or oils are present in the synthesis gas feedstock. Tar conversion/removal processes are required for the products from a number of existing gasifiers. (See also pages 48-49.)

4.3.4.2 Dew Point of Hot gas, University of California at Berkeley (U. of California)

The purpose of this project is the determination of fundamental physical-chemical and thermodynamic data for condensation of tars from hot gases. The data acquired might make it feasible to design heat exchangers for the recovery of sensible heat from hot, pressurized, tar-containing gas, thereby increasing the thermal efficiency of the gasification process. (See also page 49.)

4.3.4.3 Catalytic Cracking, Clark University (Clark U.)

This project hopes to determine the reaction kinetics of catalytic cracking of tars in order to find conditions for minimizing the production of high-molecular weight hydrocarbons in a coal gasification product gas stream. This work might supply a much needed data base for the development of a process for the conversion of tars to useful product gas. (See also pages 49-50.)

4.3.4.4 Tar Conversion Over CaO, MIT

The objective of this project is to explore the technical feasibility of using CaO in: (1) converting tars produced during gasification and (2) increasing product gas yields, heating values, and desulfurization. Successful completion would indicate the possible commercial promise of thermal reaction of coal tar over CaO as a method of improving gas yields/quality and enhancing by-product liquid quality in coal gasification and pyrolysis. (See also page 50.)

4.3.4.5 Catalytic Cracking, Research Triangle Institute (RTI)

This project plans to test and evaluate potential catalysts for the vapor phase cracking of heavy hydrocarbons in raw gas streams from fixed-bed gasifiers. Elimination of heavy organics from the raw gas at high temperature would reduce operational problems downstream, permit high-quality waste heat recovery, and reduce the cost of recycle quench water cleanup. (See also pages 50-51.)

4.3.4.6 Aromatics Conversion Over CaO, MIT

The purpose of this project is to determine the effect of CaO on thermal reactions of pure aromatic compounds. Previous work has shown potential beneficial effects of passing coal pyrolysis products over CaO including selective cracking of tar aromatics. This work will lead to the better understanding of these phenomena by investigating the effects of heated CaO on model compounds. (See also page 51.)

4.3.5 Gas Separation

4.3.5.1 Hydrogen/Methane Separation, PETC

The objective of this project is to determine the feasibility of separating hydrogen/methane mixtures by adsorption on activated carbons. Hydrogen or hydrogen/carbon monoxide is currently separated from product methane (SNG) for recycling to the gasifier by means of cryogenic processes which are becoming more energy intensive because of increasing electric power costs. Adsorptive fractionation on activated carbons (hypersorption process) is being investigated for its applicability to coal-derived gases as a possible process alternative. (See also pages 51-52.)

4.3.5.2 Hydrogen/Methane Separation, State University of New York at Buffalo (SUNY)

The purpose of this project is to determine the feasibility of using heat-treated coals in place of activated carbons for a combined H_2/CH_4 separation and H_2S removal technique. This project has the potential to define an inexpensive alternative for activated carbon in a possible combined separation/cleanup process. (See also page 52.)

4.3.5.3 Separation of Medium-Btu Gas, Dravo Corporation (Dravo)

The objective of this project is to determine the engineering design and economic feasibility for application of the hypersorption process to the separation of medium-Btu gases. These calculations might define the possible applications of adsorptive fractionation on activated carbon for gas separation such as adjustment of H_2/CO ratios for indirect liquefaction or chemical manufacture. (See also page 53.)

4.3.6 Shift/Methanation

4.3.6.1 S/M Fluidized Bed, BCR

This project plans to demonstrate the feasibility of gas-phase, fluidized bed, shift/methanation with various catalysts. Combined shift and methanation in a single reactor has the potential for technical and economic benefits. Gas-phase, fluidized-bed operation has the potential for good temperature control of the exothermic reaction and inhibited rates of carbon deposition at elevated temperatures. (see also pages 53-54.)

4.3.6.2 Liquid Phase S/M, Chem Systems, Incorporated (Chem Systems)

The purpose of this project is to determine the rates of carbon formation on various shift/methanation catalysts and evaluation of the hydrodynamics of a liquid-phase, fluidized-bed shift/methanation reactor. The results might lead to improvement in catalyst activity and catalyst life, thereby reducing operating costs. (See also pages 54-55.)

4.3.7 Support Studies

4.3.7.1 Thermodynamic Tables, Dow

The objective of this project is the derivation of tables of data for thermodynamic properties of substances involved in coal conversion processes. These thermodynamic tables have an impact on the development and operation of gasifiers, gas cleanup and separation units, methanators, and other reactors. (See also pages 55-56.)

4.4 Wastewater and Effluent Handling

4.4.1 Process Wastewater, PETC

The purpose of this project is to develop environmental control strategies for gasifier wastewater through laboratory- and bench-scale studies. Included are measurement of chemical oxidation with ozone, anaerobic conversion of organic constituents to methane, solvent extraction of organics, and other biological and physiochemical treatments. The wide range of data being obtained with a variety of gasifier wastewaters shows promise for the development of an integrated treatment program that will be realistic and meet future as well as current environmental standards. (See also pages 56-57.)

4.4.2 Wastewater Treatment, Grand Forks Energy Technology Center (GFETC), DOE

The purpose of this project is investigation of the treatment of the wastewater from the GFETC slagging fixed-bed gasifier. The work includes biotreatment with activated carbon addition, solvent extraction, oxygen-activated sludge, anaerobic digestion, and leachable components from gasifier slag. The data obtained will make it possible to compare effluents process-train requirements as a function of the gasifier-operating conditions and the coals used as feed to the gasifier. Industry needs information of this sort in order to anticipate environmental problems for commercial gasification and develop/design an energy-efficient integrated treatment process. (See also page 57.)

4.4.3 Wet Oxidation, RTI

The objective of this project is the experimental evaluation of wet oxidation as a technique for removing organics from gasifier quench water and the evaluation of potential catalysts for such a process. Wet oxidation could provide a simple and economic alternative to other waste treatment techniques. See also pages 57-58.)

p

APPENDIX A — ADVANCED GASIFICATION PROJECTS

A.1 *Novel Gasification Concepts/Chemistries/ Processes*

A.1.1

Title

Development of BEACON Technology

Performer

TRW, Inc., Redondo Beach, CA

Objective

The objective is to develop catalysts, reactors, and systems to utilize the unique BEACON chemistry for the production of methane from low-Btu coal derived fuel gases.

Project History and Background

The BEACON process was developed by TRW over a period of about 4 years prior to the Cooperative Agreement with the DOE. SOHIO joined with TRW in 1978 to continue this development effort.

Proof-of-principle testing and research in small, atmospheric pressure fixed-bed reactors provide a good data base in support of the process chemistry. Additional experiments in fixed-, fluid-, and entrained-bed reactors at pressures up to 20 atmospheres provided additional global reaction rate data And led to the selection of fluid-bed reactors as a preferred mode of operation.

The chemistry involved in the BEACON process is based on the patented discovery that carbonaceous materials suitably prepared by the disproportionation of carbon monoxide over group VIII ferrous metal catalysts can be uniquely reactive with hydrogen or steam. The process being developed around this chemistry upgrades the low-Btu produced gas derived from the partial oxidation of coal in two steps. In the first step, carbon is deposited on the ferrous metal catalyst, which is then separated from the hot depleted fuel gas. The carbonaceous material is then reacted with either hydrogen or steam to produce methane in the second step of the process. The hot, depleted fuel gas is used to produce steam and/or generate electric power.

Description of Work

The DOE Cooperative Agreement is aimed at further development and improvement of catalysts and testing of these catalysts in laboratory reactors over a range of temperatures and pressures. Selected catalysts will then be further evaluated in larger bench-scale units to determine reaction kinetics and catalyst stability and regenerability over multiple cycles of carbon deposition and gasification. Sufficient data will be generated to permit realistic conceptual commercial designs and economic evaluations and to provide a data base.

Present Status

The carbon deposition reaction has been found to proceed rapidly over several different types of properly activated catalysts. Preferred temperatures are 450°-500°C with carbon monoxide conversion of over 80 percent at commercially viable gas residence times. Reaction rates are relatively insensitive to pressure.

A reasonably complete data base is now available covering the reaction sequence of carbon deposition followed by hydrogenation to methane. These data are briefly summarized in Figure 4.1.1-1, which illustrates the following results:

1. Methanation rates as a function of temperature follow a normal Arrhenius plot and are relatively insensitive to pressure.
2. Methane concentration as a function of pressure is close to

BEACON COGENERATION PROCESS

SIMPLIFIED FLOW DIAGRAM

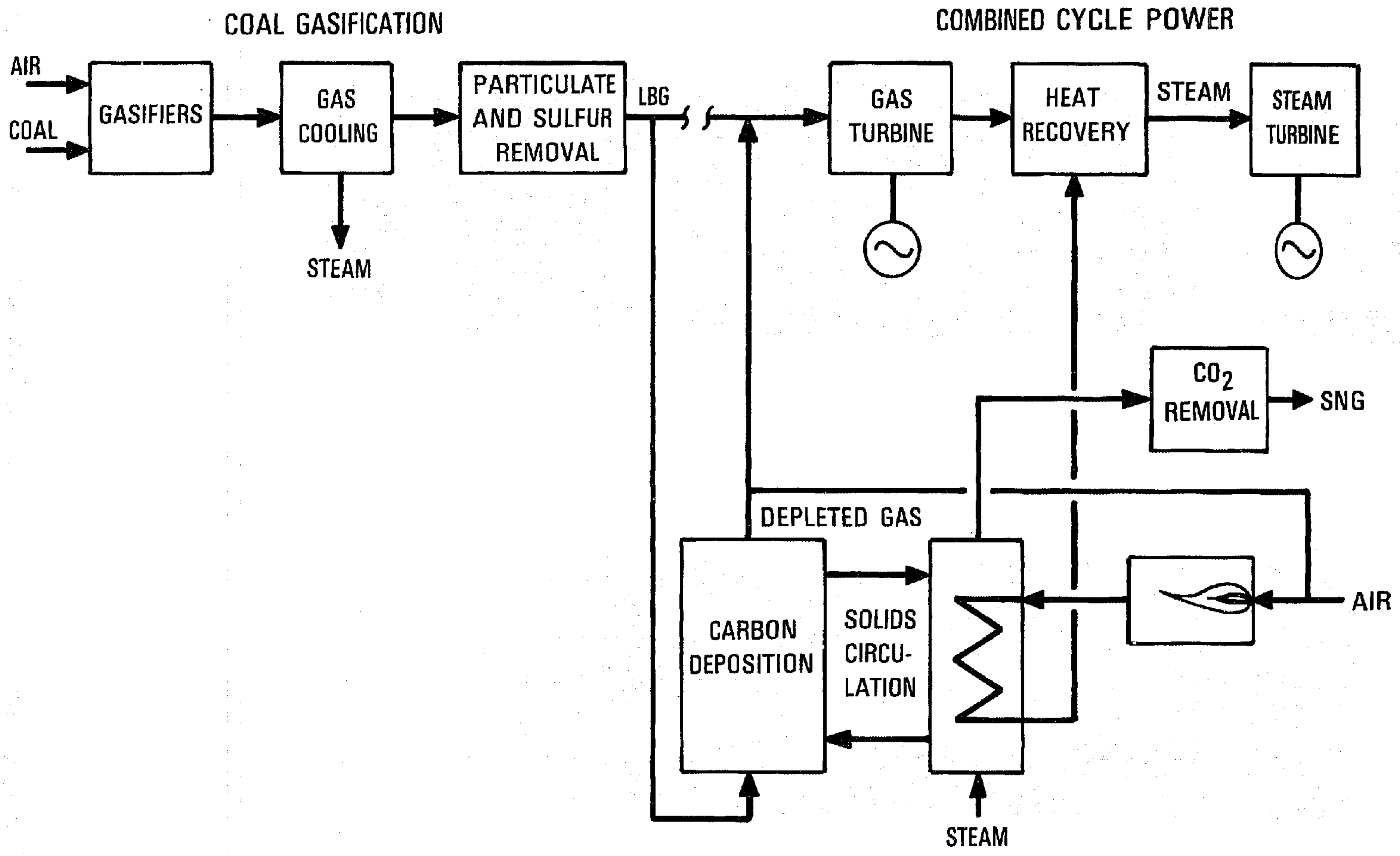

FIGURE 4.1.1-1 BEACON PROCESS

calculated equilibrium concentration, and is reached at commercially viable gas residence times.

3. The specific methanation rate increases as carbon is hydrogenated and is still increasing even after 93 percent of the original carbon is removed.

A series of 63 cycles of carbon deposition and hydrogenation demonstrated retention of catalyst activity over an extended period of time.

Catalysts suitable for direct hydrogenation of deposited carbon had a rapid loss of activity at temperatures below 800°C under steam gasification conditions. New catalysts have now been developed which exhibit excellent steam gasification activity and stability at temperatures as low as 550°C. This appears to be the most promising process route since it is independent of an external source of hydrogen. Further catalyst development efforts and bench-scale testing of selected catalysts are concentrating on this process route.

Accomplishments

Since the start of the DOE Cooperative Agreement, significant improvements have been made in catalyst formulations. A close approach to thermodynamic equilibrium gas composition is attained by steam gasification of deposited carbon at temperatures as low as 550°C with commercially reasonable gas residence time. Furthermore, two basically different types of catalysts have been tested and proven suitable for fluid-bed operation. One is a conventional type of supported catalyst, while the second is unsupported. These catalysts have been tested under carbon deposition, hydrogenation, and steam gasification conditions at pressures up to 200 psia and in fluid-bed reactors up to 4 inches in diameter.

Application

The BEACON process offers a unique method of upgrading low-Btu gases to Synthetic Natural Gas (SNG). These feed gases may come from air-blown coal or char gasification processes, underground coal gasification, or blast furnace top gas. These feed gases cannot be readily converted to methane by known conventional technologies.

