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Analysis of the Market and Product Costs for Coal-derived High BTU Gas Mercury Control Literature Survey of Properties of Synfuels Derived from Coal *Commercialization Strategies for Coal-derived Transportation Fuels* Group Contribution Methods for Coal Derived Liquids Coal Science Environmental Implications of Expanded Coal Utilization *Clean Coal Technologies* Emission and Control of Trace Elements from Coal-Derived Gas Streams The Separation and Analysis of Coal-derived Liquids *The Characterization of Coal Derived Liquids Production of Jet Fuels from Coal-Derived Liquids. Volume 15. Thermal Stability of Coal-Derived Jet Fuels* Utilisation of Coal Derived Fuel Gas at Elevated Pressure Production of Jet Fuels from Coal Derived Liquids. Volume 6. Preliminary Analysis of Upgrading Alternatives for the Great Plains Liquid By-Production Streams Production of Jet Fuels from Coal-Derived Liquids. Volume 13. Evaluation of Storage and Thermal Stability of Jet Fuels Derived from Coal Liquids Research Report on Evaluation of Alternative Uses of Coal and Coal-derived Fuels *Literature Survey of the Properties of Synthetic Fuels Derived from Coal* Emission and Control of Trace Elements from Coal-Derived Gas Streams FILTRATION OF COAL DERIVED LIQUIDS.. *X-ray Imaging of Coal Derived Products* Utilisation of Coal Derived Fuel Gas at Elevated Pressure *Separation of Hydrogen from Coal Derived Gas Mixtures Using Fe TiNi1 and LaNi4Cu Alloys* Development of Continuous Solvent Extraction Processes For Coal Derived Carbon Products *Characterization of Coal-derived Liquids and Other Fossil Fuel Related Materials Employing Mass Spectrometry Production of Jet Fuels from Coal-Derived Liquids. Volume 12. Preliminary Process Design and Cost Estimate and Production Run Recommendation* Production of High-Hydrogen Content Coal-Derived Liquids [Part 2 of 3]. *Thermodynamic Model for Calorimetric and Phase Coexistence Properties of Coal Derived Fluids. Annual Report* Flourescence spectroscopy in the characterization of coal-derived liquids Hydrotreating of Coal-derived Liquids Characterization of Coal-derived Liquids Relationships to Chemical Structures in Coal Utilisation of Coal Derived Fuel Gas at Elevated Pressure Hydrodenitrogenation of a Coal Derived Liquid Refining of Coal-Derived Synthetic Crudes Aging Studies of Coal-derived Liquid Fuels The Economical Production of Alcohol Fuels from Coal-derived Synthesis Gas. Sixth Quarterly Technical Progress Report, January 1, 1993--March 31, 1993 *Dry Syngas Purification Processes for Coal Gasification Systems* Development of Alternative Fuels from Coal-derived Syngas NOVEL SLURRY PHASE DIESEL CATALYSTS FOR COAL-DERIVED SYNGAS. *The Use of Coal Derived LNG as a Heavy Vehicle Fuel* Effects of Impurities in Coal-derived Liquids on Accelerated Hot Corrosion of Superalloys

In this reporting period, tonnage quantities of coal extract were produced but solid separation was not accomplished in a timely manner. It became clear that the originally selected filtration process would not be effective enough for a serious commercial process. Accordingly, centrifugation was investigated as a superior means for removing solids from the extract. Results show acceptable performance. Petrographic analysis of filtered solids was carried out by R and D Carbon Petrography under the auspices of Koppers and consultant Ken Krupinski. The general conclusion is that the material appears to be amenable to centrifugation. Filtered solids shows a substantial pitch component as well as some mesophase, resulting in increased viscosity. This is likely a contributing reason for the difficulty in filtering the material. Cost estimates were made

for the hydotreatment and digestion reactors that would be needed for a 20,000 ton per year demonstration plants, with the aid of ChemTech Inc. The estimates show that the costs of scaling up the existing tank reactors are acceptable. However, a strong recommendation was made to consider pipe reactors, which are thought to be more cost effective and potentially higher performance in large scale systems. The alternate feedstocks for coke and carbon products were used to fabricate carbon electrodes as described in the last quarterly report. Gregory Hackett successfully defended his MS Thesis on the use of these electrodes in Direct Carbon Fuel Cell (DCFC), which is excerpted in Section 2.4 of this quarterly report. The objective of this paper is to analyze a program that can stimulate the development of a synthetic liquid transportation fuels from coal industry, by requiring that the products be bought at their true cost of production. These coal-derived liquids will then be assimulated into the nation's fuel supply system. The cost of this program will be borne by increased cost of all fuels in the marketplace. The justification of the program is the assumption that, because of increasing demand, the world oil price (WOP) will increase to a level that will make coal-derived fuels economical in the relatively near future. However, as noted in the International Energy Outlook of 1990: ''Given current costs and Technologies, it is estimated the cost of crude oil would have to exceed $35 per barrel in 1989 dollars for at least four consecutive years for commercial production, in the range of 100,000 barrels per day, of synthetic liquids to occur. This delayed response