



**U.S. Department of Energy  
National Energy Technology Laboratory**

**Refining and End Use Study of  
Coal Liquids**

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**Final Report**

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## TABLE OF CONTENTS

	Page
1. Introduction.....	1
2. Activity 1 – Demonstration of a Refinery Accepting Coal Liquids.....	4
2.1 Basic Program.....	4
2.1.1 Fractionation and Characterization.....	6
2.1.2 Pilot Plant Testing and Correlation.....	7
2.1.3 Linear Programming Analysis.....	13
2.2 Option 1 Program.....	16
2.2.1 Economic Evaluation.....	16
2.2.2 Engine Emissions Using Fuels Containing Direct Coal Liquids.....	18
3. Activity 2 – Emissions Testing of Fischer-Tropsch Diesel.....	23
3.1 Phase I – Screening.....	23
3.2 Phase II and III – Equipment Modifications.....	25
4 Activity 3 – Biomass Gasification F-T Modeling.....	28
5 Activity 4 – Updated Gas-to-Liquids Baseline Design/Economic Study.....	29
6 Activity 5 – Upgraded Rentech FT Liquids .....	30
 Appendices	
A A List of Key Topical Report.....	A1
B Selected Project Presentations.....	B1

## 1. Introduction

This document summarizes all of the work conducted as part of the Refining and End Use Study of Coal Liquids, a study which was funded in 1993 by the U.S. Department of Energy's (DOE's) Federal Energy Technology Center (now National Energy Technology Laboratory) under Contract No. DE-AC22-93PC91029. Bechtel/Nexant was the prime contractor; subcontractors included Southwestern Research Institute (SwRI), M. W. Kellogg Co. (MWK) and Amoco. Consultants were Richard Eccles (LP Modeling) and Joseph Fox (data correlation.) There were several distinct objectives set, as the study developed over time:

1. **Demonstration of a Refinery Accepting Coal Liquids** - two direct coal liquids, produced by direct hydrogenation of an Eastern and a Western coal at the Hydrocarbon Technologies, Inc. (HTI) facility in New Jersey, and one indirect coal liquid, produced in the 1992 DOE Fischer-Tropsch pilot plant at La Porte, Texas, were pilot plant tested for inclusion in the feed to a typical PADD II Refinery, simulated by a Linear Programming (LP) Model. Once the model was finalized, gasoline, jet fuel and diesel fractions containing significant amounts of coal liquids were prepared and submitted to engine testing to ascertain the effect of the coal liquids on emissions. The product slate (55% gasoline) was designed to meet year 2000 projections of quantity and quality. The economic penalty or advantage for the coal liquids over Midwestern crude oil (a mixture of Arabian light and heavy crudes) was then determined by using the LP Model. This study consisted of several integrated parts:

The *Basic Program* of experimentation and refinery modeling, consisting of:

- Fractionation of the coal liquids into refinery cuts and characterization of same by SwRI.
- Pilot plant testing of these refinery cuts, alone and in blends with similar refinery cuts obtained from Amoco's Whiting refinery. Testing included hydrotreating and platinum reforming by SwRI, fluid catalytic cracking by MWK, hydrocracking and fluid catalytic cracking of La Porte Fischer-Tropsch wax by Amoco.
- Refinery modeling by Bechtel, using linear programming, to guide the pilot plant and emissions testing work.

The *Option 1 Program – Task 1*, consisting of:

- Economic evaluation, by Bechtel, of feed value differences, using the LP Model.
- Production runs at design conditions, by SwRI and MWK.
- Product blending and comparative engine testing for emissions by SwRI.

2. **Emissions Screening of Indirect Diesel** - When the Fischer-Tropsch (F-T) liquid from 1992 La Porte was found to have unusual and unfavorable characteristics (catalyst fines and unusually high molecular weight), the *Option 1 - Task 2 Program* was added in 1995. Three typical diesel blends were obtained from proprietary F-T process licensors, who prefer to remain unidentified. Two refinery diesel blends from petroleum were also prepared - a typical reference diesel fuel and a prototype advanced diesel fuel. All five products were then subjected to comparative emissions testing, in several phases, by SwRI.

*Phase I* – Screening of all five fuels, using an EPA Hot Start Transient Emissions Test Procedure, in a 1991 Heavy Duty Detroit Diesel Engine.

*Phase II* – Further transient emissions testing of one F-T and one petroleum diesel in a 1993 Heavy Duty Detroit Diesel Engine outfitted with DDEC II Electronic Control System.

*Phase III* - Further emissions testing using a Passive Continuously-Regenerative, particulate trap, after-treatment device.

3. **Biomass Gasification F-T Modeling** – formally titled *ASPEN Process Flowsheet Simulation. Model of a Battelle Biomass-Based Gasification, F-T Liquefaction and Combined Cycle Power Plant*, this study was added as the *Option 1 - Task 4 Program* in 1995. This was a self-contained add-on, in which Bechtel employed the modeling program developed for the Baseline Indirect Coal to Liquids Study.
4. **Updated Gas to Liquids (GTL) Baseline Design/Economic Study** – This update to the 1995 *Baseline Design/Economics of Indirect Gas Conversion Study* was added to the scope of work in 1999 as an add-on. The work was done by Nexant, successor to Bechtel's Technology and Consulting group.

This **Final Summary Report (Report 1)** is intended to wrap-up the End Use Study. Each of the above four sections is treated as a whole package with an Executive Summary of its own and reference is made to specific reports, already issued, which document the work. Where applicable, these Executive Summaries have been lifted out of the documentation reports. This was not always possible and some new material has been added to achieve continuity. No attempt has been made to update the studies other than to correct minor errors. The target product slate for **Activity 1 (Demonstration of a Refinery Accepting Coal Liquids)**, for example, is still based on year 2000 projections. Aside from the proposed phase out of the additive, MTBE, these projections are still considered valid for study purposes.