Essentially all of the exothermic heat of the carbon deposition reaction is retained in the hot depleted effluent fuel gas, which can be very efficiently used for combined-cycle power generation. In this system approach, a high and variable portion of the heating value of the low-Btu feed gas goes to cogeneration of electric power.

A.1.2

Title

Advanced Gasification Concepts

Performer

Morgantown Energy Technology Center, Morgantown, WV

Objective

The objective is to provide a technology data base for the development of advanced concepts in gasification.

Accomplishments

Site preparation work, which included the construction of high-pressure cells, blast walls, a control room, a gas cylinder room, and a bulk gas area was completed during FY81 for the in-house research facility. This facility, which has been designated the Advanced Gasification Concepts (AGC) Facility, will house two reactor systems: (1) a small-scale (3-inch ID, 10 lb/hr), high-pressure (1000 psig), high-temperature (3000°F), entrained reactor system; and (2) a small-scale (6-inch ID, 150 lb/hr), high-pressure (1000 psig), oxygen and air-blown, fluidized-bed reactor system. Both reactor systems have been designed, and the major procurements were either begun or completed by the end of FY81. Also during FY81, the structural steel for the process equipment was erected for both systems, and installation of the control room instrumentation for the entrained reactor system was started. During the early design and construction phases of the AGC facility, in-house experimental and contractor R&D activities were carried out. In-house experimentation made use of an existing thermobalance reactor to determine the effects of catalyst type, loading, and impregnation techniques/degree on coal- and char-related gasification reactivities. Eleven contracts were initiated to support DOE's overall advanced gasification program, spanning a range of subjects such as computer applications, instrumentation development, and basic studies in coal pyrolysis and agglomeration.

Current Work

The primary emphasis is being placed on completing the installation of both reactor systems in the AGC facility by the end of FY82. In conjunction with these efforts, there will be a refinement of the planned entrained reactor test program and a formulation of the fluidized-bed reactor test program.

Application

The entrained reactor system was designed, in general, to have the capability and flexibility to investigate the complex physical, chemical, and kinetic behavior of coals through a broad range of processing conditions. Areas of prominent importance will be carbonization/pyrolysis/hydropyrolysis reactions, high-temperature heterogeneous reactions, and devolatilization product stabilization reactions. In addition to strengthening the overall gasification technology data base, the studies anticipated with this system may improve the fundamental understanding of gasification reactions, and may thus aid in the development of improved or advanced gasification concepts.

The fluidized-bed reactor system was designed primarily to serve as a flexible, reliable source of coal-derived gas of widely ranging composition. This gas will be used for studies in the general areas of cleanup, instrumentation, and component testing. In addition, it is expected that the reactor will yield important data for model verification. The exact uses of the system will be defined during FY82, but researchers anticipate that studies with the system will make important contributions in advanced instrumentation and sensor testing and development of advanced cleanup concepts.

A.1.3

Title

Hydrogasification/Hydropyrolysis of Coal

Performer

Brookhaven National Laboratory, Upton, NY

Objective

The objective is to obtain process chemistry information for the rapid hydrogasification and hydropyrolysis of coal to primarily gaseous and liquid hydrocarbon products.

Accomplishments

Two subbituminous coals, New Mexico and Montana Rosebud, and two bituminous coals, Illinois No. 6 and Kentucky No. 9, have been hydrogenated in a highly instrumented 1-inch I.D. entrained downflow tubular reactor system. Coal particle residence times varied from approximately 0.5 second to greater than 6 seconds. The New Mexico coal yielded, based on carbon converted, approximately 20 percent liquid hydrocarbon products at 2000-2500 psi and 10 percent at 1000 psi. The maximum gaseous hydrocarbon yield was 85 percent at 2500 psi and 900°C. The Montana Rosebud coal, studied at less than 2 seconds residence time and 1000 psi, produced 12 percent liquid and 23 percent gaseous products.

The caking bituminous coals, all run at no greater than 1000 psi, were used with diluents of limestone or sand to prevent agglomeration. The liquid yield from the Illinois No. 6 coal was 8-13 percent and the gaseous yield 34-43 percent when researchers used limestone and 27-31 percent when they used sand. Twenty percent liquids were produced from the Kentucky No. 9 coal and 45-50 percent gaseous hydrocarbons at reactor temperature of 1000°C. Hydrogen/coal feed ratios, hydrogen partial pressure, and product concentration were also investigated. Carbon balances were made and the data correlated to obtain kinetic expressions.

Current Work

The study of the rapid hydrogenation of Kentucky No. 9 coal is being concluded using 15 percent Cab-O-Sil as a diluent to prevent agglomeration. The reactor operating conditions are 1000°C and 800 and 1000 psi. The results show the gaseous hydrocarbon yields ($CH_4 + C_2H_6$) to be as high as 60 percent of the available carbon and the maximum BTX yields to be approximately 8 percent. The use of Cab-O-Sil as a diluent, as opposed to the sand previously used, has not only reduced the amount of diluent need (15 percent vs. 60 percent), but also has eliminated the wear on the coal feeder experienced when sand is used.

Work has started on the preparation of a final report summarizing all of the accomplishments and indicating application areas.

Application

The results of these process chemistry studies and the correlations provide data upon which direct processes for conversion of coal to synthetic fuels can be designed and evaluated. This project provides reliable yield and kinetic data upon which reactors and process equipment can be designed. The information has already been used to evaluate various direct rapid hydrogenation reactions, such as those conducted by IGT, CS/RI, CUNY, and MIT.

A.1.4 *Title*

Coal Conversion Support Studies

Performer

Institute of Gas Technology, Chicago, IL

Objective

The objective of this program is to advance coal gasification technology through a series of related studies that support the ongoing development of advanced coal gasification processes. In addition, these studies will assist the greatly expanded national effort to bring synthetic fuels into commercial reality in the shortest possible time by making a large amount of missing technology available to the process designers. These studies, involving both the analytical and experimental aspects of synfuels production, will either generate missing basic design data or develop new processing techniques for direct application to overall processes with associated incentives for improving efficiency, lowering cost, and expediting process development.

Accomplishments

In this multi-task studies project, the following are the significant accomplishments:

- Colorado subbituminous coal was subjected to a mild extraction with n-hexane, benzene, or THF at their normal boiling points (152° to 176°F). Devolatilization experiments conducted with hexane-extracted coal and benzene-extracted coal in hydrogen show that the CO_x yield decreased, although the methane yield increased. Analysis of solid residue products and parent coal failed to indicate any significant differences.
- Rates of gasification of both stabilized chars and chars produced in-situ in steam-hydrogen mixtures and synthesis gas were determined. In general, the in-situ chars were more reactive than the stabilized chars. The effect of added catalysts on steam-char gasification was also measured.
- An experimental technique was developed to measure solids entrainment rate from high-pressure fluidized beds. The effect of operating parameters and entrainment rates of coke breeze and sand were measured, and appropriate design correlations were developed.

- The equipment for measuring solids flow through seal legs was constructed. The solids flow rate was correlated with the pressure drop in a solids recirculating lift line.
- In correlating the operating parameters for char sintering in high-temperature, oxygen-blown fluidized beds, researchers determined that the superficial gas velocity, in excess of the minimum fluidization velocity that is needed to prevent sintering, is linearly proportional to the average fluidized-bed temperature. The operating plot of fluidized-bed temperature versus fluidizing gas velocity, for various oxygen concentrations, is being developed to identify the sintering and nonsintering regimes.
- Void-gas stripping studies were conducted with sand and coal char to identify the optimum operating conditions to strip interstitial gases in moving beds of solids. Experimental data was also obtained on the effect of pipe diameter on void-gas stripping. A relative velocity model, useful for design and scale-up, is being developed.
- Multi-component vapor-liquid equilibria experimental data were obtained using up to nine components. The validation of available correlations with the experimental data showed that the PengRobinson correlation is slightly better than the Soave-RedlichKwong and both are better than Grayson-Stred and Chao-Seader correlations. The specific observations with the Peng-Robinson correlation are that it underestimates the solubilities of H_2, C_2H_4, H_2S, COS, and CO in C_6H_6 and the vapor phase concentration of C_6H_6, CO_2, CH_4 and C_2H_6.
- Different materials were investigated in a parametric fixed-bed experimental program to determine their suitability to high-temperature (1400° to 1800°F) fuel gas desulfurization and their specificity for elemental sulfur production during regeneration. Of the materials tested, zinc aluminate and zinc chromite were found to be effective in producing as much as 85 percent sulfur as elemental sulfur during regeneration. To determine the performance of these materials over extended desulfurization and regeneration cyclic tests, a 4-inch ID bench-scale adiabatically shielded reactor has been designed and is being constructed. The unit is designed for operation at ambient pressure and 1800°F with pre-heated gas at (up to 2000°F) space velocities ranging from 300 to 2000 hr^{-1}. To conserve synthetic gas, a recycle compressor is included along with provisions for elemental sulfur recovery. The unit is being prepared for shakedown.
- A one-dimensional process simulation model for the fixed-bed desulfurization and regeneration operations, an adiabatic gas-solid reaction system, has been formulated and solved to estimate the effect of operating parameters on the desulfurization process scheme.
- As a part of the water purification studies, a char-water slurry containing 2 weight percent solids was used at flow rates of up to 30 gal/min to test the performance of Abcor type J and Osmonics 704 filters. The Abcor ultra filter rated better than the Osmonics filter, with flux rates dropping from 720 gal/ft^2–day after 70 hours of operation.
- Simulated blowdown wastewater containing up to 17 organic and inorganic compounds was employed to determine the performance of polyamide reverse osmosis membranes. A large number of experiments were conducted in a bench-scale system using a UOP Fluid Systems' 701-PA polyamide spiral wound unit and DuPonts' 042-021 polyamide hollow fiber unit at pressures up to 1000 psig and flow rates up to 1-5 gal/min. Over a pH range

of 7 to 10, nearly complete removal of ammonium ions and rejection of 85 percent of the phenol, 74 to 98 percent of the bicarbonates, and 39 to 94 percent of the sulfide ions were achieved with the membranes.

Current Work

The objectives of the ongoing experimental work have been redirected to emphasize studies on fluid-bed phenomena, hot-gas cleanup, and shift catalyst performance and catalyst deactivators.

Application

The contributions of the IGT support studies program can be broadly divided into two categories, generation of missing data and development of efficient and economical alternatives to processes and process steps. Included in the first category are the kinetic data on subbituminous coal char gasification, solids entrainment data, solids flow through seal legs, identification of non-sintering operating regimes for oxygen-blown fluidized-bed char gasification reactors, void-gas stripping data, and multicomponent vapor-liquid equilibrium data. The pioneering work in many of these areas has resulted in models and/or correlations which can be used to design and scale-up a wide variety of coal gasification processes.

The experimental data from the evaluation of water-gas shift catalysts and high-temperature desulfurization materials have been evaluated to develop advanced gas cleaning and upgrading schemes which are potentially more efficient and economical than currently available processes. These schemes offer significant reduction in steam and waste water treatment requirements, and reductions in capital investment and savings in operating costs. They also may result in better control over effluents disposal compared to present commercial gasification plant designs. It should be noted that the advanced gas upgrading schemes are applicable for LBG, synthesis gas, MBG, and SNG production in moving, fluidized, and entrained gasifiers.

The data obtained from advanced wastewater treatment methods, including ultrafiltration and reserve osmosis, also contribute to developing efficient alternative water recovery methods. Compared to the conventional water treatment methods, the improved schemes will result in better water recovery while minimizing undesirable effluent disposal.

A.1.5

Title

Production of Hydrogen Using Coal-Water Slurries

Performer

Brookhaven National Laboratories, Upton, NY

Objective

The objective is to investigate the feasibility of producing hydrogen from coal-water slurries by pumping such slurries through the magnetic field of a permanent magnet.

Background

Superconducting magnets that can be used for such a process are available. By adding coal particulates as a slurry in water, researchers note that the voltage for the water electrolysis reaction falls to slightly below 0.3V. If a coal-water slurry flow is perpendicular to an externally applied magnetic field, sufficient voltage will be generated across electrodes to electrolyze the slurry in a magnetohydrodynamic-(MHD-) type unit.

Accomplishments

Several test runs were carried out on an MHD test unit for production of hydrogen using coal-water slurries. The linear flow of liquid through the restriction in the tube where the platinum and lead electrodes are located was about 1.1 meters per second. At a constant velocity, a linear plot of emf (volts) versus magnetic field H (Tesla) was obtained with 5N H_2SO_4 electrolyte. Construction and leak testing were completed on an electrically driven cell for measuring coal conversion efficiency. In this cell both electrodes are platinum — 10 percent rhodium, with 5 mil Nafion membrane separating the electrodes. A mixture of 5N H_2SO_4 containing 10 weight percent New Mexico subbituminous coal ground to less than 100 mesh is circulated. Runs were made in the electrically driven electrochemical cell with a 10 percent slurry of New Mexico subbituminous coal in 5N H_2SO_4. A limiting current density of 4 mA/cm^2 was observed in the recorded plots of total voltage versus current (amperes).

Current Work

Experimental results are being obtained at both room temperature (~30°C) and at 75°C in the electrically driven unit. Phosphoric acid with concentrations of 5N and 10N, as well as 5N sulfuric acid, are being studied as possible electrolytes. Sulfuric acid shows the strongest anode depolarizing effect with coal. A strong temperature dependence was shown from room temperature and 75°C curves. The limiting current density of near 12 mA/m^2 at 75°C with 10 weight percent New Mexico subbituminous coal implied that a further increase in temperature would lead to a further increase in the limiting current density.

Work has started on the preparation of a final report summarizing all of the accomplishments and indicating application areas.

Application

Results with both the MHD-type unit and the electrically driven unit indicate possible operating conditions for development of this concept to a practical stage. This research could lead to an inexpensive source of hydrogen.

