U.S. DOE INDIRECT COAL LIQUEFACTION PROGRAM: AN OVERVIEW

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INTRODUCTION

Coal is the most abundant domestic energy resource in the United States (U.S.). The Fossil Energy organization within the U.S. Department of Energy (DOE) has been supporting a coal liquefaction program to develop improved technologies to convert coal to clean and cost-effective liquid fuels to complement the dwindling supply of domestic petroleum crude. The goal of this program is to produce coal liquids that are competitive with crude at $20 to $25 per barrel. Indirect and direct liquefaction routes are the two technologies being pursued under the DOE coal liquefaction program.

In indirect liquefaction, coal is gasified in the presence of steam and oxygen to produce a synthesis gas (syngas) containing mostly carbon monoxide and hydrogen. This syngas, after being cleaned of impurities and adjusted to the desired H_2/CO ratio (if required), is converted in the presence of catalysts. A unique feature of the indirect liquefaction is its ability to produce a broad array of sulfur and nitrogen free products including motor fuels, methanol, mixed alcohols, dimethyl ether (DME), and chemicals with the use of different combinations of catalysts and process conditions. The conversion of syngas to liquid hydrocarbon fuels is known as Fischer-Tropsch (F-T) synthesis. In addition to coal, other carbonaceous feedstock also can be used in indirect liquefaction applications, including natural gas, petroleum/oil sands coke, petroleum resid, biomass, and municipal/refinery wastes.

Commercial indirect liquefaction plants to produce motor fuels have been in operation since 1955, including coal based plants in South Africa, and natural gas based plants in New Zealand, Malaysia, and South Africa. All these plants use F-T technology, with the exception of the New Zealand plant which uses a Mobil MTG (methanol to gasoline) technology. In addition, a coal to methanol plant has been in operation in U.S. since 1983. In all these plants, the syngas is converted in gas phase reactors. Because of the high exotherm (heat release) associated with the reactions, it has long been known that a liquid phase reactor could offer both cost and operational flexibility advantages over gas phase reactors due to its superior heat transfer capability and simpler reactor design. Earlier work in liquid phase reactor technology after World War II was suspended because of the cheap petroleum crude price. Interests in this technology was revived in the late 1970s with the rise in crude price. Scoping economics study supported by DOE and Electric Power Research Institute (EPRI) indicated that the capability of a liquid phase reactor to process a lean syngas (low H_2/CO ratio syngas) produced from advanced coal gasifiers could offer substantial cost advantages over the gas phase reactors (Gray et al., 1980; Brown et al. 1982). In the early 1980s, DOE began to support a R&D program to advance the liquid phase reactor technology aimed for coal based applications under joint efforts with the industries. In 1989 liquid phase methanol technology was successfully demonstrated at the proof-of-concept (POC) unit at LaPorte, Texas under cost shared contracts with Air Products and Chemicals, Inc. (Air Products). Subsequent efforts have been directed at extending the know-how to the development of liquid phase dimethyl ether (DME) and slurry phase F-T technologies. Recent publications indicate that other industrial companies also have been active in the area of slurry phase F-T technology development (Fourie 1995; Eisenberg et al. 1993). Liquid phase reactor also is known as slurry phase reactor and the two terms are considered interchangeable in this paper.

This paper will give an overview of the DOE indirect liquefaction program. More detailed discussions will be given to the F-T diesel and

DME fuels which have shown great promises as clean burning alternative diesel fuels. We also will briefly discuss the economics of indirect liquefaction and the hurdles and opportunities for the early commercial deployment of these technologies. Our discussions will be preceded by two brief reviews on the liquid versus gas phase reactors and the natural gas versus coal based indirect liquefaction.

LIQUID PHASE VERSUS GAS PHASE SYNGAS CONVERSION REACTORS

A schematic drawing of the liquid phase and the two commercial Sasol gas phase reactors now in operation in South Africa is shown in Figure 1. In a liquid phase reactor, the fine catalyst particles are suspended in a liquid medium by a syngas stream on the shell side of the reactor. In a gas phase reactor, the catalysts are packed inside the tubes in a fixed bed gas reactor, and are circulated around the loop by the syngas stream on the shell side of a fluidized bed Synthol reactor. In addition to higher transfer capability, liquid phase reactor also has the advantage that it can process a sub-stoichiometric hydrogen to CO ratio syngas, partially because of the higher hydrogen to CO ratio on the catalyst surface than the bulk gas phase due to the differences in the solubility and diffusivity between hydrogen and CO in the liquid medium. A recent publication indicates that the current know-how has deemed it feasible to design a 10,000 barrels per day slurry phase F-T reactor (Sasol 1997).

NATURAL GAS VERSUS COAL BASED INDIRECT LIQUEFACTION

Natural gas is richer in hydrogen than coal, and thus produces a syngas with a higher hydrogen to CO ratio. Depending on the technology used, natural gas can be converted to a syngas with a hydrogen to CO ratio in the 1.8 to 5.4 range. In the Shell F-T plant in Malaysia, the syngas is produced by a combination of partial oxidation (POX) and steam reforming which leads to a hydrogen to CO ratio close to the stoichiometric value of 2. Recent publications indicate that other F-T developers have opted to use a catalytic autothermal reforming technology to produce syngas from natural gas (Agee 1997). Cobalt catalyst is the choice for F-T synthesis with natural gas based syngas, partially because it does not have a concurrent water gas shift (WGS) activity which would convert CO and water to hydrogen and carbon dioxide.

Advanced POX gasifiers are now the choice for coal gasification because of the higher thermal efficiency. In these gasifiers, coal is converted to a syngas with a H_2/CO ratio in the 0.5 to 0.9 range. At the Eastman Chemical Company (Eastman) coal to methanol plant, the syngas from a Texaco gasifier is first shifted in a separate step to increase the hydrogen to CO ratio to the stoichiometric value of 2. In the Sasol coal based F-T plants in South Africa, syngas is produced from the first generation Lurgi gasifier which yields a syngas with hydrogen to CO ratio of 1.9. F-T synthesis is carried out over an iron catalyst which has a concurrent WGS activity. No separate WGS step is installed in the Sasol plants.