As a guide to the reader and for completeness of documentation, the following is a listing of the appended reports, already issued for each of the four sections:

**1. Demonstration of a Refinery Accepting Coal Liquids**

**Report 2** - Refining and End Use Study of Coal Liquids Final Report – *Basic Program* (Topical Report issued March 1999 by Bechtel.)

**Report 3** - Refining and End Use Study of Coal Liquids Topical Report – *Petroleum Refinery Linear Programming Model Design Basis* (Topical Report issued March 1995 by Bechtel and discussed in **Report 2**, the *Basic Program Report*.)

**Report 4** - Refining and End Use Study of Coal Liquids Topical Report – *Addendum to the Linear Programming Refinery Model Design Basis* (Topical Report issued October 1997 by Bechtel and discussed in **Report 2**, the *Basic Program Report*.)

**Report 5** - Refining and End Use Study of Coal Liquids Topical Report – *Option 1 Economic Evaluation* (Topical Report issued in July 1998 by Bechtel.)

**Reports 6 and 7** - Refining and End Use Study of Coal Liquids Final Report - *Option 1 Fuel Production and Engine Testing* (Final Report and Appendix issued in May 1999 by SwRI.) Production runs are correlated along with small scale test data in **Report 2**, the *Basic Program Report*.

**Report 8** - Refining and End Use Study of Coal Liquids Topical Report – *In-line Hydrotreater Simulation Study* (Topical Report issued in June 2001 by SwRI)

**2. Emissions Screening of Indirect (Fischer-Tropsch) Diesel**

**Report 9** - *Engine Evaluation of Fischer-Tropsch Diesel, Phase I* (Final Report prepared for Bechtel by SwRI and issued in October 1995)

**Report 10** - *Heavy-Duty Transient Emissions at Various Engine Timings using Fischer-Tropsch Diesel* (Final Report prepared for Bechtel by SwRI and issued in April 1997)

**3. Biomass Gasification**

**Report 11** - *ASPEN Process Flowsheet Simulation .Model of a Battelle Biomass-Based Gasification, F-T Liquefaction and Combined Cycle Power Plant* (Topical Report issued by Bechtel in May, 1998.)

**4. Gas to Liquids (GTL) Design/Economic Study**

**Report 12** - *Updated Baseline Design/Economics of Indirect Gas Conversion* (Topical Report issued by Nexant in December, 2000.)

## 2. Demonstration of a Refinery Accepting Coal Liquids

This refinery demonstration study was divided into two parts: (1) the Basic Program consisting of pilot plant testing, correlation and LP refinery modeling (*Reports 2, 3 and 4*) and (2) Option 1 - Task 1, consisting of economic evaluation, production runs and emissions testing (*Reports 5, 6A and 6B*). Owing to the lack of a good sample of indirect liquid, only the direct liquids portion was completed.

The study demonstrated that direct coal liquid DL-2, prepared by hydrogenation of sub-bituminous Western Coal in HTI's three stage coal liquefaction process, using an in-line hydrotreater as the third stage, can be fed directly to a PADD II type refinery, supplying a portion of the feed to the fluid bed catalytic cracking unit and the catalytic reformer. The other direct liquid, DL-1, was produced from bituminous Eastern coal without the third stage and had somewhat more limited processing characteristics. Either coal liquid can replace a significant portion of the crude oil when operating in a refinery expansion mode. Gasoline, jet fuel and diesel, meeting present day specifications, can be produced and their emissions characteristics are not significantly affected by the addition of coal liquid.

Direct coal liquids have an intrinsic value higher than standard PADD II crude oil due to the improved reformat yield and the lack of a heavy end. The differential versus crude oil ranges from \$0.60 per barrel in a no-expansion mode to as much as \$4.00 per barrel in an expansion mode. The value of the coal liquids is as much as \$1.00 per barrel still higher in the no-expansion scenario, when advantage is taken of their low end point to bring in cheaper, heavy, high metals crude oils. If refinery expansion is allowed, the situation is not as clearcut. The coal liquids still have an advantage but it may be desirable to increase the use of low cost crude instead.

The inclusion of the third stage, in-line, hydrotreater in the coal hydrogenation process with Western Coal made a great difference in the ability to prepare specification cat reformer feed, in improved light distillate blending characteristics and in improved fluid cat cracking yields. If the Eastern Coal had also been processed using the in-line hydrotreater, refinery processing of the resulting coal liquid would undoubtedly have given similar results but this assumption needs to be verified. The overall economics, starting from coal, should be ascertained.

### 2.1 BASIC PROGRAM

The overall objective of the Basic Program was to determine the most cost-effective method for processing direct and indirect coal liquids, in an existing PADD II petroleum refinery, in order to produce transportation fuels that meet expected year 2000+ specifications. A "petroleum-only" LP model of the required complexity was developed for a 150,000 bpd PADD-II Refinery operating under projected year 2000 product specifications and quantities with a variety of crude slates. This model is shown diagrammatically in **Report 3**, Figure 1. This was subsequently modified to include the feeding of raw coal liquids in either a no-expansion case or in an expansion to 200,000 bpd, letting the program set unit capacities using capital charge factors.