A.1.6 Photo-Assisted Electrolysis Applied to Coal Gasification, University of New Mexico, Albuquerque, NM

The objective of this work is to investigate the technical feasibility and detailed mechanisms of coal gasification by photo-assisted electrolysis. This could lead to a process which: (1) accomplishes coal gasification with the aid of solar energy rather than through the strongly endothermic carbon-steam reaction, (2) is a low-temperature operation, and (3) produces cleaner gas products. Initial studies on this 2-year project were aimed at a better understanding of the oxidation mechanism which produces carbon oxides and hydrogen from a coal slurry. It was shown that ions of iron leached into the electrolyte solutions undergo reactions which catalytically oxidize coal to carbon oxides and other products. This slow catalytic step is rate limiting, and a better catalyst is being sought.

A.2 *Improved Technologies for Gasifiers*

A.2.1 Entrained-Bed Gasification

A.2.1.1 Prediction and Measurement of Operating Parameters for Entrained-Flow Coal Gasification Processes — Characterization, Brigham Young University, Provo, UT

The objectives of this project are to develop an understanding of the physical and chemical rate processes which occur during entrained coal gasification in steam and oxygen, and to develop a data base for use by modelers in validating mathematical models of entrained-flow gasification. During earlier phases of this program, a laboratory-scale entrained coal gasifier was designed, built, and operated at atmospheric pressure to determine optimum operating conditions and to obtain detailed particle and gas profiles within the reactor. The coal gasifier is of sufficient scale to allow gas and particle samples to be removed locally from within the reactor. These local samples have been useful in optimizing operating variables and in determining the mixing and gasification rates of coal in a practical environment.

For recent tests the reactor was modified to incorporate swirl in the secondary stream and to provide increased preheat of the secondary stream. These modifications were made in an attempt to increase the carbon conversion in the reactor. Subsequent tests showed that secondary swirl and preheat had little effect on carbon conversion, but that the distribution of oxygen between the secondary stream and the primary stream had a major effect. Carbon conversion values of about 60 percent were obtained with all of the O_2 in the secondary stream. Introduction of all of the oxygen in the primary stream (premixed O_2 and coal) gave significantly higher (approximately 85 percent) carbon conversion results.

In addition to the laboratory-scale gasifier, a non-reactive, confined jet mixing test facility has been used to determine gas and particle mixing rates in the absence of chemical reaction. These data are useful when trying to deduce mixing and reaction rates separately. The current effort is to collect and analyze operating data from the gasifier for a variety of coals at pressures up to 17 atm, and to continue non-reactive, confined, two-phase jet mixing tests with a newly installed laser-Doppler velocimeter. Completion of the project is scheduled for September 1983.

A.2.2 Fluid-Bed Gasification

A.2.2.1

Title

Tri-Gas Low-Btu Coal Gasification Process

Performer

Bituminous Coal Research, Inc., Monroeville, PA

Objective

The objective is to develop a fluidized-bed coal gasification process for the production of low-Btu fuel gas from caking as well as non-caking coals without producing by-product liquids, tar, or char using three reactors connected in series for a continuous integrated operation.

Accomplishments

Key operations of a 100-lb/hr PDU have been demonstrated including the following. Illinois No. 6 caking coal has been successfully devolatilized in the Stage 1 reactor, supplying a free-flowing char to Stage 2. In Stage 2, char and volatile tars from Stage 1 have been gasified with air and steam to produce an approximately 150 Btu, tar-free fuel gas. Char from Stage 2 has been further gasified in Stage 3 to produce a high-ash solids discharge and a hot-gas effluent for the gas feed to the devolatilization stage. All three stages have been operated in a completely integrated mode with transfer of solids and gas through the successive stages.

A continuing series of equipment malfunctions, many traceable back to deficiencies in the original PDU design, resulted in only a few integrated runs and these mostly for only a few hours at steady-state conditions.

Current Work

The experimental work was concluded and a final report was published.

Application

Many observations about fluidized-bed reactor design and operation are transferrable from the reports on this project to other DOE fluidized-bed coal gasification projects, mostly in terms of problems that can arise and how to avoid or solve them. The three-stage reactor approach on balance does not appear to be an advantageous process, however, because of inherent technical complexities.

A.2.2.2

Title

High-Pressure Fluidization Cold Model

Performer

Pittsburgh Energy Technology Center, U.S. DOE, Pittsburgh, PA

Objective

The objective of this project is to develop a data base for the effect of pressure on fluidization parameters of coal and char, such as minimum fluidization velocity, complete fluidization velocity, minimum bubbling velocity, bubble size bubble velocity, jet penetration distance, and distributor design effects.

Accomplishments

A 4-inch diameter cylindrical plexiglass model contained in a 24-inch diameter pressure shell with 24 observation ports and capable of operation to 1000 psig was used to study fluidization velocities of coal and char. A series of 76 tests was completed at pressures ranging from atmospheric to 900 psig. Observations included: (1) minimum fluidization velocity decreases slightly with an increase in pressure; (2) complete fluidization velocity decreases dramatically with an increase in pressure and seems to approach a minimum value at a pressure which may depend somewhat on particle size distribution; (3) minimum bubbling velocity increases significantly with an increase in pressure, and seems to approach a maximum value at a pressure which may depend somewhat on particle size distribution; and (4) bed height normally increases with increased superficial gas velocity, but at high pressures a point is reached where the bed height actually decreases for a time before again increasing with increased superficial velocity.

Photographic studies of bubbling phenomena in fluidized beds of coal and char were recently completed in an 8-inch diameter, 0.75-inch thick "two-dimensional" plexiglass model. Photographs were taken over a pressure range of 0 to 950 psig, at gas velocities of 0 to 0.7 ft/sec, and at three different positions in the bed. Information about bubble size, shape, velocity, and frequency is being analyzed.

Current Work

The "two-dimensional" plexiglass model is being replaced by an 8-inch diameter cylinder to facilitate further bubbling phenomena studies using capacitance probes.

Application

Development of a data base for the effects of pressure on fluidization parameters is extremely important for the design and scale-up of fluidized-bed gasifiers. Availability of such data in the literature is severely limited. The fact that it is one of only two such units known to exist in the United States accentuates its value as a tool for developing a high-pressure fluidization data base.

A.2.3 Modeling

A.2.3.1

Title

Computer Modeling of Coal Gasification Reactors

Performer

Systems, Science and Software, La Jolla, CA

Objective

The objective is to develop models of coal gasification reactors which, when validated and applied, can be used to expedite the development and to aid in the scale-up and optimization of such reactors. The models will combine theoretical descriptions of the thermomechanical interactions between the solid and gas phases with a kinetic model of chemical reactions based on the best experimental data available during development.

Accomplishments

Two major computer models have been developed which include: (1) a fluidized-bed coal gasifier model and (2) and entrained-flow coal gasifier model. These models provide, respectively, two- and three-dimensional spatial descriptions of the steady and transient processes within the gasifiers and, in addition, predict the composition of the product gas from the reactors. The models are based upon finite difference and finite element numerical techniques which permit the representation of arbitrary reactor geometries.

The numerical computer codes have been delivered to DOE/METC together with descrtiptions of the models and code user's manuals, and the codes have been installed and implemented on the METC computer facilities. The entrained-flow coal gasifier code has undergone further development and has been introduced into the Electric Power Research Institute (EPRI) computer tape library.

Current Work

With the submission of the models/codes and supporting documentation, model development has been halted for the interim. Currently, researchers are analyzing and evaluating the complex computer codes using DOE/METC and other Government-sponsored computer facilities. The results of these studies can be compared to earlier studies of the U-Gas and Westinghouse fluid-bed reactors and the BiGas entrained-flow reactors to provide information for the subsequent enhancement of the models.

Application

After verification and validation, the S^3 models will provide insight into the phenomena involved during gasifier operations and, also, the models may provide needed information concerning reactor performance after scale-up.

A.2.3.2

Title

Computer Modeling of Mixing and Agglomeration in Coal Conversion Reactors.

Performer

JAYCOR, Del Mar, CA

Objective

The objective is to develop a multi-dimensional, time-dependent computer model of mixing, pyrolysis, and agglomeration processes in coal conversion reactors.

Accomplishments

A time-dependent, axisymmetric computer model/code of a fluidized-bed, agglomerating gasifier has been developed. The code describes various processes which can be generally classified into fluid dynamics, chemistry, collisions, and agglomeration. In addition, the code for each of the processes is modularized to facilitate the addition of new modules or the replacement of old ones. Both dense phase and dilute phase gasification simulations can be conducted in either an extrapolative (predictive) mode or in an interpolative mode to assist analyses of experimental data.

The numerical computer codes have been delivered to DOE/METC together with a description of the model and code user's manual, and the code has been installed and implemented on the METC computer facilities.

Current Work

Current efforts are directed toward analyzing and evaluating not only the fluidized-bed gasifier code, but also an entrained-flow gasifier code developed concurrently by JAYCOR with Government support. The results of these studies, which will be conducted using both DOE/METC and other Government-sponsored computer facilities, can then be compared to results obtained from the BiGas entrained-flow gasifier to provide information for the possible subsequent enhancement of both models.

Application

The JAYCOR fluidized-bed and entrained-flow gasifier models/codes will provide insight into the phenomena involved during gasifier operations and, after verification and validation, may provide information relative to reactor performance after scale-up.

A.2.3.3

Title

Riser Reactor Studies and Modeling

Performer

Environmental Research and Technology, Pittsburgh, PA

Objective

The objective is to develop a model that will predict the conversion of a chemical reaction occuring in a riser reactor which contains a flowing gas-solid suspension. The model is to be developed from experimental studies by ERT which include identifying wall effects by characterizing the performance of 3.-, 4.25-, and 6-inch diameter reactors.

Accomplishments

A method (device) for making the initial separation of gas from solid in a stream heavily laden with solids has been developed (greater than 98 percent efficiency). During system checkout, limited data on effectiveness of contacting between a gas and solid, solids circulation rate, gas velocity, and pressure gradient for flowing suspensions were obtained. A rate equation, based on Langmuir-Hinshelwood kinetics, was found which correlates data from ozone decomposition over a solid catalyst in the riser reactor. This is providing insight on the apparent low activation energy of the process.

Current Work

This effort was initiated, to a large degree, in support of the Hydrocarbon Research, Inc. (HRI), pilot plant, which has been shut down because of operational difficulties as well as re-directed emphasis of the gasification program. Current efforts, therefore, are directed to the analysis and evaluation of data obtained during the tests that were conducted and the preparation of a final report of results.

A.2.3.4 Stochastic Study of Local Fluctuations Around the Distributor in a Fluidized-Bed Gasifier, Kansas State University, Manhattan, KS

The objective of this new research effort is to determine the local and fluctuating phenomena around the distributor of a fluidized-bed gasifier by measuring local particle velocities, local pressure, and pressure fluctuations around the jet, using fiber optic and pressure transducer techniques coupled with correlation methods. The results will be tested against models developed for the data using a stochastic approach. A capacitance probe and a microcapacitance probe have been demonstrated to measure bubble frequency and bubble coalescence as well as local fluctuations of particle motion in a liquid-solids fluidized bed. In addition, a correlation technique has been developed to relate signals from the capacitance probes to jet penetration depth, the dead zone height, and the velocity of a relatively large particle in a two-phase flow system involving solid particles. Both the bubbling frequency in a gas-solids fluidized bed and its stochastic variation along the axial direction of the bed have been determined by means of the capacitance method. The stochastic model proposed, more specifically a pure-death process, appears to be capable of describing the stochastic variation of the bubbling frequency along the axial direction in the fluidized bed.

A.2.3.5 Analytical Modeling of Gasification Processes, University of Houston, Houston, TX.

The primary objective of this effort was to model single particle char burning and gasification with implications on fluidized-bed combustion and gasification processes. The study indicates that it is essential to analyze single particle behavior to predict particle burnout time, quenching, non-ignition, and maximum temperature. Intraparticle effects were studied with consideration of changes in local internal surface area and porosity of the particles. The intraparticle mass transport equations coupled with reaction and external structure and with reacting boundary layer were solved. Models were developed for the changing intraparticle structure based on hypotheses about the macro- and micropores and how they coalesce and combine as reaction proceeds. The results of the studies were used to develop models of diffusion limited and kinetic limited fluidized-bed char combustion.

A.2.3.6 Prediction and Measurement of Operating Parameters for Entrained-Flow Coal Gasification Processes — Modeling, Brigham Young University, Provo, UT

The major objective of this project is to validate, refine, and document a previously developed two-dimensional model for prediction of entrained-flow coal gasifier performance. Previous analytical modeling work at BYU led to the development of two separate computer codes which describe the operation of a pulverized coal gasifier/combustor. The first model is a one-dimensional, plug-flow reactor code which describes gas and particle mixing rates as input conditions but otherwise considers the devolatilization and heterogeneous reaction of the coal. The second code is a two-dimensional axisymmetric code which models gas and particle mixing as well as the coal reactions.

During the current project, subroutines for coal devolatilization, char heterogeneous reactions, radiative heat transfer, and particulate motion have been incorporated into the two-dimensional model, as have parameters for turbulence, gas-phase reactions, coal reactions, and two-phase effects. User's manuals for both models are being prepared. Current efforts are directed toward validating the two-dimensional model. Completion of the project is scheduled for September 1983.

A.2.3.7

Title

Gasification Reactions Measured with FTIR

Performer

Advanced Fuel Research, Inc., East Hartford, CT

Objective

The goal of this program is to develop the techniques to characterize a raw coal with a few simple tests and use this characterization to predict the coal's behavior in a gasifier. The program proposes the collection of data in an entrained-flow coal reactor with on-line in situ gas analysis using a Fourier Transform Infrared (FTIR) Spectrometer. The FTIR analysis will allow direct measurements of species evolution kinetics and kinetics of secondary reactions such as cracking, soot formation, char gasification, etc.