DOE INDIRECT LIQUEFACTION PROGRAM

The DOE indirect liquefaction program is aimed to develop a liquid phase reactor/catalyst system which can convert syngas from advanced POX gasifiers to various clean liquid fuels and chemicals without a prior WGS step. This technology has the advantage that it can be readily integrated into an Integrated Gasification Combined Cycle (IGCC) for power, fuels, and chemicals coproduction.

LIQUID PHASE METHANOL REACTOR TECHNOLOGY

Liquid phase methanol is the first technology developed under the DOE indirect liquefaction program. Its feasibility is demonstrated in a 120 day run conducted in 1989 at the LaPorte POC facility using a commercial methanol catalyst in a once-through mode with a 0.67 hydrogen to CO ratio syngas simulating that from a Texaco coal gasifier. The methanol from this technology has a water content less than 1%, and meets the fuel grade methanol specifications. For comparison, the methanol from commercial gas phase reactor would have a water content of 10% because of the hydrogen rich environment in the reactor. More details on the development highlights of the liquid phase methanol technology can be found elsewhere (Shen et al. 1996).

Liquid phase methanol is now undergoing commercial demonstration under a cost-shared contract jointly supported by the industry and DOE Clean Coal Technology program. This demo plant is located at the Eastman complex in Kingsport, TN, and uses a syngas produced from a Texaco coal gasifier on the site. Its construction began in October 1995 and was completed in December 1996. The plant initiated operation in April 1997 and achieved the design rate of 260 tons of methanol per day on the third day after the startup. This represents a successful 26-fold scale up from the 10 tons per day proof-of-concept (POC) scale plant. Chemical grade methanol produced from this demonstration plant has met the specifications and now accepted by Eastman for captive chemical feedstock uses in the complex.

The demonstration project is managed by the Air Products Liquid Phase Conversion Company, L.P., which is a joint venture between Air Products and Eastman. The funding mix between the joint venture and DOE is 43%/57%. It will be operated for four years to demonstrate the reactor operability over a wide range of process conditions and syngas compositions, as well as to prove out the important features which will enable the integration of this technology into an IGCC facility for power/methanol co-production. Fuel grade methanol produced from a low hydrogen to CO ratio syngas will be collected and used in a concurrent product testing program to demonstrate its various commercial applications, including fuels for transportation use and power production.

The opportunity for the commercial deployment of liquid phase methanol technology for power and methanol coproduction has recently been reviewed (Osterstock et al. 1997).

LIQUID PHASE DIMETHYL ETHER (DME) TECHNOLOGY

DME (CH_3-O-CH_3) is manufactured today by the dehydration of two molecules of methanol. In the liquid phase DME technology, the methanol synthesis and the subsequent methanol dehydration to DME are carried out in a single reactor by using a binary physical mixture of catalysts for these two separate activities. Again, this technology is aimed for coal based syngas coproduction applications. It is being developed under joint efforts between Air Products and DOE. There have been considerable industrial interests in this one-step synthesis gas-to-DME technology, which would offer cost advantages over the conventional two-stage process. DME is now primarily used as precursors for chemicals, but has shown potential as a super clean diesel fuel (Fleisch et al.1995). Haldor-Topsoe recently has reported the technology of a single step gas phase reactor to convert natural gas based syngas to DME (Hansen et al. 1995).

Feasibility of liquid phase DME technology for a 0.67 hydrogen to CO ratio syngas was first demonstrated by Air Products at the LaPorte POC unit in 1991. Continued work since then at the bench scale unit has led to the development of modified methanol dehydration catalysts with substantial improvement in activity and life maintenance over the earlier versions (Peng et al. 1996). Discussions are underway between Air Products and catalyst manufacturing companies to scale up the production of these newly developed dehydration catalysts. A demonstration run to prove out the superiority of the new binary catalyst system at the LaPorte POC unit is tentatively planned for 1998.

Recent research by Air Products shows that the DME molecules can be coupled to form a mixture called "DME soup" which would have boiling point range comparable to that of a conventional diesel. Preliminary data indicates this coupled DME mix have a cetane number over 100 and could be used as a blending component for the conventional diesel. .

SLURRY/LIQUID PHASE F-T TECHNOLOGY

F-T Synthesis Chemistry: Unlike methanol synthesis, products from F-T synthesis are a mixture of hydrocarbons with carbon number ranged from C_1 to C_{40} or higher, which can be predicted by the Anderson-Flory-Schulz distribution developed for the polymerization reactions using a single parameter called "alpha" (probability of chain growth). The basic building block, $-CH_2-$, is formed from Reaction (1). The chain growth terminates when a molecule disassociates from the catalyst surface. The probability of chain termination is defined as (1-alpha). The value of alpha in F-T synthesis is controlled by the catalyst composition and process conditions. The fraction of F-T products, which has a carbon number greater than 20, is called wax. It can easily be refined to produce gasoline and distillate. Thus, the product slate selectivity from F-T synthesis can be varied by F-T catalyst alpha, the F-T wax refining conditions, or a combination of the two. For the Shell F-T plant in Malaysia which uses a high alpha cobalt catalyst, the following product slate selectivity has been reported (Tijm et al. 1995).