The Basic Program consisted of three primary tasks: (1) fractionating and characterizing coal liquids, two direct and one indirect. (**Report 2**, Section 3), (2) conducting pilot plant tests on coal liquid and petroleum fractions and blends of the two for the various upgrading processes and correlating the results (**Report 2**, Section 5), and (3) developing a linear programming (LP) model for a PADD-II petroleum refinery and integrating the test results into it (**Report 2**, Section 4, **Report 3** and **Report 4**). The LP model was used to determine the optimum-processing scheme for the coal liquids and for economic comparisons. Because of deficiencies in the indirect liquid sample, steps (2) and (3) could only be carried to completion for the direct liquids.

Specific conclusions from the study can be summarized as follows:

- The LP model showed that the optimum route for handling direct coal liquids was to hydrotreat the naphtha along with petroleum naphtha in the refinery hydrotreater followed by platinum catalyst reforming. The distillates were not hydrotreated; the light distillate going directly to product blending and the heavy distillate blended with petroleum cuts as feed to the fluid bed catalytic cracking unit. Because of their lower end points, the direct liquids did not produce a vacuum residuum, thus freeing up heavy end processing capacity.
- Hydrotreating the naphtha was required prior to platinum reforming but, in the case of DL-2, this could be done in the same hydrotreater as the naphtha from crude oil. DL-2 could be handled in a typical low-pressure refinery naphtha hydrotreater and meet the specification for nitrogen in the catalytic reformer feed. The coal liquid of DL-1, on the other hand, would require either a separate high pressure hydrotreater or a strict limitation in the percentage of DL-1 naphtha allowed in the feed.
- The direct liquids were superior to petroleum derived fuels from the standpoint of gasoline production. The naphtha fractions from the direct liquids, after heteroatom removal, were better platinum reformer feedstocks than the petroleum naphtha.
- A key issue is the establishment of optimum catalytic reformer yields and operating pressure. The usable pilot plant data was at high pressure, whereas the original LP model used low pressure, regenerative, reforming with better selectivity. The selectivity data were recorrelated for high pressure (i.e. low severity) operation. As a result, there is some discontinuity with the original refinery LP model and the product pricing this derived. This does not effect the yield advantage for coal liquids or the enhanced differential value of the coal liquids but should be corrected in future studies using this model.
- Hydrotreating the light and heavy distillate fractions was not warranted. The neat materials were already highly hydrogenated and had low heteroatom contents, DL-2 being superior to DL-1 in these respects. The coal liquid light distillates had poorer combustion and ignition qualities than those from petroleum and these properties were not improved significantly by hydrotreating unless the pressure was raised to 2,000 psig.

- The preferred processing route for both the coal liquid heavy distillate fractions was to catalytically crack the unhydrotreated material in blends with petroleum cuts. The cat-cracking yield and conversion were improved by pre-hydrotreating DL-1 distillate but, according to the LP model, not enough to justify an extra hydrotreating step. DL-2 heavy distillate did not require further hydrotreating.
- Coal liquid heavy distillates were very amenable to catalytic cracking but, because of their low carbon production, would have to be used in blends with heavier fractions from petroleum in order to run in heat balance. This is not anticipated to be a problem and may be an advantage in some refineries
- From a practical standpoint it seems advantageous to take advantage of the high pressure and temperature in the coal liquefaction unit (2700 psig and 800 °F) and include a severe hydrotreating step on the whole syncrude than to provide multiple high pressure hydrotreating operations in the refinery. This conclusion should certainly be checked out in future studies with other coals and the overall economics developed.
- For the lighter cuts, there is no fundamental difference between coal liquids and petroleum in the types of compounds present nor in their kinetic behavior during processing. The main difference is that the coal liquids have higher nitrogen, lower sulfur and higher naphthene contents than the typical PADD II petroleum fractions supplied by Amoco. The heavy distillates, however, seem to have fundamentally different types of compounds present which affect their behavior during hydrotreating or catalytic cracking.
- Linear blending rules can be applied to feed properties to estimate heteroatom removal for the lighter fractions. For aromatics removal, however, consideration needs to be given to naphthene/aromatics equilibrium, particularly at low pressure. Heavier fractions need to be studied further but there is evidence that blends with petroleum can be processed quite satisfactorily. In fact, there are indications, which should be checked further, that blending with petroleum improves the treatment of the coal liquid.

### 2.1.1 FRACTIONATION AND CHARACTERIZATION

The differences between the two direct coal liquids can be attributed to (1) the coal source and type and/or (2) the production method. Both liquids were produced at the Hydrocarbon Technologies, Inc., facility in New Jersey. The first direct liquid (DL-1) was produced from a bituminous coal using a two-stage hydrogenation process in Proof of Concept (POC) Run 1. The second liquid (DL-2) was produced from subbituminous coal in POC Run 2, using a three-stage hydrogenation process with in-line hydrotreating as the third stage. The DL-2 liquid had the higher degree of aromatic saturation and lower heteroatom content.

Compared with earlier direct coal liquids, the two direct coal liquids had higher hydrogen contents, lower heteroatom contents, and lower end points. All of these factors enhanced the value of the liquids. The primary difference between the two coal liquids tested also lay in the degree of hydrogenation. SwRI in-line hydrotreating experiments of DL-1, **Report 8**, confirm

this effect. The results showed that the added in-line hydrotreating processing was the major factor influencing both the sulfur and the polyaromatic hydrocarbon concentrations in the product liquids. The total aromatics concentration was relatively unaffected by the processing, but the types of aromatic compounds and their distribution among the distillation fractions were affected by the additional in-line hydrotreating. The nitrogen content was influenced by both the processing and the type of coal used. The third stage, or in-line hydrotreater, was therefore an important contributor to the high quality of the produced coal liquids.