Accomplishments

The current contract was initiated in September 1981, and the program is based on a continuing research effort which has had sponsorship of the National Science Foundation (NSF), DOE, and the Environmental Protection Agency (EPA). The work has developed an important understanding of coal thermal decomposition, which was incorporated into a successful general kinetic model. The model allows the prediction of the time and temperature dependent evolution of pyrolysis products in a heated grid apparatus from a knowledge of the coal's functional group distribution using a set of kinetic rate constants which are independent of coal rank.

The current program will extend these results to coal pyrolysis under practical gasification conditions in a laboratory-scale entrained-bed reactor.

Current Work

The current work is aimed toward the determination of kinetic rates and secondary reactions using the entrained-flow reactor and the use of the data for the extension and modification of the thermal decomposition model.

Application

It is expected that the results of the program will be a significant step toward more efficient, more pollution-free, and more sophisticated gasification of coal. The results will have application to new as well as existing gasifiers. The program will also provide an opportunity to examine the FTIR as an instrument to provide on-line species and temperature data in a coal gasification plant.

A.2.3.8 Hydrodynamical Basis for Scaling Fluidization Data on Jet Penetration and Mixing Relevant to Fluidized-Bed Coal Gasifiers, University of Massachusetts, Amherst, MA

This new effort involves the development of non-dimensional relationships describing fluidization and the use of these relationships to correlate the published data on jet penetration and mixing in fluidized-bed gasifiers. The study is designed to provide a synthesis of fluidization data which can be used in reactor design and scale-up. Progress to date includes the preliminary scaling of jet data for three-dimensional and semi-circular beds which suggests that measurement of jet penetration by several investigators can be correlated by non-dimensional parameters including the Froude number, ratio of solid to gas velocity, ratio of gas to solid density, ratio of particle to jet orifice diameter, and the Reynolds number. These initial results appear to be consistent with and partially verify a non-dimensional analysis of the continuum equations of motion for gas and particle flows in a fluidized bed.

A.2.3.9 Dynamic Behavior of Moving-Bed Coal Gasification Reactors, Washington University, St. Louis, MO

The objective of this research is to develop a dynamic model of moving-bed gasifiers and to investigate the stability and controllability of the gasifier when it is subject to typical load disturbances. An understanding of the process dynamics can lead to improved design and operations which will result in increased productivity from coal conversion plants. Progress to date has resulted in the development of a mathematical model composed of partial differential equations which are solved numerically using finite difference methods. The model has been used to study the stability and controllability characteristics of a gasifier and the results confirm that gasifier operation is very sensitive to step changes in the coal, steam, and oxygen feed rates. In particular, the ash depth in the gasifier, which should be operated with as little ash layer as possible for maximum efficiency, was found to vary strongly with these same input variables.

The effect of the blast feed rate to control the ash layer thickness was studied using a feedback control loop. Control using oxygen flow was found to be difficult because of the low flow rates and high sensitivity factor. Steam flow, however, was found to be effective in maintaining a reasonably constant ash layer. Steady-state predictions from the model agree well with published data; however, the results of transient predictions have only been compared qualitatively due to a lack of published data.

A.2.3.10

Transfer of ASPEN Technology at METC, Massachusetts Institute of Technology, Cambridge, MA

The primary objectives of this work are to transfer ASPEN technology to METC and to demonstrate the ability of ASPEN to simulate coal conversion processes by modeling the CONOCO Slagging Lurgi Gasification Process. ASPEN software has been installed on the METC VAX computer system and on the Argonne IBM computer system. ASPEN models have been developed for all major sections of the CONOCO Demonstration Plant and rigorous models have been developed for the hot carbonate acid-gas removal system and the combined shift methanation section. In the future the ASPEN CONOCO models will be exercised individually and integrated to determine code stability and reliability. The models will then be validated with CONOCO design data. The ASPEN simulator will be the primary process modeling tool at METC. It is the state-of-the-art code for coal conversion process simulation. The CONOCO models can be used as stand-alone models or integrated into other gasification process simulations.

A.2.4 Catalytic Gasification

A.2.4.1

Title

Catalytic Enhancement of Coal Gasification

Performer

Columbia Gas System Service Corporation, Columbus, OH

Objective

The original objective of this project was to assess the possible benefits of using sodium carbonate catalyst in the gasification of coal in a fixed-bed reactor. However, emphasis has recently been shifted to a fluidized-bed mode.

Accomplishments

Operational problems plagued this project in 1981 and led to installation of continuous, auger-driven coal feed and ash withdrawal systems. These systems only partially alleviated the problems, and subsequent difficulties experienced with Pittsburgh No. 8 bituminous coal resulted in a switch to the fluidized-bed mode. Testing in this mode in the 3-inch i.d. reactor has yielded preliminary results for pretreated Pittsburgh No. 8 coal solution impregnated with approximately 7 percent Na_2CO_3 and gasified in oxygen and steam at 350 psig. The effect of the catalyst on gasification rate has been disappointing, with less than 80 percent increase observed in all cases. Observed temperature decreases have ranged from 5° to 70°F. The most significant result from the catalyst addition has been a large increase in steam decomposition, ranging from 57 percent to 197 percent, while the H_2/CO ratio has been observed to be 3 to 7 times greater with catalyzed coal than with uncatalyzed coal. It should be noted that only a limited amount of data is currently available and detailed evaluation has not been completed so that the information presented here must be regarded as very preliminary.

Current Work

Current plans are to perform a limited amount of additional experimental work. Efforts are being directed toward completion of a final report by April 1982.

Application

If the use of sodium carbonate catalyst can be shown to be feasible in gasifying coal at lower temperatures, several benefits will result. The lower operating temperature will require less oxygen per pound of coal than in non catalyzed gasification. Reduced steam feed will be possible because the lower operating temperature will require less steam to moderate temperatures, and the steam that is supplied will be more effectively used through catalytic action. A lower operating temperature can be expected to improve the methane yield from the gasifier as well.

A.2.4.2 *Title*

Mechanisms of Gasification Reactions in the Catalysis of Coal, Char, and Other Carbonaceous Materials

Performer

General Electric Company, R&D Center, Schenectady, NY

Objective

Although the promotional effects of alkali and alkaline earth salts on the gasification rates of carbonaceous material have been widely recognized, the mechanisms of their action have not been established. The objectives of this study are to: (1) achieve an understanding of the mechanisms of alkali and alkaline earth-based catalysis in gasification reactions of coal and char, (2) identify controlling parameters in such reactions, and (3) obtain the relative activities of alkali and alkaline earth catalysts for a variety of coals and chars.

Accomplishments

The results obtained to date indicate that catalytic gasification in CO_2 and steam involves chemical reactions between the salt phase and the carbon substrate and between the surface species and the components of the gaseous environment. Thus, on heating salt catalysts with coal char or graphite in an inert atmosphere, solid state reactions occur at tempertures in the gasification range, i.e., 700°-1000°C. The catalytic effect during gasification is interpretable on the basis of a sequence of redox reactions at a carbon site, i.e., catalyst + carbon → reduction → gasification of carbon → re-oxidation of catalyst. The solid state reactions appear to have reaction times of the order of those for steam gasification at commercial gasification conditions.

The effects of a wide variety of alkali metal and alkaline earth catalysts have been studied during gasification of anthracite, bituminous coal, and lignite. Gasification has proceeded in atmospheres of CO_2 and $H_2O(g)$ with excellent cross-checked reproducibility between two independent thermogravimetric analyzer systems. In addition to gasification, studies of surface area and pore volume distributions in coals, uncatalyzed chars, catalyzed chars, and mineral matter extracted from the coal by low-temperature ashing techniques have been conducted. Several methods of catalyst contacting have been attempted: addition "micronized" catalyst powder to lump coal and to "micronized" coal, catalyst addition to coal chars, pressure impregnation of the original parent coals, and catalyst addition to demineralized coals and to pure graphites. Gasified chars have been analyzed using scanning electron microscopy and energy dispersive x-ray techniques.

Current Work

Current efforts are to complete thermogravimetric tests on uncatalyzed and catalyzed samples of graphite, anthracite, Pittsburgh No. 8 and Illinois No. 6 bituminous, Wyodak subbituminous, and Montana lignite coal to identify and confirm mechanisms of catalysis. Parametric kinetic studies include varying the anion with constant potassium cation (K^+, K_2CO_3, $KHCO_3$, KOH, K_2O, K_2SO_4, HCOOK, HCl, and KF); varying alkali metal cation with constant carbonate anion (Li_2CO_3, Na_2CO_3, K_2CO_3, and Cs_2CO_3); varying forms of nickel as a transition metal (Ni, $NiCO_3$, and NiO); varying alkaline earth with constant carbonate anion ($CaCO_3$, $SrCO_3$, and $BaCO_3$); and binary eutectic mixtures of the above salts selected on the basis of reduced melting points and ability to utilize NaCl as an ingredient. Planned completion rate November 1982.

Application

Successful completion of this study will provide an expanded understanding of the fundamentals of catalytic gasification and will provide the basis for improved operation and control of processes based on that concept. In particular, elucidation of mechanistic aspects has the potential of leading to new concepts in catalysts — in the method by which they are dispersed, in the composition of desirable catalytic salts, or by simplifying their recovery from the residue coal ash.

A.2.4.3

Title

Mechanism of Catalytic Gasification of Coal Char

Performer

SRI International, Menlo Park CA

Objective

Although the promotional effects of alkali and alkaline earth salts on the gasification rates of carbonaceous materials have been widely recognized, the mechanisms of their action have not been established. The objectives of this study are to: (1) achieve an understanding of the mechanisms of alkali, alkaline earth, and transition-metal salts in the catalysis of gasification reactions of coal char; (2) identify controlling parameters in such reactions; and (3) obtain the relative activities of alkali, alkaline earth, and transition-metal catalysts for a variety of coal chars.

Accomplishments

The experimental results to date point to the operation of redox cycle in the potassium carbonate-catalyzed char gasification reaction. The alkali salt or its derivative is reduced by the carbon with the release of CO and subsequently reoxidized by the gaseous reactant (CO_2 or H_2O). Such a process must occur at a catalyst-carbon interface and thus requires extensive dispersal of the catalyst over the surface of the char.

Investigations have focused on one char from Illinois No. 6 bituminous coal, and one catalyst cation, K, primarily in the forms of K_2CO_3 and KOH. Two principal experimental techniques have been used to provide information about chemical pathways in char gasification reactions. One, temperature programmed reaction (TPR), reveals the rate of formation of stable gaseous products resulting from the reaction of a gaseous reactant with the coal char as a function of temperature, mass of char, and gaseous reactant pressure. The other, high-temperature Knudsen mass spectrometry, complements TPR experiments by revealing the partial pressures of vapor species in equilibrium with the solid char as a function of temperature and the gaseous environment. This information has been supplemented by: (a) examination of the char by scanning electron microscopy and x-ray diffraction to determine structural characteristics and changes, (b) BET gas adsorption measurements to determine internal surface areas of fresh and partially gasified char samples, and (c) evaluation of free-radical densities in chars and carbons exposed to various pretreatments by in situ electron paramagnetic resonance spectroscopy (ESR). A thermogravimetric analyzer (TGA) has been used to assess overall gasification rates.

Current Work

Current work at SRI is focusing on completion of studies of steam, CO_2 and H_2 gasificiation of a variety of coal chars. Catalysts to be studied include potassium, sodium, calcium, and iron in the form of water-soluble carbonates, bicarbonates, hydroxides, or other salts. Parametric tests will gather information on product distribution, reaction intermediates, surface morphology, and gasification reaction rates as a function of degree of catalyst impregnation. Planned completion date is September 1982.

Application

Successful completion of this study will provide an expanded understanding of the fundamentals of catalytic gasification and will provide the basis for improved operation and control of processes based on that concept. In particular, elucidation of mechanistic aspects has the potential of leading to new concepts in catalysts — in the method by which they are dispersed, in the composition of desirable catalytic salts, or by the simplificiation of their recovery from the residue coal ash.

A.2.4.4

Title

Coal Gasification Catalysis Reaction Mechanisms

Performer

Rockwell International, Canoga Park, CA

Objective

Although the promotional effects of alkali and alkaline earth salts on the gasification rates of carbonaceous materials have been widely recognized, the mechanisms of their action have not been established. The objectives of this study are to: (1) achieve an understanding of the mechanisms of alkali and alkaline earth-based catalysis in gasification reactions of coal char, (2) identify controlling parameters in such reactions, and (3) obtain the relative activities of alkali and alkaline earth catalysts for the gasification of Illinois No. 6 bituminous coal char.

Accomplishments

Gasification rate experiments have produced results generally consistent with other published data. The more significant results obtained thus far in this portion of the program include: (1) the discovery of the highly pyrophoric nature of partially gasified catalyzed char produced by steam gasification in contrast to that yielded by CO_2 gasification, (2) the transient high-catalytic effect of the OH^- ion, (3) the catalytic activity of K_2SO_4, (4) the contrasts between the rates of methane formation in the presence or absence of effective catalysts during steam gasification, and (5) the dependence of the gasification rate on the cation of the alkali metal carbonate used as a catalyst.

Studies to date have concentrated on CO_2 gasification of Illinois No. 6 bituminous coal char with K_2CO_3 catalyst and steam gasification of the same char with a variety of alkali metal and alkaline earth catalysts. Reaction rates have been measured directly by thermogravimetric analysis and gas chromotography with mass spectral analysis. Additional data on the char-catalyst mixtures at various stages of gasification have been obtained by nuclear magnetic resonance spectroscopy, x-ray photoelectron spectroscopy, electron paramagnetic spectroscopy, infrared spectroscopy, BET surface area measurements, and porosimetry.

Current Work

Current efforts are to complete the study of cation and anion effects of alkali metal catalysts, to study alkaline earth catalyzed steam gasification, to study the effects of reaction products (CO and CH_4) on gasification kinetics, to study the K_2CO_3 catalysis of hydrogasification, and to develop mathematical models of identified catalytic mechanisms. Planned completion date is July 1982.