of production to price increases reflects the planning and construction time required to complete a coal liquefaction plant''. This program is designed to reduce this time lag so that coal-derived fuels will be available when they are needed. This timely production capability of coal liquids may be able to limit future world oil prices to the actual cost of synthetic alternatives. In addition, the program is structured so that it will provide synthetic fuel producers with a cushion in the event that the WOP continues to remain low. Amoco and Lummus Crest have developed seven cases for upgrading by-product liquids from the Great Plains Coal Gasification plant to jet fuels, and in several of the cases, saleable chemicals in addition to jet fuels. The analysis shows that the various grades of jet fuel can be produced from the Great Plains tar oil, but not economically. However the phenolic and naptha streams do have the potential to significantly increase (on the order of $10-15 million/year) the net revenues at Great Plains by producing chemicals, especially cresylic acid, cresol, and xylenol. The amount of these chemicals, which can be marketed, is a concern, but profits can be generated even when oxygenated chemical sales are limited to 10 percent of the U.S. market. Another concern is that while commercial processes exist to extract phenolic mixtures, these processes have not been demonstrated with the Great Plains phenolic stream. Keywords: Turbine fuel; JP-4; JP-8; High density fuel: Great plains gasification plant; Crude phenols; Naphtha; Tar oil; Linear programming; Economics. (MGM). On September 1, 1989 work was initiated on a project to extend the available vapor-liquid equilibrium (VLE) model for coal fluids to allow satisfactory predictions of excess enthalpies of coal liquids at high pressures. The available vapor liquid equilibrium model was developed with support from previous grant from DOE-PETC (Grant no. DE-FG22-89PC90541). The current project also involves measurement of some model compound VLE data and chromatographic characterization of coal liquids for distribution of heteroatoms. A computational thermodynamic model for VLE, excess enthalpies and heat capacities of coal derived liquids has been developed. The model uses the modified UNIFAC correlation for the liquid phase. Some unavailable UNIFAC interactions parameters have been regressed from experimental VLE and excess enthalpy data. The computations are carried out using the method of continuous thermodynamics. Mode is used to derive interesting conclusions on the effect of oxygen, nitrogen, and sulfur

heteroatoms on the thermodynamic properties of coal liquids. When compared with limited experimental data available for coal liquids the model shows good agreement. Some progress has been made on binary VLE measurements and size exclusion chromatography of coal liquids. Coal Science, Volume 3 presents and evaluates selected fundamental scientific areas on coal structure, reactivity, and utilization. This book describes the organic geochemistry of coal, role of oxygen functionality in coal and coal liquids reactivity, chemistry of hydrocarbon syntheses from carbon monoxide and hydrogen, and chemistry of coal in carbon monoxide/water systems. Other topics discussed include intermediates and mechanisms of the FTS of hydrocarbons; synthesis of oxygenates; and structural features of vitrinite macerals. The molecular weight determination for coal derivatives; thermal reactions of oxygen compounds; and alternative methods for removing oxygen compounds from coal-derived liquids are also elaborated. This publication likewise covers the aqueous coal conversions and conversion mechanism. This volume serves as a valuable source of information and guide to scientists and researchers interested in the coal literature. Dry Syngas Purification Processes for Coal Gasification Systems illustrates the promising development status of dry syngas purification for various power generation systems based on coal gasification. The core advantages of dry syngas purification, methodologies for impurity measurement, sorbents development, and evaluation of process performance are described in-depth, and from a practical perspective that is based on current research and development. Reviewing key findings from process integration, the book encompasses scale-up strategies from pilot processes to achieve dry syngas processing for new build plants. The book provides researchers and engineers with practical information to realize dry syngas purification processes for each context. Delivers pathways to realize dry syngas purification processes customized to specific power plant contexts Provides analytical tools to facilitate plant operators in examining and interpreting the relevant impurities of coal gasification and gas treatment processes Illustrates rational strategies for developing capable and durable dry removal sorbent for syngas impurities Describes process design and integration through key engineering evaluation Describes scale-up strategies of dry syngas processing for their deployment in new plants Provides prospects on the development of future coal energy conversion system adopting dry syngas purification processes This report describes and summarizes a literature survey of the properties of synthetic fuels for ground-based turbine applications, compiled up to October 1980. The major