The indirect coal liquid (IL-1) was made, using iron catalyst Fischer-Tropsch (F-T) technology, in DOE's Process Demonstration Unit at Air Products and Chemicals, Inc.'s plant in LaPorte, Texas. Because of the catalyst separation problems, the heavy end (wax) of the F-T product was contaminated with catalyst fines. Preliminary cleanup and characterization of the indirect coal liquid were successfully completed but, because of concerns over the quality of the liquid, there was no fractionation and no final characterization work or pilot plant testing conducted on any indirect coal liquid fractions other than the wax.

## 2.1.2 PILOT PLANT TESTING AND CORRELATION

### Direct Liquids

Hydrotreating, reforming and catalytic cracking tests were carried out in a small scale pilot plant on the direct coal liquids, typical petroleum fractions and blends of the two. The data were correlated to determine the processing conditions required to meet specifications. Larger scale production runs were undertaken to provide feed for further processing or emissions testing (described in **Reports 6A** and **6B**.) These production runs data were used to check the correlations. Results were as follows:

- *Naphtha* Naphtha was processed to high-octane gasoline by a combination of hydrotreating and platinum reforming.

Hydrotreating The target specifications of 0.5 ppmw on sulfur and nitrogen in the hydrotreater products used for platinum reformer feed were often at or below the limit of detection with the analytical methods employed. The DL-1 naphtha contained more sulfur and nitrogen than the DL-2 naphtha, the latter being close to meeting the nitrogen specification, as produced. In the production runs, in which feed was prepared for platinum reformer testing, DL-1 was hydrotreated at 1600 psig, 720 °F and 1.4 LHSV. DL-2, with considerably less sulfur and nitrogen, was processed at 700 psig, 500 °F and 1.36 LHSV. Both reformed satisfactorily in a high-pressure (450 psig) catalytic reformer.

Small-scale hydrotreating test work on DL-1 and a 33 vol% blend of DL-1 and petroleum naphtha was inconclusive as to whether the higher pressure used for DL-1 hydrotreating was actually necessary to meet the required reformer feed specifications of 0.5 ppmw nitrogen. Limited information was obtained on sulfur removal but this did indicate that the 0.5 ppmw sulfur specification could be met on

neat DL-1 naphtha and on a petroleum naphtha containing 1630 ppmw of sulfur under typical mild refinery hydrotreating conditions.

Platinum Reforming DL-1 and DL-2 hydrotreated naphthas were successfully upgraded in platinum reforming operations at 450 psig and these results were used for the LP model. This relatively high reforming pressure was used because rapid aging occurred in earlier 250 psig test work. While SwRI's 250 psig reformer test results, corrected for aging, confirmed a yield advantage for low pressure reforming (**Report 2**, Figure 5-65, reproduced below) the data were too inconclusive to be used for design. The LP reformer model was revised to check observed 450 psig selectivities.

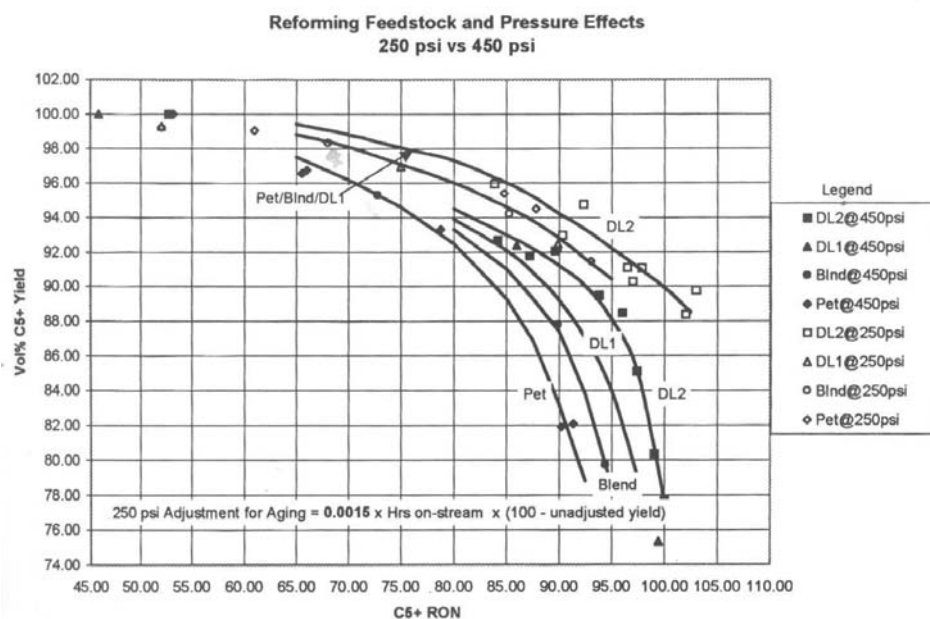


Figure 5-65 Combined Run 9 and Run 13 Correlation Showing Effects of Pressure and Feedstock

Predictions using the platinum reforming yield-octane relationship built into the original refinery LP model (the PIMS model, using N+2A content as the correlating parameter) checked the corrected low pressure selectivities (**Report 2**, Figure 5-66, reproduced below), providing a possible alternative design tool for future use. Lower pressure, regenerative reforming, used in many modern refineries and simulated in the original refinery LP model, would have given an additional five percent greater C5+ reformat yield of a given octane rating, at the expense of a somewhat higher investment cost.

Both the original LP Model (based on N+2A) and the correlated 450 psig test results confirmed the superiority of the coal liquid naphthas over the petroleum naphtha as

platinum reformer feedstock. Both of the direct coal liquids showed a significantly higher C5+ yield at a given severity (octane) level than the petroleum naphtha feed. The yield advantage can clearly be attributed to the higher naphthene and aromatic levels of the direct liquid feed materials.