Product slate % wt	Diesel mode	Kerosene mode
Naphtha	15	25
Kerosene	25	50
Diesel	60	25

For F-T iron catalyst which also has WGS activity, Reaction (2) occurs in parallel with Reaction (1). A combination of Reactions (1) and (2) yields Reaction (3), indicating that F-T synthesis could proceed with a syngas having a 0.5 hydrogen to CO ratio in case an iron catalyst is used. The feasibility of processing a 0.67 hydrogen to CO ratio syngas in a slurry phase F-T reactor with an iron catalyst was successfully demonstrated at the bench scale unit by Mobil under cost-shared contracts with DOE. More detailed review of the Mobil work can be found elsewhere (Shen et al. 1996). It should be noted that the wax fraction of the F-T products would remain in the slurry phase reactor and has to be removed after separation from the catalysts.

$$2H_2 + CO \rightarrow -CH_2- + H_2O \qquad (1)$$

$$H_2O + CO \rightleftharpoons H_2 + CO_2 \qquad (2)$$

$$H_2 + 2CO \rightarrow -CH_2- + CO_2 \qquad (3)$$

Slurry Phase F-T Operations at LaPorte POC Unit: Three slurry phase F-T runs have been made at the LaPorte POC unit between 1992 and 1996, with costs shared by different industrial consortiums headed by Air Products. The first two runs used iron catalysts and their results have been reviewed in details (Bhatt et al. 1995a, 1995b, 1995c). The third run used a cobalt catalyst and its data workup is now in progress. All three runs indicate that catalyst/-wax separation remains to be a challenging problem for slurry phase F-T reactor technology development.

F-T Catalyst Development: In the F-T catalyst development area, the Kentucky Center for Applied Energy Research (CAER), in conjunction with the United Catalyst, Inc., has reported successful results at bench scale unit of a low alpha iron catalyst with improved activity and life maintenance using a 0.67 hydrogen to CO ratio syngas (O'Brien et al. 1996). Our immediate future effort is to modify this catalyst to increase its alpha value to an intermediate value to produce straight chain alpha olefins in the C_5 to C_{15} range. This represents our continued effort to improve the iron catalyst versatility to produce a broader array of high value chemicals in addition to fuels to further enhance the profitability of plants based on this technology.

Synthesis Gas to Oxygenates and Chemicals :

Novel catalyst R&D cost shared with industry and universities has been underway to explore the use of synthesis gas as an alternative feedstock to produce oxygenate octane enhancers and oxygenate based chemicals which would offer cost advantages over the conventional technologies. The products include mixed alcohols including isobutanol (Xu et al. 1996), vinyl acetate monomer (Tustin et al. 1996), methyl methacrylate (Spivery et al. 1996), and dimethyl carbonate (Hagen 1996). The industrial participants in this effort include Air Products, Eastman, and Amoco.

Slurry-Phase Bubble Column Reactor (SBCR) Hydrodynamics: A five-year engineering development study for the SBCR system has been underway since 1995 under a cost-shared contract with Air Products. The two subcontractors are: Ohio State University and Washington University (St. Louis, MO). Sandia National Lab, through a separate contract with DOE, also is a participant to this project. The expertises of these participants will be joined to develop an improved SBCR design data base by combining the know-how gained from the hydrodynamics studies conducted in the non-reacting and reacting systems under the commercially prevalent conditions. A second objective of this study is to gain a better fundamental understanding of the SBCR hydrodynamics. More detailed descriptions of the proposed contract work can be found elsewhere (Degaleesan et al. 1996; Jackson et al. 1996). Separately, an in-house research group at the DOE/Federal Energy Technology Center has been developing new diagnostic techniques to aid the SBCR hydrodynamics studies (Soong et al., 1995)

ENVIRONMENTAL PREMIUMS FOR DME AND F-T DIESEL

DME and F-T diesel, which are free of sulfur and aromatics and have high cetane number, are both known to have potential as a cost-effective, super clean diesel fuels. Engine testing with DME supported by an industrial consortium shows that the emissions from DME fuels would meet the California Ultra Low Emissions Vehicle (ULEV) regulations for medium-duty vehicles (Fleisch et al.1995). In a separate study funded under cost-shared contracts with DOE, emissions from F-T diesel are reduced by up to 40% when compared with a conventional petroleum diesel (Montalvo1995). More recent data indicate that the emissions from a F-T diesel used in advanced diesel engines also would meet the ULEV regulations (Starr 1997). Review of the earlier diesel engine testing with blends of petroleum and F-T diesel fuels can be found elsewhere (Shen et al. 1996).

ECONOMICS OF INDIRECT LIQUEFACTION

A DOE supported study by Bechtel indicates that indirect coal liquefaction is competitive with conventional crude oil production and refining at a crude cost of $34 per barrel based on the current status of slurry F-T technology. The conceptual commercial plant, which is located at an Illinois #6 coal mine site, produces 50,000 barrels/day of gasoline and diesel fuels meeting and/or exceeding market specifications. This product cost represents a value in reference to a crude used by a typical refinery in the local area, and is called crude oil equivalent (COE) price. Subsequent studies show that this cost could be reduced to $27 per barrel with continued R&D in both slurry phase F-T synthesis and the upstream syngas production steps. In special cases where the F-T plant is located adjacent to an existing refinery, the COE price could be reduced to the $20-25 per barrel range (Gray et al. 1995; Gray et al. 1996). A schematic drawing of the COE prices for different cases is shown in Figure 2.

HURDLES AND OPPORTUNITIES FOR THE COMMERCIAL DEPLOYMENT OF INDIRECT LIQUEFACTION TECHNOLOGY

The DOE liquid phase reactor technology development has been focused on its integration into an IGCC plant to coproduce power, fuels, and chemicals. Our analysis shows this mode of operation offer the best promise for the early commercial deployment of this technology in the U.S. One of the main hurdles for this deployment strategy is the technical risks inherent in the individual gasification and F-T synthesis steps, and also in the system integration. The technical risks associated with the gasification step should be greatly reduced with the ongoing commercial demonstration of several advanced gasification technologies in the IGCC projects supported by the DOE Clean Coal Program (DOE 1996a, 1996b, 1996c). Because of the current federal budget constraints, financing for the commercial demonstration of slurry phase F-T technology could pose a challenging problem. We have explored the concept of a pioneer plant which would employ a single commercial train slurry phase F-T reactor and located adjacent to a facility with existing infrastructures. We feel that the formation of an industry led consortium would be an appropriate vehicle to undertake this pioneer plant project. We also feel that financial incentives would be needed for the first few pioneer plants to compensate for the technical and market risks associated with these projects. One of the important features of these pioneer plants will be their capability to process feedstock beyond coal to include other carbonaceous materials like petroleum coke, wastes, and biomass. We are considering joining with industry to conduct a preliminary feasibility study for this pioneer plant which would include site selection, a financial plan, the types of incentives needed, and additional R&D support required. More discussions on this subject can be found elsewhere (Gray et al., 1997; Schmetz et al. 1996; Schmetz et al. 1997). Results have been reported on several case studies which deploy the indirect liquefaction technologies in commercial applications to coproduce power and fuels (Osterstock et al. 1997; Gray et al. 1997; Tam 1993).