processes for coal liquefaction (solvent extraction, catalytic liquefaction, pyrolysis, and indirect liquefaction) and coal gasification (fixed bed, fluidized bed, entrained flow, and underground gasification) are described. Processes for upgrading coal-derived liquids are discussed, and some property data for some coal-derived liquid and gaseous fuels are presented. The primary goal of this project has been to evaluate and compare the effect of the intrinsic differences between cobalt (Co) and iron (Fe) catalysts for Fischer-Tropsch (FT) synthesis using coal-derived syngas. Crude oil, especially heavy, high-sulfur crude, is no longer the appropriate source for the additional, or marginal, amounts of middle-distillate fuels needed to meet growing US and world demand for diesel and jet fuels. Only about 1/3 of the marginal crude oil barrel can be made into diesel and jet fuels. The remaining 2/3 contributes further to global surpluses of by-products. FT can produce these needed marginal, low-sulfur middle-distillate fuels more efficiently, with less environmental impact, and from abundant US domestic resources. Cobalt FT catalyst is more efficient, and less expensive overall, than iron FT catalyst. Mechanisms of cobalt FT catalyst functioning, and poisoning, have been elucidated. Each of these primary findings is amplified by several secondary findings, and these are presented, and verified in detail. The most effective step the United States can

take to begin building toward improved long-term national energy security, and to reduce dependence, over time, on imported crude oil from unfriendly and increasingly unstable areas of the world, is to begin producing additional, or marginal amounts of, middle-distillate-type fuels, such as ultralow sulfur diesel (ULSD) and jet fuel (not gasoline) from US domestic resources other than petroleum. FT synthesis of these middle distillate fuels offers the advantage of being able to use abundant and affordable US coal and biomass as the primary feedstocks. Use of the cobalt FT catalyst system has been shown conclusively to be more effective and less expensive than the use of iron FT catalyst with syngas derived from coal, or from coal and biomass combined. This finding is demonstrated in detail for the initial case of a relatively small FT plant of about 2000 barrels per day based upon coal and biomass. The primary feature of such a plant, in the current situation in which no commercial FT plants are operating in the US, is that it requires a relatively modest capital investment, meaning that such a plant could actually be built, operated, and replicated in the near term. This is in contrast to the several-billion dollar investment, and accompanying risk, that would be required for a plant of more than an order of magnitude greater capacity, which has been referred to in the technical literature on fuel production as the capacity required to be considered "commercial-scale." The effects of more than ten different potential poisons for cobalt FT catalyst have been studied extensively and in detail using laboratory continuous-stirred tank reactors (CSTRs) and bottled laboratory syngas "spiked" with precisely controlled amounts of the poisons, typically at the levels of 10s or 100s of parts per billion. This data set has been generated and interpreted by world-renowned experts on FT catalysis at the University of Kentucky Center for Applied Energy Research (UK-CAER), and has enabled unprecedented insight regarding the many molecular-scale mechanisms that can play a role in the "poisoning" of cobalt FT catalyst. In September 1986, the Fuels Branch of the Aero Propulsion Laboratory of WPAFB, OH, began an investigation of the potential of the production of jet fuel from the liquid by-products streams produced by the gasification of lignite at the Great Plains Gasification Plant (GPGP) in Beulah, North Dakota. Funding was provided to the Department of Energy, Pittsburgh Energy Technology Center, to administer the experimental portion of this effort. This report details the program with the National Institute for Petroleum and Energy Research of the IIT Research Institute to study the storage and thermal stability of a JP-8 fuel produced from the GPGP liquid by-products streams. Sediments and deposits from stability tests were analyzed by IR and probe microdistillation/high resolution mass spectroscopy. Results were compared with corresponding results from a conventional petroleum-derived JP-8 fuel. Keywords: Jet engine fuels; Turbine fuels, Coal liquids; Storage stability; Thermal stability; Mass spectrometry; Sediment analysis; Deposit analysis. (EDC). This essential handbook and ready reference offers a detailed overview of the existing and currently researched technologies available for the control of mercury in coal-derived gas streams and that are viable for meeting the strict standards set by environmental protection agencies. Written by an internationally acclaimed author team from government agencies, academia and industry, it details US, EU, Asia-Pacific and other international perspectives, regulations and guidelines. Considerable activity was devoted to resolving problems preventing the attainment of optimum performance from the mass spectrometer /data acquisition system. These activities included electronic modifications to various sections of the mass spectrometer, providing an excellent ground to the mass spectrometer, NOVA 3/12 minicomputer, and other peripheral instrumentation, and the distribution of well-regulated 120 V AC to the power supplies in the various instruments used to produce DC. The increase in the useful static resolution of the mass spectrometer from ca. 21,000 to at least 33,000 is indicative of the quality of the results obtained from these activities. In