Application

Successful completion of this study will provide an expanded understanding of the fundamentals of catalytic gasification and will provide the basis for improved operation and control of processes based on that concept. In particular, elucidation of mechanistic aspects has the potential of leading to new concepts in catalysts — in the method by which they are dispersed, in the composition of desirable catalytic salts, or by the simplification of their recovery from the residue coal ash.

A.2.4.5

Title

Coal Gasification Using Chemically Incorporated Catalysts

Performer

Battelle-Columbus Laboratories, Columbus, OH

Objective

The objective is to evaluate the hydrogasification and steam-oxygen gasification characteristics of caking coals subjected to a mild pretreatment process involving lime and small amounts of sodium hydroxide in the presence of water to determine the effectiveness of this impregnation pretreatment for enhancing gasification while preventing agglomeration of caking coals.

Accomplishments

Caking coals such as Illinois No. 6, when impregnation pretreated with 0.15 part lime and 0.01 part sodium hydroxide in water to 1 part coal, showed steam reactivities up to 10 times greater and hydrogasification reactivities up to 50 times greater than the raw coal. The agglomerating index was reduced, and there were no caking problems in at least some runs in the 4-inch fluidized-bed steam-oxygen gasifier at PETC and in the 2.8-inch continuous tubular hydro-gasification reactor at Battelle. Mild to severe caking was observed on some runs due to either tar condensation during hydrogasification or coal particle size in excess of 50 mesh during steam-oxygen gasification.

A series of tests was completed to obtain correlations between treatment conditions for chemically incorporated catalysts in caking coals and their effectiveness in promoting gasification with either steam/oxygen or hydrogen in the absence of agglomeration of feedstock.

Current Work

A comprehensive final report

was prepared, summarizing all the project work.

Application

The results of this study are complementary to some other studies on coal gasification with catalysts, such as that being conducted at PETC. Due to the potentially favorable economics of a lime-based catalytic process, other gasification processes might benefit by use of a cheaper catalyst and/or by the use of eastern caking coals. However, technical problems appear to limit these potential applications of the Battelle process.

A.2.4.6

Title

Catalytic Effects in Coal Gasification

Performer

Sandia National Laboratories, Albuquerque, NM

Objective

The objective is to conduct a study of catalytic effects of coal minerals in coal gasification. Emphasis will be placed on determining the role of inherent mineral matter on the devolatilization and subsequent gasification of coal. The work will be directed toward a fundamental understanding of the mechanisms of catalytic gasification and will attempt to correlate the properties of several coals with their behavior under various gasification conditions. The ultimate objective will be to develop an understanding of mineral matter effects and other catalytic effects in coal gasification.

Accomplishments

Five high-volatile bituminous coals whose mineral matter content varies from about 5 to 25 percent have been selected for this study. Each coal has been chemically and and physically characterized. Base line studies of the gasification rates of these coals in nitrogen and hydrogen have been completed at 600°, 800°, and 1000°C. A gas-sampling device for a thermogravimetric analysis (TGA) system sampled the product gas stream at selected time intervals, followed by gas chromatographic (GC) determination of gas composition. The gasification rates of demineralized coals, prepared using float sink techniques, were measured under gasification conditions used in the baseline studies. The effect of added mineral matter on demineralized coals and on low-ash coals for the gasification rate and product gas distribution was determined. Detailed studies have shown that pyrite in coal acts as an effective hyrdogasification catalyst via conversion to metallic iron. The iron crystallite size, number of active sites (possibly defects) on the crystallite surface, and the hydrogen dissociation on the surface have all been shown to be critical by studies with model iron compounds.

Current Work

Inherent hydrogasification experiments involve the rate of methane production as influenced by inherent minerals and coal catalyst interactions. Kinetic studies of coals and separated coal minerals include determination of rate of weight loss by thermogravimetric analysis (TGA) at pressures from 1 atm to

1000 psig and determination of apparent activation energies by the change in rate with temperature of reaction. Rates of methane and other product formations are being followed by gas chromatography. Conditions are 15 to 1000 psig at temperatures ≤1000°C.

Application

This program is providing technical support to coal gasification processes in general by clarifying the effect of mineral matter in the gasification of coal. The primary thrust for this work is to obtain a fundamental understanding of the mechanism of catalytic action of mineral matter in coal gasification.

A.2.4.7

Title

Catalytic Gasification

Performer

Pittsburgh Energy Technology Center, U.S. DOE, Pittsburgh, PA

Objective

The objective of this work is to establish a catalytic gasification data base on the effects of a wide variety of cation-anion combinations for use as gasification catalysts to enhance reaction rates and to reduce caking in bituminous coals.

Accomplishments

A series of 180 experiments covering an extensive test matrix of 80 potential catalysts was performed in a bench-scale, fixed-bed, steam gasifier. Chemicals of various anion-cation combinations were impregnated in a water slurry into the coal at a pressure of 1000 psig and a temperature of 285°C in a 300 cc autoclave. Monocatalysts at 5 weight percent loading and bicatalysts at 2.5 weight percent loading were impregnated into Illinois No. 6 coal. The bicatalysts were selected to decake the coal and increase its reactivity. The bench-scale gasification tests were performed at a pressure of 300 psig and a temperature of 800°C.

Test results indicated that ammonium carbonate has a synergistic effect on the reactivity of Illinois No. 6 coal when combined with alkali or alkaline earth catalysts. The rate of steam gasification of Illinois No. 6 coal in a fixed-bed reactor was shown to vary with carbon conversion in a manner consistent with the unreacted, shrinking-core model of gas-solid reactions. It was found that 10 weight percent loading of potassium carbonate, applied to the coal by solution impregnation, accelerated the reaction rate by a factor of 3.1-4.6 for reaction temperatures ranging from 800°-900°F. The acceleration was brought about through a decrease in the overall activation energy.

Current Work

All experimental work has been completed and current efforts are aimed at preparation of a final report with a planned completion date of March 1982.

Application

This study provides information on a wide variety of potential coal gasification catalysts which will be useful in the development and evaluation of catalytic gasification processes.

A.2.4.8

Title

Catalytic Coal Conversion Support

Performer

Los Alamos National Laboratory, Los Alamos, NM

Objective

The objective is to determine the changes in coal structure produced by heating in the presence of catalysts and gas atmospheres typical of various candidate processes for catalytic coal conversion.

Accomplishments

Various coals were heated in the presence of atmospheres of He, N_2, H_2, CO, CO_2, or H_2O to fixed temperatures over the range of 100° to 600°C. The same coals were impregnated with aqueous solutions of various alkaline, alkaline earth, and transition metal salts before heating. Comparisons in coal-structure changes were made by means of fragmentation of the coal structure by beams from CO_2 and Nd lasers, and analysis of the fragments was made by gas-liquid chromatography and mass spectrometry. Significant changes in the proportions of aliphatic, aromatic, and heteroatom (S,O,N) building blocks in the coal structure occuried by heating in the presence of the catalysts. These results indicate that specific changes in coal structure catalyzed by materials used in catalytic processes under study by other contractors (such as Battelle-Columbus and Columbia Gas) can possibly be determined and these processes, thereby, can be better understood.

The structural changes in coal were compared with those in polymeric models of known structure simulating that of coal. For example, the natural polymeric precursor of coal, wood lignin, not only yields remnants of its building blocks, such as methoxyphenol, during heating, but also yields indene, a product of ring closure reactions, which is produced by heating coal as well.

Current Work

Work is underway on statistical analysis and interpretation of the data from about 650 tests representing about 65 test mixtures of coal, graphite, lignite, and model substances heat treated at several different temperatures in various gaseous atmospheres in the presence of 16 different catalysts. Work has also been started on the preparation of a final report.

Application

This project has the potential for elucidating hitherto unknown changes in coal structure during heating and the catalysis of these changes during coal-conversion processes. This information could be used to direct the production of heteroatom derivatives into innocuous forms, such as elemental nitrogen in place of ammonia, or increased yields of desired heteroatom products, such as carbon monoxide.

A.2.5 Gasification Support Studies

A.2.5.1 The Role of C-CO_2 Reactions in the Gasification of Coal and Char, West Virginia University, Morgantown, WV

Work is almost complete on this 3½-year study of fundamental phenomena related to coal gasification. The purposes of this project were: (1) to obtain basic kinetic information on the reactions of coal, char, and pure carbon with CO_2 and steam; (2) to investigate the fluidization phenomena which are important to the design and scale-up of gasification systems; and (3) to correlate the data obtained for use in the design and prediction of performance of fluidized-bed gasification systems. During this work it was found that extent of pyrolysis depends on particle size, pressure, and temperature. The temperature dependence occurs in three stages according to whether chemical reaction kinetics or internal or external diffusion is the rate-limiting process. Char properties were determined including diffusion coefficients of CO_2 in char. Reactivity of char with steam or CO_2 did not depend strongly on pressure over the range tested, but inhibition by CO and H_2 increased rapidly with pressure. It was found that elutriation of particles in a hot bed can be determined from low-temperature results if they are compared at the same value of excess fluid velocity above minimum fluidization. Bubble size and numbers change only slightly with pressure. A basic fluidized-bed gasification model was developed.

A.2.5.2 Kinetics of Coal-Char Gasification at Process Conditions, Case Western Reserve University, Cleveland, OH

The objective of this research is to gain a better understanding of and a data base for practical coal gasification processes. Major problem areas being addressed are: (1) lack of data at practical operating conditions, (2) lack of parallel measurements of specific surface area and pore volume distribution on coal-char samples, (3) a need for knowledge of the detailed chemistry and mechanics of gasification reactions, and (4) a need for a more realistic kinetic model. The heart of the experimental portion of this effort is a novel hanging bed reactor for obtaining thermogravimetric kinetic data. The entire reactor plus contents are weighed during the course of a run. Surface area, porosity, and morphology of the samples used are also being determined. The results of the experimental work are being used to obtain correlations between gasification rate, physical characteristics, and process conditions. Attempts are being made to develop mechanistic interpretations of the results. All data are being obtained at conditions of temperature, pressure, and gaseous atmosphere characteristic of practical gasification processes.

A.2.5.3 Studies Toward Improved Techniques for Gasifying Coal, City College, The City University of New York, New York, NY

The objective of this research is to provide an experimental basis for improving the economic attractiveness of coal gasification process by the cogeneration of gaseous fuel and high market value, light liquid fuel, such as BTX, through flash pyrolysis in steam and steam-hydrogen mixtures. In work to date in laboratory-scale experiments on the flash (1-second) hydrolysis of Illinois No. 6 coal in 50 atmospheres of pure steam, a yield of 68 percent carbon conversion to liquid product was obtained at 900°C (120 seconds of coal heating). The gas yield was 20 percent, consisting of approximately equal amounts of methane, carbon monoxide, and carbon dioxide. The residual char was only 12 percent. These conditions may prove to be optimum for maximum liquids production. Currently, determinations are being made of relative yields of liquid, gas, and char, and the gas composition and the variation of these with reactant gas composition (steam, steam/hydrogen), reactant gas pressure (1 to 100 atm), heating rate (20° to 2000°C per second), vapor residence time (0.1 to 100 seconds), and solids contact time (2 to 300 seconds).

A.2.5.4 Kinetics and Modeling of the Oxidative Pretreatment of Coal, University of Pennsylvania, Philadelphia, PA

The objective of this research was to investigate the rates at which a variety of coals change their properties when subjected to moderate temperature drying and mild gas-phase oxidation, and to correlate the effectiveness of such treatment on the agglomerative properties of the coals. The coals pretreated at various conditions of temperature, pressure, and particle size were evaluated by a thermomechanical expansion test for correlation with the oxidative changes. Models were developed that can be used to explain, predict, and interpret practical results for a wide range of coals. The physical properties of a variety of coals, specifically, the reduction in caking propensity as the result of mild oxidative pretreatment and the change in porosity and surface area as the result of moderate-temperature drying and oxidation, were determined. Highly caked coal was rendered virtually noncaking by oxidation at 200°C. Coal drying generally reduced coal porosity, surface area, and particle-size distribution. The degree of change varied directly with original water content of the coal. This project has been completed.

A.2.5.5 Process Development Studies in Coal Gasification, University of Utah, Salt Lake City, UT

This project consists of two studies. In the first, the objective is to optimize a single-stage catalytic coal gasification concept which would use direct hyrdogenation of coal to form high-Btu gas. In this process, coal is being slurried with tetralin, and several catalysts and process variables are being investigated to optimize production of methane. Process-derived liquids are also being tested as the solvent. Success of this developmenight lead to a more thermally neutral process in which the heat of methanation is used rather than rejected. The second study focuses on experimental investigation of the steam reforming of aromatic liquids to produce hyrdogen or synthesis gas. This could lead to the use of the liquefaction and subsequent steam reforming of coal to replace the use of natural gas and naphtha for this purpose.

A.2.5.6 Influence of Changing Particle Structure on the Rate of Gas-Solid Gasification Reactions, Vanderbilt University, Nashville, TN

The objective of this research is to determine the changes in the particle structure of coal as it undergoes the reaction $C + CO_2 \rightarrow 2CO$. Changes in the structural parameters, such as surface area available for reaction, porosity, and pore size distribution, will markedly affect the rate of gas-solid reactions. Accompanying these changes in structural parameters are changes in the resistance to diffusion of gaseous products and reactants through the pores of the solid. An experimental system, which combines a pulse reactor with a flow-type BET apparatus, is being used to study the influence of a changing coal-solid structure on the gas-solid reaction.

Progress to date has demonstrated that the pore structure of coal char is greatly affected by the temperature increase used in the production of that char. Internal surface area of the char increased by two to threefold upon devolatilization. This increase in surface area should make chars more reactive than the parent coals since the reaction rate is proportional to the available surface area.

However, the increase in available surface produced during devolatilization generally causes a shift in the pore size distribution towards smaller pores. Measurement of the effective diffusivity shows a decrease on the order of approximately twofold.