Recent publications also indicate that the deployment of IGCC for power, hydrogen and syngas production has received more commercial commitments and/or interests with choices of feedstock including natural gas, petroleum coke, refinery wastes, and petroleum residue (Chemical Week 1996; Rhodes 1996; Aalund, 1996; Oil & Gas Journal 1997). These projects are case specific and have been undertaken for a variety of reasons including the needs to dispose byproducts, to reduce plant emissions in com-pliance with environmental regulations, and to meet the niche market demands in the local areas. With more and more IGCC systems in place and/or under considerations, the opportunity to add an indirect liquefaction component to coproduce premium transportation fuels and chemicals in addition to power could offer the best prospects for the early commercial deployment of the indirect liquefaction technologies. With the learning experience gained from these early entrant operations, a transition to a coal based indirect liquefaction could be underway with greatly reduced technical risks between 2010 and 2015 when coal liquids would become competitive with crude.

CONCLUSIONS

We have presented an updated summary of the work performed under the DOE indirect liquefaction program since 1994. We also have summarized the recent diesel engine emission data with DME and F-T diesel as the test fuels. Finally, we have discussed the prospects for the early commercial deployment of indirect liquefaction in an IGCC facility to coproduce power, fuels, and chemicals. We feel that the appeal for coproduction concept would be enhanced with continued R&D to develop more versatile iron catalysts to produce a broad array of high value chemicals in addition to fuels.

REFERENCES

1. Aalund, L.R., "Italian Refinery Gasification Project to Make Electricity, Steam, and Hydrogen from Tar", Oil & Gas Journal, P. 33, October 21, 1996

2. Agee, M.A. 1997 "Economic Conversion of Natural Gas to Synthetic Petroleum Liquids", Paper Presented at the ACS National Meeting, San Francisco, CA, April 14-17, 1997

3. Bhatt, B.L., R. Frame, A. Hoek, K. Kinnari, V.U.S. Rao, and F.L. Tungate 1995a "Catalyst Processing Scale-up for Fischer-Tropsch Synthesis", Topics in Catalysis 2 (1995) 235-257.

4. Bhatt, B.L. 1995b, "Liquid Phase Fischer-Tropsch (II) Demonstration in the LaPorte Alternative Fuels Development Unit", topical Research Report, Prepared by Air Products and Chemicals for the US. DOE, contract No. DE-AC22-91PC90018, September, 1995

5. Bhatt, B.L., D.M. Brown, E.C. Heydorn, Hoek, A., and G.J. Stiegel 1995c "Productivity Improvements for Fischer-Tropsch Synthesis", 14th North American Meeting of the Catalysis Society, Snowbird, Utah, June 11-16, 1995

6. Brown, R.E., et al. 1982. "Economic Evaluation of the Co-Production of Methanol and Electricity with Texaco Gasification-Combined-Cycle Systems", EPRI AF-2212, Project 239-2, Final Report, January 1982

7. Chemical Week 1996. "Texaco and Praxair in syngas Venture", Pg. 15, March 27, 1996

8. Degaleesan, S., S. Kumar, M.P. Dudukovic, B.A. Townsend, and B.L. Bhatt 1996 "Progress in Understanding the Fluid Dynamics of Bubble Column Reactors", Paper Presented at the DOE First Joint Power and Fuels Systems Contractors Conference, July 9-11, 1996

9. DOE Clean Coal Technology Topical Report 1996a "The Tampa electric Integrated Gasification Combined-Cycle Project", Topical Report No.6, October 1996

10. DOE Clean Coal Technology Topical Report 1996b "The Wabash River Coal Gasification Repowering Project", Topical Report No.7, November 1996

11. DOE Clean Coal Technology Topical Report 1996c "The Pinon Pine Power Project", Topical Report No.8, December 1996

12. Eisenberg, B., G.C. Lahn, R.A. Fiato, and G.R. Say 1993 "Exxon AGC-21 Advanced Gas Conversion Technology", Paper Presented at the at the Council on Alternate Fuels' Alternate Energy '93, April 27-30, 1993

12. Fleisch, T., C. McCarthy, A. Basu, C. Udovich, P. Charbonneau, W. Slodowske, S. Mikkelsen, and J. McAandless 1995. "A New Clean Diesel Technology: Demonstration of ULEV Emissions on a Navistar Diesel Engine Fueled with Dimethyl Ether", SAE Paper Series No. 950061, February 27-March 2, 1995

13. Fourie, J.H., 1995 "Sasol Update 1995", Paper Presented at the Council on Alternate Fuels 15th Annual Spring Conference, May 1-4, 1995

14. Gray, D., et al. 1980 "The Impact of Developing Technology on Indirect Liquefaction", MTR-80W326, Mitre Corp., November, 1980

15. Gray, D. and G. Tomlinson 1995 "Rationale for Continuing R&D in Indirect Coal Liquefaction", Proceedings for the Coal Liquefaction and Gas Conversion Contractors Review Conference, Pittsburgh, PA, August 29-31, 1995

16. Gray, D. and G. Tomlinson 1996 "Rationale and Proposed Strategy for Commercial Deployment of Coal-Derived Transportation Fuels", MP 96W0000209, Mitretek Systems, June 1996

17. Gray, D., and G. Tomlinson 1997 "Opportunities for Early Commercial Deployment of Indirect Liquefaction", Paper Presented at the American Chemical Society Meeting, San Francisco, CA, April 13-17, 1997 .