regard to development of micromolecular probe distillation in combination with field-ionization mass spectrometry for quantitative analysis, development of algorithms to permit acquisition of both probe temperatures and FI/MS data was initiated. Initial designs for the interface between the NOVA 3/12 and the comparator /microdensitometer were prepared. A manuscript describing our detailed investigation of the sensitivities for FI of saturates was prepared and accepted for publication. Progress on a report ''Current State-of-the-Art in Mass Spectral Analysis of Alternate Fossil Fuels'' is summarized. Preliminary economic investigations have focused on cost reduction measures in the production of syngas from coal. A spread sheet model has been developed which can determine the cost of syngas production based upon the cost of equipment and raw materials and the market value of energy and by-products. In comparison to natural gas derived syngas, coal derived syngas is much more expensive, suggesting a questionable economic status of coal derived alcohol fuels. While it is possible that use of less expensive coal or significant integration of alcohol production and electricity production may reduce the cost of coal derived syngas, it is unlikely to be less costly to produce than syngas from natural gas. Fuels evaluation is being conducted in three parts. First, standard ASTM tests are being used to analyze the blend characteristics of higher alcohols. Second, the performance characteristics of higher alcohols are being evaluated in a single-cylinder research engine. Third, the emissions characteristics of higher alcohols are being investigated. The equipment is still under construction and the measurement techniques are still being developed. Of particular interest is n-butanol, since the MoS2 catalyst produces only linear higher alcohols. There is almost no information on the combustion and emission characteristics of n-butanol, hence the importance of gathering this information in this research. Samples of jet fuel (JP-4, JP-8, JP-8X) produced from the liquid by-products of the gasification of lignite coal from the Great Plains Gasification Plant were analyzed to determine the quantity and type of organo-oxygen compounds present. Results were compared to similar fuel samples produced from petroleum. Large quantities of oxygen compounds were found in the coal derived liquids and were removed in the refining process. Trace quantities of organo-oxygenate compounds were suspected to be present in the refined fuels. The thermal stability of organo-oxygen compound and the coal derived jet fuels was determined. (KR). A preliminary design for the production of JP-8 jet fuel and other salable products from the Great Plains by-products is given. The design incorporates experimental results from Tasks 2 and 3 with the scoping design from Task 1. The experimental results demonstrated the need for more severe hydrotreating conditions to convert the tar oil to jet fuel than was estimated in Task 1. As a result, capital costs for the revised design are significantly higher and the plant is less profitable than estimated in Task 1 work. The increase in capital costs is offset somewhat by a higher phenol value in the current market. Refined estimates for the cost of an aromatics recovery unit preclude its economical construction in the new estimate, consequently the revised product slate includes no BTX. Turbine fuel, JP-4, JP-8, High density fuel, Great Plains gasification plant, Tar oil, Economics, Design. (eg). Emission and Control of Trace Elements from Coal-Derived Gas Streams presents an up-to-date and focused analysis on Trace element (TEs) emissions and control strategies during coal utilization. This book provides insights into how TE’s in coal are distributed from different coal-forming periods, coal ranks and coal-bearing regions. As the emission and control of TEs during coal utilization are a significant concern, this book introduces TEs in coal and pollution in an accessible way before discussing why they occur and how they are distributed during various stages of coal forming, also considering various regions and countries. Specific types of TEs in relation to partition in coal combustion, coal fires, gasification and coal feed furnace are