A.2.5.7 Heterogeneous Kinetics of Coal Gasification, Brown Univeristy, Providence, RI

The objective of this research is to conduct fundamental experimental kinetic studies of the heterogenous gas-coal-char gasification reactions at high-temperature and pressure (up to 1400°F at 550 psig), using transient techniques in a novel, continuous flow apparatus. To date, work has been focused on the design and development of the experimental apparatus consisting of a continuous gas flow, fixed solids, gradient-less autoclave reactor, coupled with supersonic, modulated molecular beam sampling of the reactant and product gases. Currently, the entire experimental apparatus has been designed, constructed, interfaced, and is undergoing preliminary testing. Data for the coal-char-carbon dioxide-carbon monoxide reaction system will be generated initially with commercial chars. Once the system is sufficiently understood, coal-char will be introduced to the reactor. The resultant data will contribute significantly to the design, optimization, and evaluation of all types of coal gasifiers.

A.2.5.8

Title

Coal Flow Test Facility

Performer

Pittsburgh Energy Technology Center, U.S. DOE, Pittsburgh, PA

Objective

Since an accurate and reliable measurement of coal flow is essential in most coal conversion processes, development of suitable flow monitoring devices is of critical importance. The overall objective of this project is to test and evaluate various devices for monitoring and measuring the pneumatic transport of coal in pipes.

Accomplishments

After an extensive survey of commercially available flow monitoring devices, an Auburn monitor and a Micro Motion flow meter were selected and tested. The Auburn monitor relates the dielectric properties of solid/gas mixtures to mass flow rate, while operation of the Micro Motion flow meter is based on the Coriolis force exerted by the solid/gas mixture passing through a U-tube. Both candidate devices provide instantaneous mass flow information. Moreover, the Auburn monitor uses a patented rotating electric field technique, which provides a better volume average of the coal/gas mass flow in pipes than is usually obtained with uni-directional property measurement devices.

Conclusions drawn from the tests conducted are:

1. The Auburn Monitor can be used for monitoring coal/nitrogen mass flow. Variations in particle size distribution of coal between 30 percent and 70 percent minus 200 mesh and in coal moisture content up to 4.6 percent have no apparent effect on its peformance. A coal moisture content of 7.4 percent enhances the voltage signal from the Auburn monitor, presumably due to the large dielectric constant of water.
2. Insertion of the Micro Motion monitor into the test loop reduces the mass flow rate as well as the solid/gas loadings. Preliminary data so far indicate that the voltage signal from the Micro Motion monitor can be used to monitor the coal flow.
3. Analysis of pressure loss data indicates that existing theoretical models of Yang or Konno-Saito are not valid for dense phase coal flow. New correlations that fit the entire range of solid/gas loadings were developed.
4. A particle size effect on pressure loss data was also observed.

Current Work

Current efforts are concentrated on performing tests on a modified Micro Motion flowmeter for Sandia National Laboratories and evaluating a prototype of a Southwest Research Institute combined electron and nuclear magnetic resonance flowmeter.

Application

Because of the great importance of reliable coal flow measuring systems to coal conversion processes, several Governmental and private groups are involved in developing new flow monitoring techniques. The Coal Flow Test Facility provides a test ground for evaluating these new instruments as well as for those already commercially available.

A.2.6 Pyrolysis

A.2.6.1 Critical Studies in the Rapid Pyrolysis and Hydropyrolysis of of Coal, Massachusetts Institute of Technology, Cambridge MA

The objective of this work, which is almost completed, has been to perform systematic studies of the effects of operating conditions on product yields, compositions, and rates of formation in three critical areas of rapid coal pyrolysis and hydroprolysis: (1) effects of variables such as coal type, temperature, hydrogen partial pressure, and coal particle size;

(2) effects of secondary reactions of volatiles; and (3) catalytic effects of the inherent mineral matter of coal and of low-cost additives. Results have shown that almost all of these factors influence product distributions and compositions. Calcium minerals and alkali or alkaline earth ions affect tar and methane yields from pyrolysis, but few effects of clay, quartz, and iron sulfur mineral were observed. The presence of coal reduces the temperature of decomposition of calcium carbonate. The presence of this carbonate or of calcium oxide sharply increases CO yields. Transport of hydrogen in molten coal particles affected hydropyrolysis yields. By increasing particle size, agglomeration in entrained-flow hydropyrolysis retarded the hydrogen-coal reaction.

A.2.6.2 Kinetics of Coal Pyrolysis and Gasification, Pennsylvania State University, University Park, PA

The objectives of this research are: (1) to measure continuously the major gases produced during the pyrolysis and gasification of as-received and pretreated coals in nitrogen, steam, and syngas atmospheres following their rapid heating to maximum temperature; (2) to measure the catalytic activity of chars derived from as-received and pretreated coals for the concurrent methanation and hydrogasification reactions; and (3) to cross-correlate all data. Results thus far have shown that under the conditions tested, methane production was from the methanation rather than hydrogasification reaction. Carbon monoxide was found to inhibit the hydrogasification reaction as catalyzed by iron and the carbon-steam reaction when catalyzed by sodium, potassium, or calcium. Hydrogen inhibits the carbon-steam reaction when catalyzed by calcium. Theoretical and experimental results have shown that heat transfer and chemical reactions can cause significant temperature gradients within a reacting coal particle. Removal of ion-exchangeable cations resulted in an increase in both the quantity and rate of release of pyrolysis products.

A.2.6.3 Short Residence Time, Hyrdopyrolysis of Coal, Princeton, University, Princeton, NJ

The objective of this research is: (1) to collect experimental data to formulate a comprehensive understanding of coal hydropyrolysis and (2) to complete development of kinetic models to describe rate phenomena. Two types of coal, psoc 190 and psoc 102, were tested in a novel laboratory reactor that is specially designed for this research project. The results from runs at reduced pressure (0.1 torr) with 125 μm particles at temperatures up to 900°C, heating rates to 10^3 °C/s, and isothermal reaction times of 0-30s indicate no major differences. Currently, testing of a third type coal is under way. The studies will provide information toward the understanding of rapid hydropyrolysis of coal.

A.2.6.4 Rapid Pyrolysis of Coal by Hot Solids from a Fluidized-Bed Combustor, Massachusetts Institute of Technology, Cambridge, MA

This project is motivated by the potential commercial application of a process in which coal or oil shale is pyrolyzed in a fluidized bed by hot dolomitic or calcium oxide stones from a fluidized-bed combustor operating in parallel. The objective of this project which is nearly complete is then to help investigate technical feasibility by assessing the effects of the presence of such stones or the yields, heating values, and sulfur and nitrogen contents of pyrolysis products. For coal, results have shown almost complete removal of H_2S. CO_2 was removed at the same conditions, thereby increasing product gas heating value. Tar yields were reduced and gas yields were increased. A comparison of liquid yields from coal and oil shale pyrolysis with CaO showed a 25-30 percent reduction for the coal but only 0-5 percent for the shale. This is consistent with the view that CaO is specific for the removal of polycyclic aromatics. Thus, CaO use might reduce the mutagenic potency of coal pyrolysis tar products. Economic analysis showed that the implementation of the combined pyrolyzer/fluidized-bed combustor would provide good quality gaseous and liquid fuels from coal at an economically attractive cost.

A.3 Gas-Stream Treatment and Processing

A.3.1 Novel Acid Gas Removal

A.3.1.1

Title

Development of the CNG Acid-Gas Removal Process

Performer

CNG Research Company,
Cleveland, OH
Subcontractor: Helipump, Inc.,
Cleveland, OH

Objectives

This project is aimed at completing the basic data required for process development. Thus, there are four principal tasks: (1) build and operate a single stage crystallizer for separation of sulfur compounds to produce pure CO_2 and concentrated H_2S; (2) obtain basic equilibrium and handling data relative to absorption, crystallization, pumping, etc.; (3) examine process concepts for feed gases of low CO_2 concentration; and (4) determine the fate of trace constituents in the process.

Accomplishments

It has been demonstrated that, although it is technically viable, the CNG Acid Gas Removal Process appears to be less economical as CO_2 partial pressure in the feed gas is reduced below about 75 psia. Crystallization separation factors have been confirmed for H_2S/CO_2 at values from 500 to 1000. Work was conducted on COS, CS_2, C_2 and × C_2 versus CO_2. Vapor-liquid-solid equilibrium data acquisition has been completed. It was shown that the CNG crystallizer can be incorporated into any modified, selective, physical absorption process to deal with lower feed gas concentrations of CO_2 and to improve sulfur recovery economics. All work to date continues to indicate a successful process.

Current Work

Major equipment items in the bench-scale crystallizer are being designed and specified. Apparatus for slurry pumping is being reactivated. A mass flow-meter capable of measuring mass flows for liquids, slurries, and slurries containing a uniformly dispersed gas phase is being incorporated. The effect of trace contaminants on the process molecular sieves used for dehydration of feed gas is under study.

Application

Acid-gas removal from medium-Btu gases intended for various applications, i.e., high-Btu manufacture and indirect liquefaction or chemical synthesis, is one of the more costly unit operations in different gasification processes. The development of novel, more efficient, and less capital-intensive acid-gas removal processes would improve the economics of existing and new gasification processes.

A.3.2 Alkali/Particulate Removal

A.3.2.1

Title

Performance of Gas-Atomized Spray Scrubbers at High Pressure.

Performer

Air Pollution Technology, Inc., San Diego, CA

Objective

The objective is to determine the performance of venturi scrubbers in removing particulates from high-pressure gas streams in terms of collection efficiency and power consumption.

Accomplishments

A.P.T., Inc., has done an exploratory, experimental, and theoretical evaluation of venturi scrubbers operating at high gas pressures. The experimental results confirm the prediction that collection efficiency decreases and pressure drop for a given efficiency increases dramatically at high gas pressures. At pressures higher than 10 atm, the venturi scrubber cannot clean the gas to meet the compressor and turbine requirements.

Current Work

The high-pressure test program experiments were completed, and the final report is in final assessment and revision.

Application

The study assesses the applicability of gas-atomized spray scrubbers for removal of particulates from high-pressure gas streams. This is of importance because a large number of coal gasification development projects propose to use high-energy venturi scrubbers for particle removal at pressures as high as 100 atm.

A.3.2.2

Title

Laminar Flow-Cyclone Development Program

Performer

General Electric Company, Schenectady, NY

Objective

The objective was to develop a laminar flow-cyclone concept so as to achieve relatively high operating Reynolds numbers such that high-inlet velocities could be obtained in realistically sized cyclones.

Accomplishments

An exploratory investigation was conducted into the feasibility of maintaining laminar flow in a cyclone separator. Various experimental models were used to simulate the essential flow requirements, and observations were conducted on the turbulent-laminar character of the flow. From these observations, it was concluded that laminar flow could be maintained up to relatively high Reynolds numbers (3.8×10^5) in the radially inward swirl flow regime. However, a large-scale instability occurs in turning to the axial swirl flow regime. All present attempts to suppress this instability failed, and the investigation was terminated.

Current Work

This contract expired on May 31, 1981.

Application

This work was an attempt to generate a concept for affecting a marked reduction in collection "cut" size, to improve collection efficiency, to increase throughput per unit volume, and to reduce cost relative to more conventional high-efficiency collectors.

A.3.2.3

Title

Simultaneous High-Temperature Removal of Alkali and Particulates in a Pressurized Gasification System

Performer

Westinghouse Electric Corporation, Pittsburgh, PA

Objective

The objective is to perform experimental and analytical investigations, system designs, and cost estimates to ascertain the feasibility of using aluminosilicate-based getters for controlling alkali in pressurized gasification systems and to develop a comprehensive plan for evaluating a scale-up version of the getttering process as a unit operation or as an integrated part of a particulate removal device. A candidate getter will be identified by bench-scale studies as well as comprehensive thermogravimetric analysis (TGA) studies and attrition studies. The gettering kinetics, such as reaction rate, getter capacity, effect of low bulk gas alkali concentrations, regeneration for the selected getter, will be defined. System performance projections for an alkali gettering process will be developed and be used to define a plan for concept scale-up.

Accomplishments

A more detailed understanding has been developed with respect to the stoichiometry and mechanism of the gettering reaction. Also, a firm thermodynamic data base has been developed, which allows reliable projections to be made with respect to system and getter performance.

Parametric correlations have been developed with respect to the size of the packed bed required for alkali removal in a given hot-gas cleaning application for either a gasification or PFBC system. Modeling studies as part of this effort have shown that a packed bed is preferred to either a granular bed filter or entrained type system.

The most significant device developed has been the dual/balance TGA system. This enables a simultaneous monitoring of the weight gain of a reacting getter pellet along with the quantity of alkali evaporated from a platinum boat, i.e. the concentration of alkali in the bulk gas stream.

Current Work

Work is being continued to complete getter selection and qualification, which involved additional kinetic studies using both the bench-scale reactor and the TGA unit on a number of getters including 14 candidate materials subjected to a special screening test. System performance projections will provide a data base to the program definition for concept scale-up.

Application

The development of the alkali entrapment process will fill one of the necessary technology gaps in evolving an advanced low- or medium-Btu gasification system for integration with a combined-cycle power generation plant. The removal of alkali from hot medium- or low-Btu gas streams intended for use in turbines is necessary to prevent corrosion and deposition problems on turbine materials.

A.3.3 Sulfur Removal

A.3.3.1

Title

Development of a Solid-Absorption Process for Removal of Sulfur from Hot Fuel Gases

Performer

Battelle Pacific Northwest Laboratories, Richland, WA

Objective

The objective is to develop and demonstrate on a bench-scale level a process for removing sulfur from reducing gases at temperatures above 700°C. The process being developed is based on the use of molten alkali and alkaline earth eutectics within the pores of selected support materials. Preliminary system performance analysis will be conducted following completion of bench-scale sulfur removal and sorbent salt regeneration experiments.

Accomplishments

Significant progress was made on development of the process. The process concept was demonstrated using gases produced by gasification of coal. Over 99.9 percent sulfur removal efficiency was demonstrated as was sorbent regenerability and durability through 31 absorption/regeneration cycles on a single bed of sorbent. Regeneration runs demonstrated that a concentrated H_2S stream could be produced.