18. Hagen, G.P. 1996 "Synthesis of Oxygenate Products for High Volume Fuels Applications", Paper Presented at the First Joint Power & Fuel Systems Contractors Conference, Pittsburgh, PA, July 9-11, 1996

19. Hansen, J.B., B. Voss, F. Joensen, and I.D. Siguroardottir 1995. "Large Scale Manufacture of Dimethyl Ether - a New Alternative Diesel Fuel from Natural Gas", SAE Paper Series No. 950063, February 27-March 2, 1995

20. Jackson, N., J.R. Torczynski, K.A. Schollenberger, T.J. O'Hern, and D.R. Adkins 1996 "Sandia Support for PETC Fischer-Tropsch Research: Experimental: Characterization of Slurry Phase Bubble Column Reactor Hydrodynamics", Paper Presented at the DOE First Joint Power and Fuels Systems Contractors Conference, July 9-11, 1996

21. Montalvo, D.A. 1995 "Engine Evaluation of Fischer-Tropsch Diesel Fuel, Phase I", Final Report, Prepared for Bechtel Group by Southwest Research Institute under DOE Contract DE-AC22-93PC91029, October 1995

22. O'Brien, R.J., Raje, A., R.L. Spocer, L. Xu, S. Bao, R.A. Keogh, S.H. Lambert, S. Liaw, S. Chokkaram, D.J. Houpt, and B.H. Davis 1996, "Technology Development for Iron Fischer-Tropsch Catalysts", Paper Presented at the DOE First Joint Power and Fuels Systems Contractors Conference, July 9-11, 1996

23. Oil & Gas Journal 1997. "Cogeneration: Star Enterprises .....", April 7, 1997

24. Osterstock, E.R., J. Klosek, and K.W. Guy 1997. "Dispatchable IGCC Facilities: Flexibility through Coproduction", Paper Presented at the Power-Gen Europe 97, Madrid, Spain, June 17-19, 1997

25. Peng, X.D., G.E. Parris, B.A. Toseland, and R.P. Underwood 1996 "Some Advances in Catalysts for alternative Fuels", Paper Presented at the DOE First Joint Power and Fuels Systems Contractors Conference, July 9-11, 1996

26. Rhodes, A.K., "Kansas Refinery Starts Up Coke Gasification Unit", Oil & Gas Journal, P. 31, August 5, 1996

27. Sasol 1997. "Natural Gas to Liquids in Qatar", a Sasol Limited Media Reelease, March 19, 1997

28. Schmetz, E., J. Shen, and D. Gray 1996 "Coal Liquids: A Domestic Option for Liquid Transportation Fuels", Paper Presented at the Pittsburgh Coal Conference, September 4, 1996

29. Schmetz, E., J. Shen, G. Stiegel, and R. Tischer 1997 "DOE Indirect Coal Liquefaction Program - Hurdles and Opportunities for its Early Commercialization", Paper Presented at the American Chemical Society National Meeting, April 1997

30. Shen, J., G. Stiegel, and A.C. Bose 1996 "DOE Indirect Coal Liquefaction Program - An Overview". Fuel Sciences & Technology Int'l., 14(4), 559-576 (1996)

31. Soong, Y., I.K. Gamwo, F.W. Harke, A.G. Blackwell, and M.F. Zarochak 1995 "Fischer-Tropsch Slurry Reactor Modeling", Proceedings of Coal Liquefaction and Gas Conversion Contractors Review Conference, August 29-31, 1995

32. Spivery, J.J., M.R. Gogate, J.R. Zoeller, R.D. Colberg, G.N. Choi, and S.S. Tam 1996 "Synthesis of Methyl Methacrylate from Coal-Derived Syngas", Paper Presented at the First Joint Power & Fuel Systems Contractors Conference, Pittsburgh, PA, July 9-11, 1996

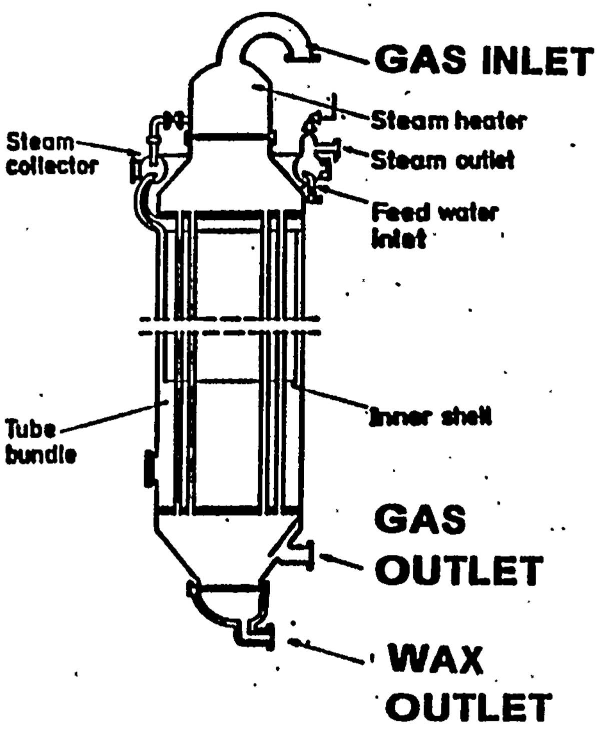
33. Starr, M.E. 1997. "Heavy-Duty Transient Emissions at Various Engine Timings Using Fischer-Tropsch Fuel", Final Report, Prepared for Bechtel Group by Southwest Research Institute under DOE Contract DE-AC22-93PC91029, April, 1997

34. Tam, S.S. 1993. "Indirect Coal Liquefaction Via Fischer-Tropsch Technology for the Baseload IGCC Plant", IEA Second International conference on the Clean and Efficient Use of Coal and Lignite: Its Role in energy, environment and Life", November 30-December 3, 1993