then analyzed, providing the reader with practical knowledge to apply to their own research or projects. This book is an essential reference for energy engineers researching and working in coal technology, with a specific focus on emission control, as well as graduate students and researchers in energy engineering, environmental, thermal and chemical engineering who have an interest in trace element emission and control from coal utilization. Presents characteristics of TE emissions during coal utilization in laboratory-scale experiments, industrial furnaces and power plants Considers different legislation and case studies from various regions and countries Includes contributions from world renowned experts Presents a concise and focused analysis on TE emissions and control strategies This report describes research conducted to support the DOE program in novel slurry phase catalysts for converting coal-derived synthesis gas to diesel fuels. The primary objective of this research program is to develop attrition resistant catalysts that exhibit high activities for conversion of coal-derived syngas. Emission and Control of Trace Elements from Coal-Derived Gas Streams presents an up-to-date and focused analysis on Trace element (TEs) emissions and control strategies during coal utilization. This book provides insights into how TE's in coal are distributed from different coal-forming periods, coal ranks and coal-bearing regions. As the emission and control of TEs during coal utilization are a significant concern, this book introduces TEs in coal and pollution in an accessible way before discussing why they occur and how they are distributed during various stages of coal forming, also considering various regions and countries. Specific types of TEs in relation to partition in coal combustion, coal fires, gasification and coal feed furnace are then analyzed, providing the reader with practical knowledge to apply to their own research or projects. This book is an essential reference for energy engineers researching and working in coal technology, with a specific focus on emission control, as well as graduate students and researchers in energy engineering, environmental, thermal and chemical engineering who have an interest in trace element emission and control from coal utilization. Environmental Implications of Expanded Coal Utilization focuses on the increasing consideration of coal as an alternative source of energy. This book comes as an answer to the issues on health and environment regarding the extraction, production, and use of coal. Composed of nine chapters, the selection starts by underlining the potential prospects for coal, which plays a vital role in meeting energy demands. The book also shows that problems have evolved regarding the use of coal, including land disturbance and increased land occupation due to mining. The text also notes that the international trade of coal will surely generate waste products, and some of which can be the result of poor transportation and handling. The book focuses on coal gasification and liquefaction and emphasizes that the processes involved must be carefully understood in order to avoid the environmental impacts of coal use. Attempts have been made to establish a conceptual framework to be used in assessing the health and environmental health impacts of the conversion and utilization of coal. Relative to this, discussions that follow include the trace elements that are the products of coal combustion and conversion and also coal derived carbon compounds. Another sector is focused on the evaluation of the effects of emissions on human health, especially of workers in the industry. The effects of the utilization of coal on communities are also considered. The text is a vital source of information to those involved in the research on the use of coal as alternative source of energy. The overall objectives of this program are to investigate potential technologies for the conversion of coal-derived synthesis gas to oxygenated fuels, hydrocarbon fuels, fuel intermediates, and octane enhancers; and to demonstrate the most promising technologies at DOE's LaPorte, Texas, Slurry Phase Alternative Fuels Development Unit (AFDU). BASF continues to have difficulties in scaling-up the new isobutanol synthesis catalyst developed in Air Products' laboratories.

Investigations are proceeding, but the proposed operation at LaPorte in April is now postponed. DOE has accepted a proposal to demonstrate Liquid Phase Shift (LPS) chemistry at LaPorte as an alternative to isobutanol. There are two principal reasons for carrying out this run. First, following the extensive modifications at the site, operation on a relatively benign'' system is needed before we start on Fischer-Tropsch technology in July. Second, use of shift catalyst in a slurry reactor will enable DOE's program on coal-based Fischer-Tropsch to encompass commercially available cobalt catalysts-up to now they have been limited to iron-based catalysts which have varying degrees of shift activity. In addition, DOE is supportive of continued fuel testing of LaPorte methanol-tests of MIOO at Detroit Diesel have been going particularly well. LPS offers the opportunity to produce methanol as the catalyst, in the absence of steam, is active for methanol synthesis. The U.S. Environmental Protection Agency (EPA) was introduced on December 2, 1970 by President Richard Nixon. The agency is charged with protecting human health and the environment, by writing and enforcing regulations based on laws passed by Congress. The EPA's struggle to protect health and the environment is seen through each of its official publications. These publications outline new policies, detail problems with enforcing laws, document the need for new legislation, and describe new tactics to use to solve these issues. This collection of publications ranges from historic documents to reports released in the new millennium, and features works like: Bicycle for a Better Environment, Health Effects of Increasing Sulfur Oxides Emissions Draft, and Women and Environmental Health.

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