Current Work

Experiments on the parametric/cycling test will be completed by mid-January 1982. The final report on this project should be available in April 1982.

Application

The process being developed could provide one of the elements necessary for the hot-gas sulfur cleanup of low- or medium-Btu gas for use in combined cycle power generation applications.

A.3.3.2

Title

Improved Methods of Removal or Recovery of Major, Minor, or Trace Elements in Coal Conversion Processes

Performer

Institute of Gas Technology, Chicago, IL

Objective

The objective is to continue the work on the removal of COS, NH_3, and H_2S from syngas. The syngas is to be desulfurized at high temperatures.

Accomplishments

The previous work on COS and NH_3 removal shows that the most effective catalysts are based on beryllia, calcium oxide, and magnesia. HCN removal was also feasible with catalysts suitable for decomposing COS. The hot-desulfurization process being developed is based on regenerable

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solid sorbents. The solid sorbent is a mixture consisting of conventionally proven zinc oxide and other additives being developed by IGT. During the regeneration of such a sorbent, elemental sulfur is produced. When such a desulfurization process is fully developed, the by-product will be only sulfur and no oxides of sulfur.

Current Work

Exploratory studies under DOE sponsorship have revealed that the group IIA elements (calcium, magnesium, strontium, and beryllium) have activity greater than or equal to alumina-type catalysts for hydrolyzing COS. These studies are conducted over the temperature range of 500° to 900°F and pressures between atmospheric and and 300 psig with both simple mixtures of gases and clean synthesis gas. Experiments are in progress to determine the tolerance of these catalysts toward impurities under extended operation. A work plan for continuation of this study is being developed.

Application

An extensive effort is being made at IGT for syngas desulfurization and for the removal of other contaminants, i.e., COS and NH_3. The development of such technology is expected to have widespread application in low- to high-Btu gas production, combined-cycle, and fuel-cell programs. The removal of NH_3 is becoming important because NH_3 is considered a source of nitrogen-oxide emissions in combined-cycle systems. Presently the H_2S hot gas cleanup results are being used by METC for its hot gas cleanup program.

A.3.4 Tar Conversion

A.3.4.1

Title

Bench-Scale Development of Catalysts for Reforming Aromatic and Heterocyclic Hyrdocarbons

Performer

R. M. Parsons, Pasedena, CA

Objective

The objective is to develop catalysts capable of converting coal-derived organic and heterocyclic liquids boiling above 400°F to synthesis gas (H_2, CO, CO_2, and some CH_4) and lighter liquids in the presence of sulfur.

Accomplishments

The catalyst development work is being conducted by Engelhard Industries under contract to R. M. Parsons. Over 20 catalysts on steam-stabilized alumina supports have been tested. Approximately half of these are nickel-containing species, the remainder containing metals of the platinum group. These catalysts have been characterized for metal content, BET and active metal areas, and pore size distribution. Additional characterization has included evaluation for steam stability in a reactor constructed for this purpose and a study of coke formation via thermogravimetric means. Screening tests have been performed to determine catalyst activities, and selected catalysts have been subjected to long-term aging tests. Spent catalysts have been characterized and results compared to those obtained with fresh samples.

Results to date indicate that sulfur poisoning rather than sintering or coking is the primary cause for deactiviation.

p

While all nickel catalysts tested deactivated rather rapidly, excellent stability has been achieved with some platinum group metals. However, activities have been unacceptably low for these catalysts.

Current Work

Efforts are now concentrated on improving catalyst activities through increased metal loading or presulfidation of the catalyst. The feasibility of employing tar derived from a slagging, fixed-bed gasifier to evaluate a high-metal loading rhodium catalyst is being determined. If it appears experimentally feasible, such an evaluation will be conducted. Completion of the final report for this project is scheduled for March 1982.

Application

Development of a successful catalyst system will make it possible to convert the tars and oils present in some gasification streams to fuel gas components prior to shift, methanation, and other downstream processing.

A.3.4.2 Dew Points of Hot Gases Containing Condensible Tars, University of California, Berkeley, CA

The objective of this research was to obtain the fundamental physical-chemical and thermodynamic data for condensation of tars required for rational design of heat exchangers to recover sensible heat from hot, pressurized, tar-containing gases produced by coal gasification. Coal tars have been characterized and fugacity coefficients obtained for dew-point calculation. Vapor pressures have been obtained for high molecular-weight hydrocarbons and their nitrogen or sulfur analogues, including the use of a group-contribution method. The calulation of dew points under equilibrium conditions has resulted in a thermodynamic analysis of the dew-point phenomenon at high pressures. Experiments were conducted to obtain fundamental understanding and direct experimental data on the conditions under which tars condense from hot gases from coal gasification processes. Appropriate theoretical models were developed to provide a firm thermodynamic basis for the experimental information. This project was completed.

A.3.4.3 Thermal and Catalytic Cracking of Tars from Coal Gasification, Clark University, Worcester, MA

The objective of this research is: (1) to investigate the kinetics and mechanism of pyrolysis as well as catalytic decomposition of tar obtainable from various coal gasifiers, (2) to carry out a systematic study of catalytic cracking of tars in the presence of various catalysts at different conditions (with temperatures up to 1500°C) for the purpose of elucidating the reaction kinetics, (3) to screen catalysts for tar cracking and to observe the extent and rate of carbon deposition on the surface of catalyst particles, and (4) to apply the kinetic model of Weekman which was successful in describing the petroleum crude cracking, to the results of tar cracking experiments in order to find conditions for minimizing the low-boiling aromatics and maximizing gases and coke. Current and future work will continue to perform tar and model compound cracking experiments to optimize the operating conditions for maximizing gas and char production and eventually to develop a kinetic model which describes the rate of cracking reaction. Preliminary results available at this time indicate that firebrick is the best catalyst for cracking METC gasifier tar, and the aluminum catalyst gives the best results for cracking model compound. The work on the cracking of tars could result in the development of a less expensive and more environmentally acceptable approach to certain coal gasification processes.

A.3.4.4 Coal Gasification and Tar Conversion Reactions Over Calcium Oxide, Massachusetts Institute of Technology, Cambridge, MA

The objective of this work is to explore the possible use of CaO as an additive for improving coal gasification and pyrolysis products. Recent results in the contractor's laboratory have shown that fluidized-bed pyrolysis of coal in the presence of calcium oxide results in: (1) desulfurization of the product gases, (2) enhanced conversion of the coal heat content to gas, and (3) product gas of increased heating value. Further study showed that the cracking activity of CaO is more selective for aromatic than aliphatic hydrocarbons. This suggests that tars from coal gasification could have reduced mutagenic potency. In this project fresh pyrolysis tars are generated by passing a flux of carrier gas over a thin bed of coal particles subjected to a preset temperature-time history. These tars are then contacted with an independently temperature-controlled bed of CaO particles. Data are being obtained on rates and extents of tar conversion, on product compositions, on stone activity loss, and on stone regeneration.

A.3.4.5

Title

Pollutant Control in Coal Gasification — Catalytic Cracking

Performer

Research Triangle Institute, Durham, NC

Objective

This project addresses a potential method for reducing the quanities of environmental pollutants in gasifier quench water, namely vapor-phase cracking of undesirable components prior to quenching the raw gas. The objectives of this effort are to evaluate the effectiveness of potential catalysts and to determine their ability to withstand the severe conditions and poisons which exist in such a gas stream.

Accomplishments

Installation of the hardware for testing the vapor-phase cracking of heavy hydrocarbons was nearly completed. Seven catalysts were selected for screening, including a Wyoming subbituminous char, an ammonia synthesis catalyst, an iron-chromium shift catalyst, and four silica or silica-alumina supported metals. In addition, researchers anticipate that a lignite char will be included in the screening tests.

Current Work

Efforts in the vapor-phase cracking study are focused on completion of the hardware installation. Laboratory experiments will then be conducted on vapor-phase catalytic cracking (at 400° to 600°C and 300 to

1000 psi) of organic compounds, including polycyclic aromatic hydrocarbons and tars, over the various catalysts. The amount of reaction of compounds in simulated gases and of gaseous compounds and tars tars generated in an existing laboratory-scale coal gasifier will be determined for specified catalysts. The amount of carbon deposition and sulfur increase in the catalysts will be determined, and the regenerability of selected catalysts will be evaluated.

Application

A successful vapor-phase cracking process would have advantages over the traditional quench-then-treatment approach since eliminating heavy organics from the raw gas at high temperature would reduce operational problems downstream of the gasifier, permit the recovery of high quality waste heat, and reduce the cost of condensate cleanup for reuse of this stream in the gasification process.

A.3.4.6 Thermal Reactions of Aromatics with CaO, Massachusetts Institute of Technology, Cambridge, MA

The overall objective of this project is to perform a detailed study of the chemistry of thermal reactions of pure aromatic compounds in the presence of calcium oxide. This will allow the assessment of the technical feasibility of using this chemistry to achieve selective cracking of aromatic-rich liquids. Specific questions being studied include the rates, extents, and stoichiometry of the conversion reactions, effects of stone physical and chemical properties, and the processes which determine stone lifetime and activity. These objectives are addressed by determining the extent of conversion and composition of resulting products when pure compounds are passed in an inert carrier gas over packed beds of CaO. Bed temperature, pressure, and contact time are controlled, and special attention is given to the method of stone preparation.

A.3.5 Gas Separation

A.3.5.1

Title

Hydrogen/Methane Separation

Performer

Pittsburgh Energy Technology Center, Pittsburgh, PA

Objective

The objective is to determine the feasibility of separating gas components by adsorption using activated carbons as an alternative to cryogenic separation in coal gasification processes. Experiments in bench-scale hardware will be conducted using synthesized gas mixtures representative of hydrogasifier product streams and operating pressures.

Accomplishments

Construction of the experimental unit designed to investigate hydrogen/methane separation by adsorption on activated carbon was completed. Shakedown testing was conducted upon completion of unit construction. Calgon provided samples of the three activated carbons that were recommended for their capacity, ease of regeneration, and physical strength. Mixtures of hydrogen and methane were tested under various conditions of pressure, temperature, etc., for separation on the different activated carbons. The experiments on the three activated carbons (BPL, BPX, and PCB) have been completed with pressure-swing and temperature-swing responses tabulated for all experiments.

Current Work

Plans are nearing completion for granting an award to State University of New York, Buffalo, for help in planning the concluding experimental work, data analysis, and report preparation. The planned work by SUNY required single-compound tests for isotherms at PEC on the BPL and BPX carbons. SUNY has already obtained this data on PCB carbon under their contract with METC.

Application

Data on the rate and amount of adsorption of hydrogen and methane on the different activated carbons can be used to design and operate a process development hypersorber unit for practical separation tests.

A.3.5.2 Low-Energy Process for Separating Hydrogen and Methane, State University of New York at Buffalo, Buffalo, NY

The objective of this research is: (1) to compare heat-treated coals (300° to 800°C) with activated carbons for the fixed-bed adsorptive separation of methane from hydrogen and hydrogen sulfied from methane/hydrogen over the temperature range of 50° to 300°C and pressures up to 1000 psig, and (2) to conduct a preliminary cost analysis and technical assessment of a combined separation cleanup process. This work is based on experimental determinations of the adsorption and desorption isotherms and isoteric heats of adsorption for methane, hydrogen, and hydrogen sulfide on heat-treated Pittsburgh bituminous and Montana lignite coals and a commercial-activated carbon. The coal type and the heat treatment temperature which gives the highest capacity for methane sorption and the lowest temperature difference between adsorption and stripping will be identified. An analysis of energy requirements will be made based on this temperature difference, and the separation process with the lowest energy requirements and costs will be defined. Preliminary design and assessment of the combined separation cleanup process will be made.

Adsorption isotherms were measured in the range of 22° to 207°C and 0 to 1000 psig on char obtained by carbonizing Montana Rosebud lignite at 800° in nitrogen. The adsorbates were methane, hydrogen, and their mixtures. The methane adsorption on char is much higher than that on raw coal, the adsorption increase being three-fold. The bulk density of the Montana char is about twice as high as that of activated carbon so that the methane capacity of the char is quite close to that of activated carbon. The lignite char performed well in the temperature-swing fixed-bed equipment at 500 psig with the temperatures being 25°C during the low-temperature-cycle and 200°C during the high-temperature cycle. With a 50/50 CH_4/H_2 feed, the CH_4 concentration was 90 percent during the high-temperature cycle and 10 percent during the low-temperature cycle.

A.3.5.3

Title

Feasibility of Hypersorption for Separation of Medium-Btu Gas

Performer

Dravo Engineers and Constructors, Pittsburgh, PA

Objective

The objective is to evaluate and determine the feasibility of using the hypersorption adsorptive fractionation process for the separation of the components of gas derived by gasification of coal.

Accomplishments

From values supplid by Calgon Corporation of adsorptivities and adsorptive capacities of selected activated carbons for the components of medium-Btu gas at various temperatures and pressures, engineering calculations have been made for their theoretical separability and the operating parameters for hypersorber towers. Energy and mass balances for a Lurgi gasification system with hypersorption separation have been obtained. Hypersorption schemes for Texaco and Foster-Wheeler gasification systems have been received from a consultant. Activiated carbon rates as high as 9 × 10^6 lb/hr of carbon are required to effect separation of some components. Initial tower diameters have been calculated for one train. Dravo's material handling experts have determined the maximum amount of activated carbon that can be practically handled in one hypersorption unit which includes the activated carbon recirculation loop.

Current Work

This study is being continued for the remainder of the contract period to determine the feasibility of the separation of H_2 from CO obtained by oxygen-blown gasifiers. The separation of acid gases such as CO_2 and H_2S from the other components is also being examined.