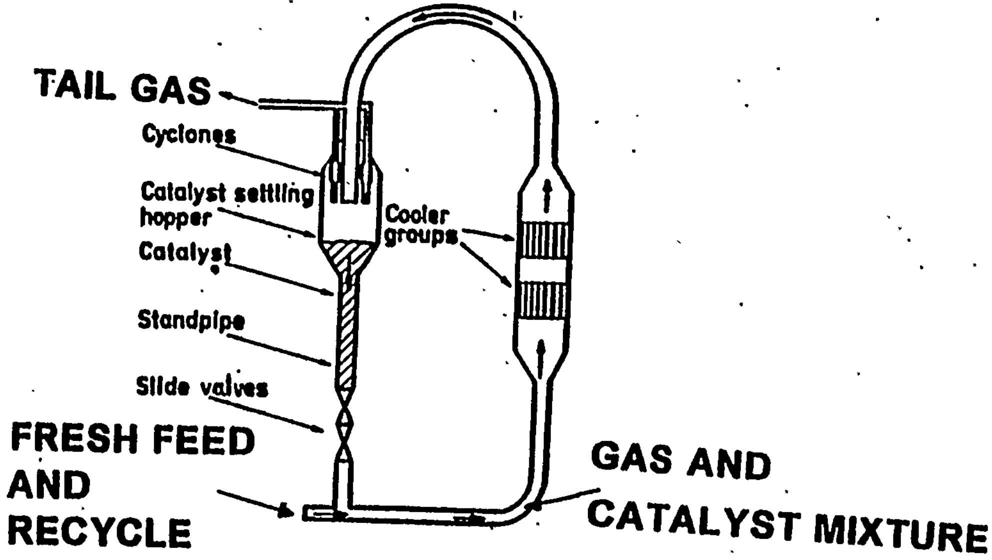
35. Tustin, G.C., J.R. Zoeller, and L. DePew 1996 "Synthesis of Vinyl Acetate Monomer from Synthesis Gas", Paper Presented at the First Joint Power & Fuel Systems Contractors Conference, Pittsburgh, PA, July 9-11, 1996

36. Xu, M., B.L. Stephens, M.J.L. Gines, and E. Iglesia 1996 "Reaction Pathways and Catalyst Requirements in the synthesis of Isobutanol from CO and Hydrogen", Paper Presented at the First Joint Power & Fuel Systems Contractors Conference, Pittsburgh, PA, July 9-11, 1996