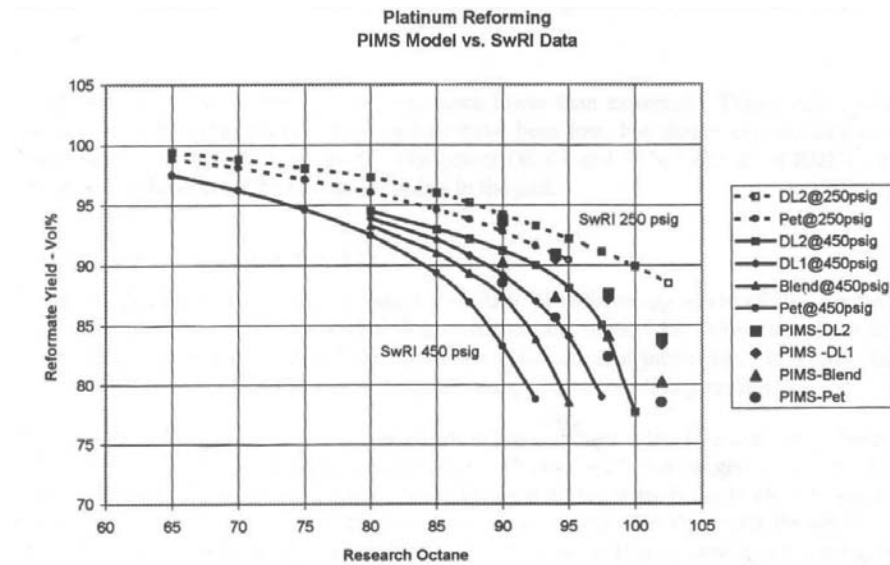


Figure 5-66 Comparison of LP Reformer Model with Run 9 and Run 13 Results

- *Light Distillate* Required levels of sulfur and nitrogen removal were achieved under relatively mild conditions. A good correlation of nitrogen removal data for all light distillate feeds was obtained using a pseudo-first-order kinetic model with a pressure correction (Report 2, Figure 5-40, reproduced below). In other words, the DL-2, DL-1 and petroleum light distillates and the DL-2/petroleum blend all showed the same behavior when expressed in terms of percent nitrogen conversion

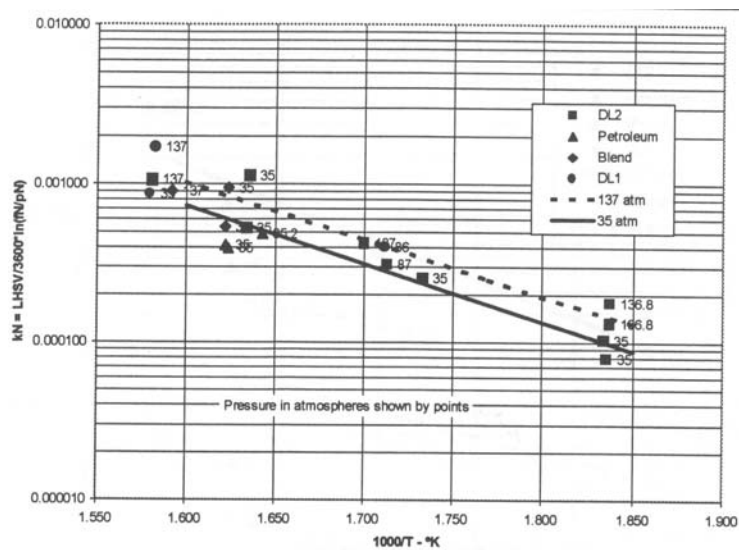


Figure 5-40 Nitrogen Removal in Light Distillate Hydrotreating Run 55

Low pressure (500 psig) hydrotreating did not improve the smoke point and the cetane number of any of the distillate fuels significantly and there was evidence of an equilibrium limit on aromatics conversion for the coal liquids as temperature was increased. Under high pressure (2000 psig) hydrotreating conditions, good aromatics removal was achieved at 680 °F and 1 LHSV, but ignition properties still did not fully meet specifications. While DL-2 was superior to DL-1, it was concluded that both the direct liquid light distillates could best be used for blending purposes without hydrotreating.

- *Heavy Distillate* Heavy distillates were processed by a combination of hydrotreating and fluid-bed catalytic cracking (FCC).

**Hydrotreating** DL-1 and petroleum heavy distillates were hydrotreated under a range of severities, the highest being 1800 psig, 730 °F and 0.43 LHSV. Again, nitrogen removal was well correlated, using pseudo-first-order kinetics, with a pressure correction (**Report 2**, Figure 5-8, reproduced below). In this case, the petroleum naphtha and the blend showed somewhat superior conversions to neat DL-1 distillate. The main objective, however, was to increase the hydrogen content and examine the effects on FCC performance (see below). DL-2 heavy distillate was deemed already sufficiently hydrotreated.