Application

This study is complementary to a bench-scale experimental study at the Pittsburgh Energy Technology Center on the separation of H_2 and CH_4 by the hypersorption process using Calgon Corporation activated carbons and to a laboratory-scale experimental study at the State University of New York at Buffalo on separation of H_2, CH_4, and H_2S, using pretreated coals as adsorbents. The hypersorption process has possible advantages over other separation processes, and a thorough determination of its capabilities and limitations has not previously been made for gases derived from coal.

A.3.6 Shift/Methanation

A.3.6.1

Title

Combined Shift and Methanation in a Fluidized-Bed Reactor

Performer

Bituminous Coal Research, Inc., Monroeville, PA

Objective

The objective is: (1) to demonstrate the feasibility of employing a gas-phase fluidized-bed catalytic reactor to carry out simultaneous shift and methanation reactions in a single pass and (2) to conduct bench-scale and PDU tests with various catalysts at about 1000 psig and 800° to 1100°F, using

H_2/CO of 2 (without steam addition) and H_2/CO of 1 with a steam/dry gas ratio of about 0.1 to 0.2.

Accomplishments

The major portion of the experimental work involved PDU-scale tests in a 6-inch ID reactor, operating at 1000 psig and temperatures in the range of 900° to 1000°F with a nominal catalyst charge of 1 cubic foot. These tests included operation for extended time periods (35 to 40 hours) with feed H_2:CO ratios of 2:1 in the absence of steam and 1:1 using steam: gas ratios of 0.1:1 to 0.2:1. Five different catalysts were evaluated. Bench-scale tests, each of approximately 10 days duration, were also conducted. At H_2:CO = 2:1 (without steam), no significant carbon deposition occurred at temperatures of 800° and 950°F. At 1100°F, however, considerable carbon formation did occur, possibly due to the onset of CH_4 pyrolysis. At H_2:CO × 1:1 and 950°F, carbon deposition took place readily in the absence of steam. Small amounts of steam in the feed (i.e., steam:gas ratio × 0.1:1) were effective in inhibiting carbon formation, although larger amounts (steam:gas ratio × 0.5:1) resulted in deactivation and loss of metal surface area through sintering. Results of auxiliary studies at Brigham Young University on rates of carbon formation, and removal were obtained. As to the relative tendencies of the various catalysts to undergo carbon deposition, results of the BYU studies generally confirmed observations made during PDU testing at BCR. Catalyst regeneration tests at BYU with 10 percent O_2 in N_2 showed that 80 to 96 percent of the original metal surface could be restored at temperatures of 572° to 662°F.

Current Work

All experimental work has been concluded, and a final report has been published.

Application

Results from this work can be of value in the development of processes for upgrading medium-Btu gas from the gasification of coal to pipeline quality synthetic natural gas. By combining the shift and methanation steps in a single reactor, these processes may obtain technical and economical benefits. Gas-phase fluidized-bed operation has shown good temperature control of the exothermic reaction, and inhibited rates of carbon formation at elevated temperatures (950° to 1050°F) have been shown.

A.3.6.2

Title

Liquid Phase Methanation/Shift Process Development

Performer

Chem Systems, Inc., Fairfield, NJ

Objective

The objective was to advance the development of the Chem Systems liquid phase shift/ methanation process by determining the rates of carbon formation on various catalysts and by evaluating the hydrodynamics of a three-phase fluidized-bed reactor.

Accomplishments

Five commercially available catalysts were tested for 100, 300, 600, and 1,200 hours at 900°F and 1,000 psig with a feed gas of 63 percent hydrogen, 19 percent carbon monoxide, 2 percent carbon dioxide, and 16 percent methane (0.15 mole percent steam added). The nominal space velocity in the bench-scale test unit was 10,000 per hour. Samples of the carbon-depositied catalysts produced in these time tests were evaluated for methanation activity. Regeneration tests of the 1,200-hour catalyst samples obtained both with and without steam addition involved decoking by means of combustion with low-oxygen content gas, reduction with hydrogen, and determiniation of the methanation actitivy level.

It was established during this study that carbon will form under reaction conditions that are thermodynamically unfavorable to carbon deposition. The addition of steam to the feed gas, however, altered this behavior so that carbon deposition was inhibited. Carbon levels in excess of 10 percent were formed in very short time periods of 2 months or less; however, the carbon can be removed in situ by controlled oxidation. After the carbon was re-reduced, it was found that the catalyst was restored to its initial activity level. During this operation it was noted that the crush strength of the catalyst decreased significantly.

Current Work

All work on this effort has been completed, and a final report has been submitted for review.

Application

A thorough assessment of catalyst properties and composition for minimum carbon deposition, and determination of the rate of carbon deposition on various catalysts can lead to significant improvement in catalyst activity and catalyst life in combined shift/methanation reactors. The fluid dynamics of a three-phase system can allow poor contacting of the reactant gas with the surface of the catalyst solids suspended in the liquid. Therefore, the evaluation of the hydrodynamics of a three-phase fluidized bed could lead to a significant improvement in catalyst activity for this type of reactor.

A.3.7 Support Studies

A.3.7.1

Title

Compilation of Thermodynamic Tables

Performer

Dow Chemical Company, Midland, MI

The objective is to produce and distribute critically evaluated tabulations of thermodynamic properties for various chemical species that are currently relevant to the interests of the United States Department of Energy (DOE). These tabulations are to be made available as part of the JANAF Thermochemical Tables. The present DOE contracts extends the scope of the JANAF Thermochemical Tables to cover chemical species occurring in chemical reactors such as gasifiers, methanators, combustors, MHD generators, fuel cells, and gas turbines, which use coal or other fossil fuel products as their feedstocks.

Accomplishments

The project has produced over 300 new tables since the contract was signed in 1976. These tables include, for example: (1) the first coverage of the elements zinc, nickel, argon, helium, krypton, neon, xenon, deuterium, and copper; (2) a much broadened coverage of sulfur compounds including K_2S, K_2SO_4, FeS_2, Li_2SO_4, and SCl_2; and (3) tables for certain special liquids such as $Ni(CO)_4$ and H_2SO_4 at various aqueous dilutions. Information on many organic and inorganic compounds was collected and used. Information of direct interest to the work included results on some alkaline earth halides, oxides, hydroxides, and copper sulfides.

Current Work

Work is continuing in the effort to collect and evaluate data for the chemical species of interest and to calculate tables for this data in a manner that is consistent with the standard known as JANAF Thermochemcial Tables. Upon completion of the current chemical species, the third hardbound edition of the JANAF Thermochemcial Tables will be published.

Application

This work is aimed at securing certain data tabulations, in a widely respected and easily used form, which are consistent with thermodynamic principles and with such reliable measurements as have been made. More specifically, the chemical species for which thermodynamic tables are to be prepared will be species occurring in fossil fuel use processes. The application for the data produced is in practically all areas of chemical engineering.

A.4 Wastewater and Effluent Handling

A.4.1

Title

Process Wastewater

Peformer

Pittsburgh Energy Technology Center, U.S. DOE, Pittsburgh, PA

Objective

The objective is to develop environmental control strategies for wastewater through bench-scale treatment studies with gasifier effluents including physicochemical and biological (aerobic and anaerobic) treatments.

Accomplishments

A study was conducted to determine the effectiveness and practicability of using chemical oxidation for tertiary treatment of coal gasification wastewater. Wastewater which has undergone biological treatment will be oxidized under controlled conditions to remove trace organic compounds, using both ozone and a combination of ozone and ultraviolet radiation. The investigation of the ozonation of 10 model compounds was conducted.

Wastewater was extracted with methyl isobutyl ketone (MIBK) in a 36-stage, countercurrent extraction column to provide raffinate as feed to a series of five 7-liter, activated sludge reactors. Michaelis-Menten kinetic model coefficients, oxygen requirements, and sludge production rates will be developed for the biochemical oxidation of coal gasification wastewaters pretreated by solvent extractions. The kinetic model will be compared with one previously developed for coal gasification wastewaters that had not been pretreated.

Operation of the integrated wastewater treatment unit involved ammonia stripping, oil and tar removal by pH depression, biological treatment, and activated carbon adsorption to investigate the treatment of fixed-bed gasifier wastewaters. Operation with METC and GFETC wastewaters was completed.

Pilot-scale feasibility studies were performed on GFETC slagging fixed-bed gasifier process wastewater under conract with Celanese Chemical Company, using their proprietary CELROBIC® anaerobic wastewater treatment process. The attempt to acclimate two 20-liter, upflow anaerobic filters had little success.

Current Work

Work on chemical oxidation, biochemcal oxidation of solvent extraction raffinate, and integrated wastewater treatment unit operation is currently being concluded.

Application

A wide range of data is being obtained that has application to the development of an integrated treatment program for coal gasification wastewater. Wastewaters from the METC, PETC, GFETC, and Holston Army Ammunition gasifiers have been used in these studies to establish a realistic data base. The best possible overall wastewater treatment plan is required for meeting future environmental standards.

A.4.2

Title

Wastewater Treatment Studies

Performer

Grand Forks Energy Technology Center, U.S. DOE, Grand Forks, ND

Objective

The existing environmental program at GFETC has the following objectives: (1) to assess the adequacy and efficiency of commercial wastewater treatment processes to render gasifier wastewater amenable for reuse as feed to a cooling tower or boiler; (2) to evaluate conventional biological treatment techniques for SFBG wastewater; (3) to test alternate/novel physical, chemical, or biological wastewater treatment processes; and (4) to evaluate disposal methods for biological, physical, and chemical wastewater treating sludges and characterize their leachates employing Resource Conservation and Recovery Act (RCRA) guidelines.

Accomplishments

The University of Pittsburgh conducted characterization of slags and their leachates according to RCRA guidelines. Work at Carnegie-Mellon University included determination of their nature and fate of trace organics after various chemical/physical biological treatment processes and development of a method for predicting the partitioning of organics during wastewater processing.

The University of North Dakota conducted an assessment of activated sludge treatment of solvent-extracted wastewater.

Current Work

Liquid and solid wastes from the pilot slagging gasifier are being evaluated for GFETC by in-house analytical procedures and through contracts with major universities on methods of treatment and disposal that will be environmentally acceptable.

Application

This work will make it possible to demonstrate an integrated process to treat gasifier effluents. Also, it will be possible to compare effluent process train requirements as a function of the gasifier and of the coals used as feed to the gasifier. By these means industry can anticipate environmental problems for commercial gasification and can develop and design an energy-efficient process train.

A.4.3

Title

Pollutant Control in Coal Gasification — Wet Oxidation

Performer

Research Triangle Institute, Durham, NC

Objective

This project addresses a potential method for reducing the quantities of environmental pollutants in gasifier quench water, namely oxidation of the condensate. The objectives of this work are to determine the conditions under which that technique is feasible for the treatment of gasifier condensate, and to determine the effectiveness of potential catalysts in promoting that method of treatment.

Accomplishments

Catalyst screening for the wet oxidation studies was begun; six catalysts have been tested to date. These include copper oxide on alumina, cobalt on calcium aluminate, nickel oxide on calcium aluminate, copper on silica, silver on granular carbon, and an Illinois No. 6 coal char. The copper oxide catalyst was the most effective, reducing the phenolic content of a solution of 10,000 mg/1 phenol by 95 percent in 30 minutes. The coal char showed little, if any, catalytic activity.

Current Work

Testing is being continued on the wet oxidation of organic compounds in aqueous solutions of phenol at 150° to 350°C and 250 to 500 psi in the presence of gasifier ash and various supported metal oxide catalysts. These tests will indicate the most promising catalysts which will then be tested with actual gasifier condensate to determine the effectiveness of each of these catalysts for use in wet oxidation. The amount of reaction will be determined, including changes in total organic carbon (TOC), carbon oxygen demand (COD), and colored matter. Oxygen consumption versus effective removal of organic compounds will also be determined.

Application

The use of wet oxidation to treat gasifier condensate could provide a more efficient and economic alternative to other water treatment techniques.

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APPENDIX C — GLOSSARY OF TERMS FOR ABBREVIATIONS

Glossary of Terms for Abbreviations Used in Sections 4.1 Through 4.5

Abbreviations used in Sections 4.1 through 4.4 are defined below:

AFR — Advanced Fuel Research, Incorporated.
APT — Air Pollution Technology, Incorporated.
Battelle NW — Battelle Pacific Northwest Laboratories.
BCL — Battelle-Columbus Laboratories
BCR — Bituminous Coal Research, Incorporated.
BNL — Brookhaven National Laboratory.
Brown U. — Brown University
BYU — Brigham Young University
CCNY — City College (the City University) of New York.
Chem Systems — Chem Systems, Incorporated.
Clark U. — Clark University.
CNG Research — Consolidated Natural Gas Research Company.
Columbia Gas — Columbia Gas System Service Corporation.
CWRU — Case Western Reserve University.
Dow — Dow Chemical Company.
Dravo — Dravo Corporation.
ERT — Environmental Research and Technology.
GE — General Electric Company.
GFETC — Grand Forks Energy Technology Center, U.S. Department of Energy.
IGT — Institute of Gas Technology.
JAYCOR — JAYCOR, Incorporated.
Kansas State — Kansas State University.
LANL — Los Alamos National Laboratory.
METC — Morgantown Energy Technology Center, U.S. Department of Energy.
MIT — Massachusetts Institute of Technology.
RMP — Ralph M. Parsons Company.
Penn State — Pennsylvania State University.
PETC — Pittsburgh Energy Technology Center, U.S. Department of Energy.
Princeton U — Princeton University.
RTI — Research Triangle Institute.
Rockwell — Rockwell International.
Sandia — Sandia National Laboratories.
SRI — SRI International.
S^3 — Systems, Science, and Software.
SUNY — State University of New York at Buffalo.
TRW — TRW, Incorporated.
U. of California — University of California at Berkeley.
U. of Houston — University of Houston.
UNM — University of New Mexico.
U. of Mass — University of Massachusetts.
U. of Penn — University of Pennsylvania.
U. of Utah — University of Utah.
Vanderbilt — Vanderbilt University.
Washington U. — Washington University.
Westinghouse — Westinghouse Electric Corporation.
WVU — West Virginia University.