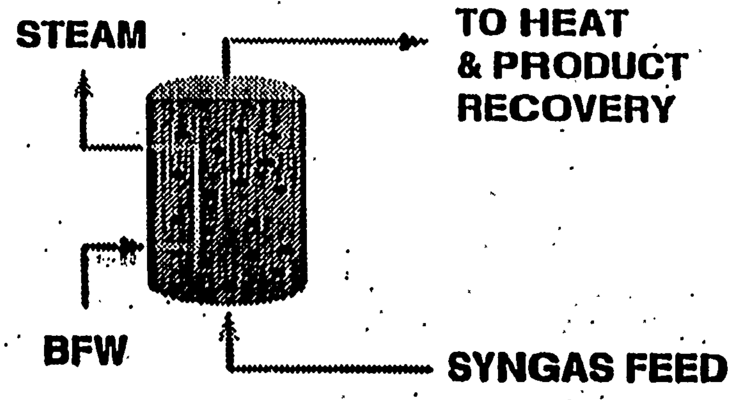
FIGURE 1 GAS AND LIQUID PHASE REACTORS



SASOL FIXED BED REACTOR



SASOL SYNTHOL REACTOR



LIQUID PHASE REACTOR

FIGURE 2 Continued R&D Can Significantly Reduce Fuel Cost and Time to Deployment

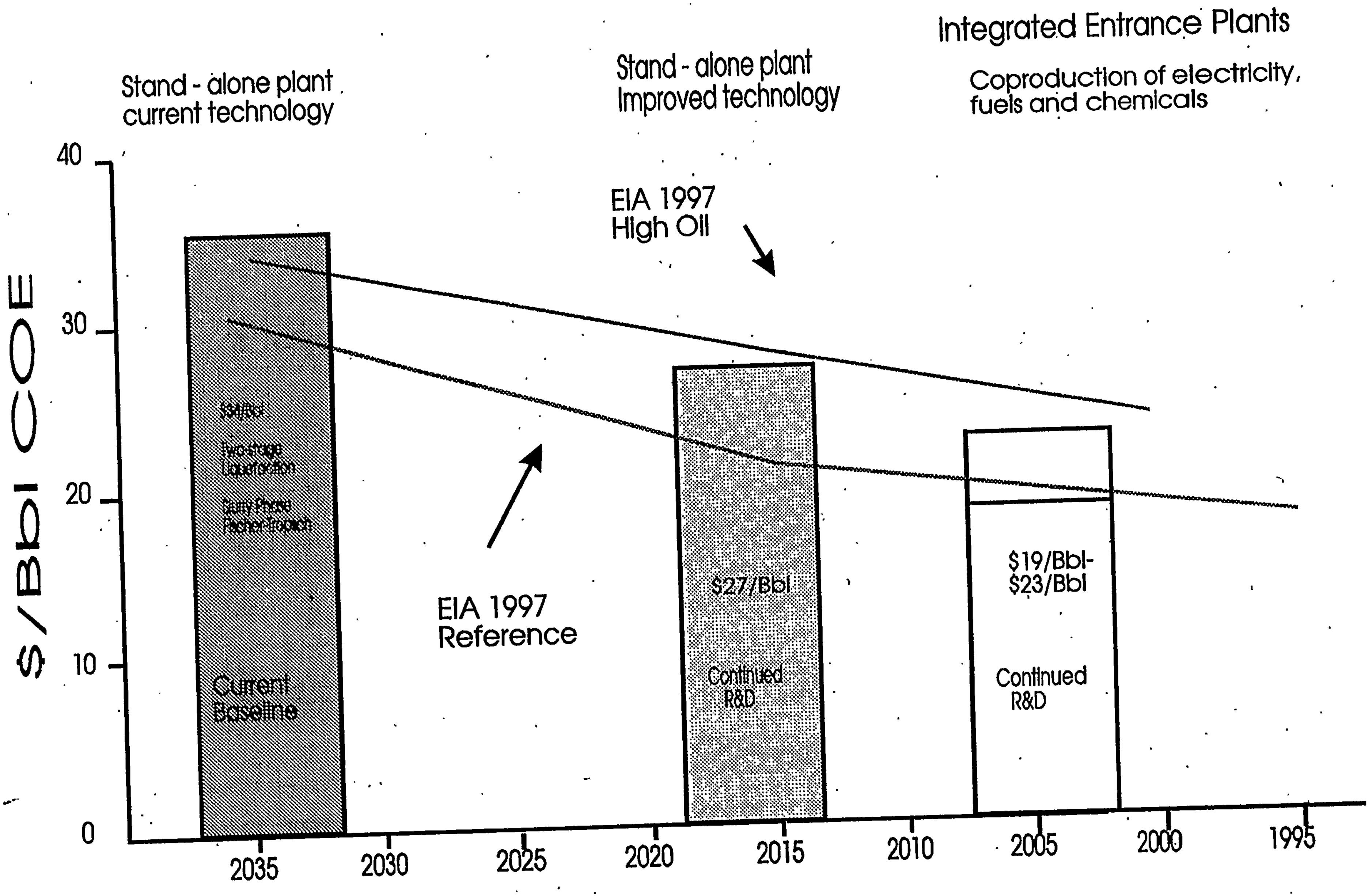


FIGURE 3: STATUS (INDIRECT LIQUEFACTION)

COMMERCIAL (GAS PHASE REACTOR)

■ SOUTH AFRICA:	SASOL (COAL TO MOTOR FUELS) & MOSSGAS (NATURAL GAS TO MOTOR FUELS)
■ NEW ZEALAND:	MOBIL MTG (NATURAL GAS TO GASOLINE)
■ U.S.A.	EASTMAN CHEMICALS (COAL TO METHANOL)
■ MALAYSIA:	SHELL (NATURAL GAS TO MOTOR FUELS)

UNDER DEMONSTRATION (LIQUID/SLURRY PHASE REACTOR)

■ SOUTH AFRICA:	SASOL (COAL TO MOTOR FUELS)
■ U.S.A.:	EXXON (NATURAL GAS TO MOTOR FUELS)
■ U.S.A. :	DOE/AIR PRODUCTS/EASTMAN (COAL TO METHANOL)

PRE-DEMONSTRATION/BENCH UNIT DEVELOPMENT
- NG BASED: SYNTROLEUM, RENTECH, SHELL, TEXACO, CONOCO/DUPONT, ENI
- COAL BASED: CHINA

FIGURE 4: INDIRECT LIQUEFACTION TECHNOLOGY PORTFOLIO

LIQUID PHASE METHANOL

- HIGHLIGHTS OF POC OPERATIONS
  - – 0.67 H_2 TO CO RATIO SYNGAS (TEXACO GASIFIER)
  - – RAW METHANOL MEET FUEL GRADE SPEC
  - – ACHIEVED 10 TONS/DAY (TPD) RATE
- COMMERCIAL DEMONSTRATION UNDERWAY

LIQUID PHASE DIMETHYL ETHER (DME)

SLURRY PHASE FISCHER-TROPSCH (F-T)

ALL THREE TECHNOLOGIES AIMED FOR CO-PRODUCTION APPLICATIONS

FIGURE 5 FUTURE WORK AT LAPORTE

SLURRY PHASE F-T IV RUN
- PARTICIPANTS: DOE/AIR PRODUCTS/SHELL OIL
- PRODUCE F-T DIESEL FOR ENGINE EMISSION TESTING
- COBALT F-T CATALYST

LIQUID PHASE DME RUN
- PARTICIPANTS: DOE/AIR PRODUCTS/EASTMAN CHEMICALS
- PROVE OUT IMPROVED CATALYST SYSTEM
- EQUIPMENT UPGRADING UNDER CONSIDERATIONS TO ALLOW FOR DME PRODUCTS COLLECTED FOR ENGINE EMISSION TESTING

FIGURE 3: STATUS (INDIRECT LIQUEFACTION)

COMMERCIAL (GAS PHASE REACTOR)

■ SOUTH AFRICA:	SASOL (COAL TO MOTOR FUELS) & MOSSGAS (NATURAL GAS TO MOTOR FUELS)
■ NEW ZEALAND:	MOBIL MTG (NATURAL GAS TO GASOLINE)
■ U.S.A.	EASTMAN CHEMICALS (COAL TO METHANOL)
■ MALAYSIA:	SHELL (NATURAL GAS TO MOTOR FUELS)

UNDER DEMONSTRATION (LIQUID/SLURRY PHASE REACTOR)

■ SOUTH AFRICA:	SASOL (COAL TO MOTOR FUELS)
■ U.S.A.:	EXXON (NATURAL GAS TO MOTOR FUELS)
■ U.S.A. :	DOE/AIR PRODUCTS/EASTMAN (COAL TO METHANOL)

PRE-DEMONSTRATION/BENCH UNIT DEVELOPMENT

- NG BASED: SYNTROLEUM, RENTECH, SHELL, TEXACO, CONOCO/DUPONT, ENI
- COAL BASED: CHINA

FIGURE 4: INDIRECT LIQUEFACTION TECHNOLOGY PORTFOLIO

LIQUID PHASE METHANOL

- HIGHLIGHTS OF POC OPERATIONS
  - – 0.67 H_2 TO CO RATIO SYNGAS (TEXACO GASIFIER)
  - – RAW METHANOL MEET FUEL GRADE SPEC
  - – ACHIEVED 10 TONS/DAY (TPD) RATE
- COMMERCIAL DEMONSTRATION UNDERWAY