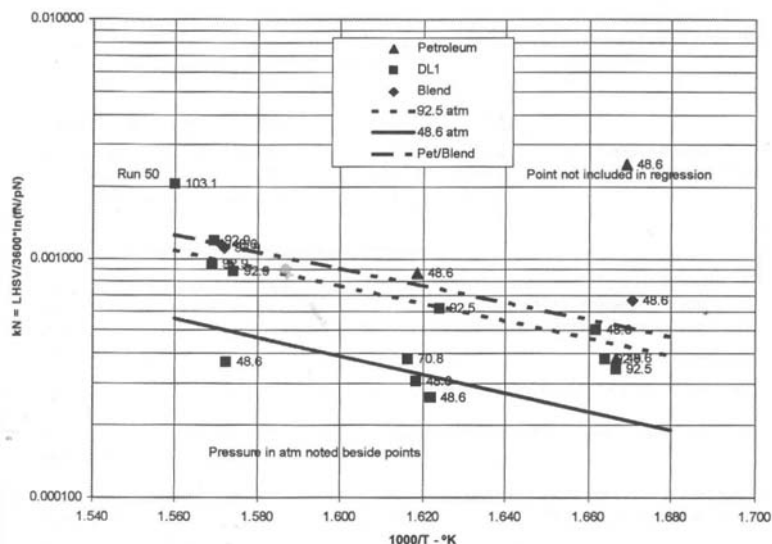


Figure 5-8 Nitrogen Removal in Distillate Hydrotreating Runs 49 & 50

**Fluid Catalytic Cracking (FCC)** Microactivity (MAT) testing was done on both raw DL-1 and DL-2 heavy distillates, on hydrotreated DL-1 heavy distillate, on petroleum VGO and on blends. It was found that the coal liquids followed different kinetics but gave maximum conversions and gasoline yields similar to VGO from petroleum. Results depended on the level of hydrogenation of the feed. In each case, the more severely hydrotreated material produced higher FCC gasoline yields and conversions but the raw DL-2 material was roughly equivalent to severely hydrotreated DL-1 distillate in this respect. Since LP modeling indicated that hydrotreating of DL-1 was not economically justified, despite the improved yields, pilot plant testing of DL-2 was carried out using the neat coal liquid. **Report 2**, Table 5-56 (reproduced below) compares the FCC pilot plant performance of petroleum VGO, hydrotreated DL-1 and raw DL-2 heavy distillates and blends with petroleum VGO. Again, DL-2 was roughly equivalent to severely hydrotreated DL-1. Because of the lower coke yields when using the coal liquids, they would have to be run in combination with higher coke producing feeds in a heat balanced, commercial unit.

**Table 5-56 Comparison of Hydrotreated DL1 and DL2 (Pilot Plant)**

Item	Run No. H-2006-			Run No. H-2038-		
	1	2	3	1	2	3
Feed Material	VGO	HT DL1	Blend	VGO	DL2	Blend
Catalyst/oil ratio	12.2	12.2	12.0	10.0	10.2	10.3
Temperatures, °F:						
Oil preheat	212	212	214	224	222	221
Catalyst inlet	1265	1253	1252	1254	1252	1255
Riser average	984	987	983	984	985	985
Material balance:						
Closure, wt%	98.5	98.5	98.5	99.9	101.9	100.7
Conversion, wt%	74.1	74.2	73.2	77.1	77.0	76.2
Total C2 and lighter	3.34	2.03	2.83	2.47	1.76	2.21
Total C3's	5.99	5.18	5.69	7.22	6.14	6.78
Total C4's	9.38	8.55	9.33	12.38	10.34	11.45
Total gasoline	50.52	55.17	51.01	49.99	55.06	51.20
Total cycle oil	25.87	25.80	26.82	22.90	23.04	23.85
Coke	4.90	3.27	4.32	5.04	3.66	4.51

- *Blends.* In all cases, performance on blends fell between that of pure coal liquids and the corresponding petroleum stock. For the light distillates (and presumably for naphthas as well) the source of the feed did not affect heteroatom conversion kinetics. In other words, hydrotreating results could be predicted from the feed composition. Petroleum heavy distillates hydrogenated more readily than the coal liquids but results on 33 vol% blends with coal liquid approached those obtained with the neat petroleum cut. For modeling purposes, linear blending was assumed and test results, within experimental accuracy, did not contradict this assumption.

### Indirect Liquid

Preliminary catalytic cracking and hydrocracking pilot plant tests were conducted by Amoco on the indirect liquid wax, after catalyst filtration by SwRI, with the following results:

- *Filtration.* A factor of 10 reduction in catalyst particles was achieved without disturbing the hydrocarbon distribution. The wax end point, before and after filtration, was much higher than expected, however. This may have been due to the use of a settling tank for catalyst/wax separation in the La Porte Demonstration Unit, which allowed the wax to be recycled back to the reactor and thus undergoing further polymerization.

- *Catalytic Cracking.* The indirect wax exhibited very high conversions with good gasoline yields and low coke make.
- *Hydrocracking.* The indirect wax showed poor conversions, which declined over a short period of time.

### 2.1.3 LINEAR PROGRAMMING ANALYSIS

There were two basic objectives to the LP modeling work.

- Determine the optimum petroleum refinery processing scheme with coal liquids addition to the facility.
- Determine the value of the coal liquids to the refiner relative to a typical crude oil.

The development and implementation of the LP model is described in **Report 2**, Section 4 but further details are given in **Report 3** and **Report 4**. First, a linear programming (LP) model was developed which simulates a PADD II petroleum refinery being expanded from 150,000 B/D to 200,000 B/D capacity (**Report 3**.) The model was then modified to process the coal liquids, either with or without expansion, based on the results from the pilot plant testing (**Report 4**). Further modifications are described in **Report 2**, Section 4.

The refinery was designed to meet projected future product specifications and product demand using a variety of crudes and includes C5/C6 isomerization, a naphtha reformer, a fluid bed catalytic cracker handling atmospheric resid and vacuum gas oil in various proportions with provisions for hydrotreating the atmospheric resid, delayed coking of the vacuum resid, a hydrocracker for the coker distillates and various hydrotreaters as required. The LP model is capable of optimizing alternative flows through the plant to optimize an economic objective function while meeting restrictions on product specifications and product make. A diagram showing the refinery model is given in **Report 3**, Figure 1. An updated product slate and product pricing relative is given in **Report 4**. This table is abbreviated below:

Unleaded regular gasoline	54,600 BPSD	28.25 \$/Bbl
Unleaded premium gasoline	18,200 BPSD	29.16 \$/Bbl
Reformulated regular gasoline	18,200 BPSD	29.03 \$/Bbl
Reformulated premium gasoline	6,070 BPSD	29.76 \$/Bbl
Kerosene/Jet fuel	12,840 BPSD	19.36 \$/Bbl
No. 2 fuel oil	13,100 BPSD	19.08 \$/Bbl
Low sulfur diesel	15,770 BPSD	19.08 \$/Bbl
High sulfur diesel	13,990 BPSD	19.46 \$/Bbl

Product pricing is marginal relative to \$18/Bbl crude (a mixture of Arabian Light and Arabian Heavy) and was based on the marginal values given by the LP model when running to achieve a profit margin consistent with historical refinery experience.

The key aspects of the model used for the Refining and End Use study were:

- The feedstock coal liquids were raw liquids and were upgraded, as required, in the refinery. Thus, the petroleum refinery and the coal liquids upgrading process were jointly optimized once the petroleum refinery configuration had been set.
- Product slate, volumes, and specifications, as well as process unit capacities, were year 2000 projections (the only major change known to have occurred since then is MTBE phase-out in California.)
- Unit expansion was allowed with capital costs reflected as daily expenses.
- Process unit yields for coal liquids were initially predicted from literature data and updated with actual pilot plant data from this study.
- Coal liquid properties, before and after processing, were obtained by characterizing the feeds and products for the pilot plant operations of this study.

The following model changes were made to make the petroleum refinery model more responsive to future markets and specifications:

- The fluid catalytic cracking (FCC) yield was made to vary depending on the Conradson Carbon Residue (CCR) of the feed.
- End points of the medium naphtha and light distillate were lowered to meet future gasoline and jet fuel specifications. A swing 325-350 °F cut is taken which can go either to gasoline or to jet fuel.
- Provision was made to produce a premium grade anode coke by desulfurizing atmospheric bottoms prior to coking. This is realistic and gives another outlet for heavy ends which is important when heavy crudes are added to the crude slate.
- Provision was made for adjusting hydrotreating yields to reflect cracked feeds and lower severity.
- Provision was made alternatively to put hydrocracker kerosene into jet fuel.
- The gasoline specification included meeting the EPA complex model predictions for emissions.
- Enhancement of the capital charge adjustment factor permitted the model to allow for expanding capacity of a specific unit or building a new unit.
- Improvements were made in the base unit capacities and product slate to meet year 2000 market requirements and specifications.
- A number of minor changes were made to develop a more flexible model.

Two scenarios were devised for future optimization of the refinery model when coal liquids are added later on:

Case 1 – No expansion of a 150,000 bpd refinery with all process units operating at full capacity. Coal liquids displace a portion of the petroleum crude.

Case 2 – Expansion of the refinery from 150,000 to 200,000 bpd by letting the program set individual unit capacities. Adjustment of the objective function by means of a capital charge factor permits the program to determine the nature of the expansion required.

Using only the base crude mix, comparison of Case 1 and Case 2 at the same objective function provided a way of establishing product values at a given crude oil price. Alternative heavy crudes were also introduced into the two LP cases to provide estimates of relative crude value. These estimates were valuable in later use of the model for coal liquids co-processing.

After the petroleum LP model was developed, modifications were made to enable the model to process coal liquids (**Report 4**.) This primarily involved incorporating the yield and product property data from the Task 4 pilot plant testing. Further details are given in **Report 2**, Section 4.

Key results from the LP analysis showed:

- Hydrotreating the naphtha was required prior to platinum reforming but, in the case of DL-2, this could be done in the same hydrotreater as the naphtha from crude oil. Results on DL-1 were inconclusive.
- The gasoline yield advantage over petroleum naphtha, as platinum reformer feeds, was significant for both of the hydrotreated direct liquids
- Hydrotreating the light and heavy distillate fractions was not warranted. The neat materials were already highly hydrogenated and had low heteroatom contents, DL-2 being superior to DL-1 in these respects. The combustion and ignition qualities did not improve significantly with hydrotreating until hydrotreating severity was quite high (1800 psig pressure or higher).
- The preferred processing route for both the coal liquid heavy distillate fractions was to catalytically crack the material without hydrotreating.
- Because of their lower end points, the direct liquids did not produce a vacuum residuum, thus freeing up heavy end processing capacity.
- A key issue is the establishment of catalytic reformer yields. Since the pilot plant data was at high pressure, whereas the model used low pressure reforming, the data were recorrelated, as described in **Report 2**, for high pressure (i.e. low severity) operation. As a result, there is some discontinuity with the original refinery LP model. This does not affect the yield advantage for coal liquids or the enhanced value of the coal liquids but should be corrected in future studies using this model.

## 2.2 OPTION 1 PROGRAM

This portion of the Refinery Optimization Program had to do with (1) the economic comparisons between coal liquids and conventional petroleum as refinery feeds in the optimized refinery (**Report 5**) and (2) the emissions characteristics of the refinery products from each source when used as transportation fuels (**Reports 6A and 6B.**) The work involved LP modeling of the refinery with coal liquids addition, use of the model to determine the differential value of coal liquids versus crude oil, larger scale pilot plant simulation of each refining step in production runs, blending the products into gasoline, diesels and jet fuel and then emissions testing in vehicles and test engines.

### 2.2.1 Economic Evaluation

The two direct coal liquids described above were evaluated by linear programming analysis to determine their value as petroleum refinery feedstock. The results are described in **Report 5**.