LIQUID PHASE DIMETHYL ETHER (DME)

SLURRY PHASE FISCHER-TROPSCH (F-T)

ALL THREE TECHNOLOGIES AIMED FOR COPRODUCTION APPLICATIONS

FIGURE 5 FUTURE WORK AT LAPORTE

SLURRY PHASE F-T IV RUN

- PARTICIPANTS: DOE/AIR PRODUCTS/SHELL OIL
- PRODUCE F-T DIESEL FOR ENGINE EMISSION TESTING
- COBALT F-T CATALYST

LIQUID PHASE DME RUN

- PARTICIPANTS: DOE/AIR PRODUCTS/EASTMAN CHEMICALS
- PROVE OUT IMPROVED CATALYST SYSTEM
- EQUIPMENT UPGRADING UNDER CONSIDERATIONS TO ALLOW FOR DME PRODUCTS COLLECTED FOR ENGINE EMISSION TESTING

FIGURE 6: DME FUEL PROPERTIES

PROPERTY	DIESEL	DME	PROPANE /BUTANE
FORMULA	——	CH3COCH3	C3H8/C4H10
BOILING POINT RANGE, °C	191-344	-25	-42/-0.5
VAPOR PRESSURE @ 20°C, BAR	LOW	5.1	8.4/2.1
LIQUID DENSITY @ 20°C, G/ML	0.8-0.84	0.668	0.501/0.610
LOWER HEATING VALUE, MJ/kg	42.5	28.4	46.4/45.7
CETANE NUMBER	40-55	55-60	—/—
IGNITION TEMP, °C	—	235	470/365

FIGURE 7: DIESEL FUEL PROPERTIES

PROPERTY	2D DIESEL	PSEUDO CARB DIESEL	F-T DIESEL
DENSITY G/ML @15°C	0.845	0.842	0.780
DISTILLATION RANGE			
IBP, °C	191	210	201
EP, °C	344	344	358
SULFUR, PPM	330	345	N.D.
CETANE NO.	46	50	76
FLASH POINT, °C	71	82	88
AROMATICS, V%	30	9	N.D.
CLOUD POINT, °C	-17	-16	1
POUR POINT, °C	-26	N.A.	N.A.

N.D. = NOT DETECTABLE
N.A. = NOT AVAILABLE

FIGURE 8: PIONEER PLANT CONCEPT FOR COMMERCIAL DEMONSTRATION

- LIQUID PHASE DME AND SLURRY PHASE F-T TECHNOLOGIES REQUIRE COMMERCIAL DEMONSTRATION TO MITIGATE TECHNICAL RISKS
- PIONEER PLANT PROPOSED TO CARRY OUT COMMERCIAL DEMO
  - – A SINGLE COMMERCIAL TRAIN
  - – INDUSTRY LED EFFORTS (TEAMING ARRANGEMENT)
  - – FEEDSTOCK FLEXIBILITY BEYOND COAL
  - – DOE TO COFUND FEASIBILITY STUDY
    - ** DEFINE ISSUES RELATED TO TECHNICAL & MARKET RISKS
    - ** SITE SELECTIONS
    - ** FINANCIAL PLAN
    - ** SUPPORT R&D

FIGURE 9: COAL VS NATURAL GAS BASED INDIRECT LIQUEFACTION

	COAL/COKE	NATURAL GAS
ATOMIC H/C RATIO	0.5-0.8	4.0
H_2 TO CO RATIO IN SYNGAS	0.5-0.7	1.75 - 5
CATALYSTS (F-T)	IRON & COBALT	COBALT & IRON
IMPURITIES IN SYNGAS	USE GUARD BED	—
PRODUCTS	FUELS, WAX, CHEMICALS	FUELS, WAX, CHEMICALS

FIGURE 10: PARTNERSHIP BETWEEN INDIRECT LIQUEFACTION AND OTHER DOE PROGRAMS

POTENTIAL PARTNERS	RELATIONSHIP W. IND . LIQ.	AREAS OF JOINT WORK
FE/IGCC POWER	SYNGAS/POWER PRODUCER	■ POWER/FUELS COPRODUCTION ■ SYSTEM INTEGRATION
FE/GAS TO LIQUIDS	SYNGAS/ FUELS PRODUCER	■ FUELS PRODUCTION ■ SYSTEM INTEGRATION ■ FUELS EMISSION TESTING
EE/HEAVY VEHICLE TECHNOLOGIES	FUELS USER	■ FUELS PRODUCTION ■ FUELS EMISSION TESTING

FIGURE 11: POLICY ISSUES

CO2 EMISSIONS FROM INDIRECT LIQUEFACTIONS

- COAL BASED TECHNOLOGY
- NATURAL GAS BASED TECHNOLOGY
- ISSUES: BENCH MARKING FUELS, ENVELOPE OF LIFE CYCLE ANALYSIS

FIGURE 11: CONCLUSIONS

- THE 260 TONS/DAY COMMERCIAL DEMONSTRATION PLANT FOR LIQUID PHASE METHANOL WAS SUCCESSFULLY STARTED UP IN 4/97.
- LIQUID PHASE DME AND SLURRY PHASE F-T ARE SCHEDULED FOR PROOF-OF-CONCEPT (POC) SCALE DEMONSTRATION IN 1998.
- F-T DIESEL AND DME SHOW PROMISE AS CLEAN ALTERNATIVE DIESEL FUELS WHICH WOULD MEET ULEV EMISSION SPEC.
- AN INDUSTRY-LED PIONEER PLANT CONCEPT HAS BEEN PROPOSED TO UNDERTAKE THE COMMERCIAL DEMONSTRATION OF LIQUID PHASE DME AND SLURRY PHASE F-T TECHNOLOGIES.
- ACTIVITIES SUPPORTED BY THE PROGRAMS OF INDIRECT COAL LIQUEFACTION, NATURAL GAS TO LIQUIDS, AND HEAVY VEHICLE TECHNOLOGIES OFFER BROAD COMMON GROUND FOR COOPERATIONS.