The coal liquids were compared against a generic petroleum crude feedstock under two scenarios. In the first scenario, it was assumed that the refinery capacity and product slate/volumes were fixed. The coal liquids would be used to replace a portion of the generic crude. The LP results showed that the DL-1 material had essentially the same value as the generic crude. Due to its higher quality, the DL-2 material had a value of approximately 0.60 \$/barrel higher than the petroleum crude.

In the second scenario, it was assumed that a market opportunity exists to increase production by one-third. This requires a refinery expansion. The feedstock for this scenario could be either 100% petroleum crude or a combination of petroleum crude and the direct coal liquids. Linear programming analysis showed that the capital cost of the refinery expansion was significantly less when coal liquids are utilized. In addition, the pilot plant testing showed that both of the direct coal liquids demonstrated superior catalytic cracking and naphtha reforming yields. Depending on the coal liquid flow rate, the value of the DL1 material was 2.5-4.0 \$/barrel greater than the base petroleum crude, while the DL2 material was 3.0-4.0 /barrel higher than the crude.

Co-processing the coal liquids with lower quality, less expensive petroleum crudes that have higher sulfur, resid and metals contents was also examined. The coal liquids have higher values in the no-expansion scenario since they permit the use of more cheap crude. Under the expansion scenario, the coal liquids still performed well but the LP model indicated that expansion of capacity of the cheaper crudes was an attractive alternative. This depends greatly on the actual crude cost and on the various capital factors used for process unit capacity expansion.

### Description of Methods Used

The key features of this model are:

- Each of the individual processing units in the refinery operates at the maximum capacity.
- A provision was added for estimating a capital charge for expanding the capacity of a process unit or adding a new unit. If it is economically warranted, the model will calculate a daily capital charge for this type of change to the base refinery.
- Since product consumption data was not available specifically for PADD II, data for determining the product slate for the refinery model was based on a DOE Energy Information Administration report<sup>1</sup>.
- Gasoline fuel specifications were based on the 1990 Clean Air Act Amendment (CAAA) Phase II requirements. Both reformulated and conventional gasolines are produced. The EPA Complex Model is used to estimate emissions from gasoline fuels.
- Specifications for diesel fuels were based on estimates of future fuel requirements (higher cetane number, etc.)

After the model was established for an all-petroleum feed, the model was adapted to incorporate pilot plant data from **Report 2**. Separate submodels were added to the model to handle each of the direct liquids.

A detailed description of the development of the LP Model and the method for determining the value/price of the products and the alternatives crudes is given in **Report 2**, Section 4, **Report 3** and **Report 4**. The key point that should be noted is that these prices reflect the capital costs of processing in the Case 2 - Expansion Allowed scenario.

In all of these scenarios, the method for determining the value of the direct coal liquids was basically the same. The LP model was initially run with petroleum crude only to determine the objective function. In simple terms, the objective function is the daily profit for the refinery and is defined as follows:

$$\text{Objective Function} = \text{Revenues} - \text{Purchases} - \text{Utilities} - \text{Capital charges}$$

The PIMS LP Model maximizes the objective function based on the constraints placed on the model (e.g. feed qualities, unit capacities, process yields, fuel specifications, product slate, etc.)

Once the objective function is established for the petroleum feed, one of the direct coal liquids is “forced” into the model at a given rate and at zero value and is used to replace a portion of the petroleum crude. Since the coal liquid initially has a zero value, the “Purchases” component of the objective function decreases and the overall objective function increases. The increase in the objective function divided by the amount of coal liquid forced into the model is the value of the coal liquid at that feed rate. The difference between the value of the coal liquid and the

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<sup>1</sup> “Supplement to the Annual Energy Outlook 1995”, Department of Energy/Energy Information Agency, February, 1995, DOE/EIA-0554(95)

petroleum crude is the amount of money that a refiner would be willing to pay above the cost of the petroleum crude

## **2.2.2 Engine Emissions Using Fuels Containing Direct Coal Liquids**

Engine emissions tests were performed on potential coal derived products from direct hydrogenation. This work is described in **Reports 6A** and **6B**. Results showed that coal hydrogenation liquids can be incorporated into the refinery mix without significantly changing emissions characteristics of the fuels produced.

LP modelling of a 150,000 BPSD PADD II refinery with direct liquids addition, without unit expansion, showed how much direct liquid could replace a portion of the standard petroleum crude while still meeting a fixed product slate and meeting specifications. Results were similar for the two direct liquids with the final refinery feed composition being about 50.5% PADD II crude mix, 37.2% coal liquid and 12.5% MTBE plus butanes. The gasoline, diesel and jet fuel blends thus all contained significant quantities of coal derived material. Except for one diesel blend containing untreated DL-1 distillate, the emissions testing was done entirely on products derived from the second direct liquid (DL-2), since it met light and heavy distillate specifications without further hydrotreating. This was in agreement with the recommendations of the Basic Program, which indicated that it was better to use a third stage hydrotreater in the coal hydrogenation plant to treat the whole liquid rather than running separate hydrotreating steps in the refinery.

## **Fuel Preparation**

Gasoline, diesel and jet fuel blends meeting ASTM specifications were prepared from the products of four pilot plant production runs, which included:

- (1) Naphtha hydrotreating/catalytic reforming of a 52/48 vol.% blend of heavy virgin naphtha and DL-2 medium naphtha. Hydrotreating conditions were 557 °F, 800 psig, 1.84 LHSV, 2200 SCFB. Reforming conditions were 875 °F, 500 psig 2.0 LHSV and 1920 SCFB. Product octane number was 90.4 RON and 81.1 MON.
- (2) Straight run light distillate hydrotreating at 560 °F, 500 psig, 1.46 LHSV.
- (3) Heavy distillate hydrotreating of a 63.5/36.5 vol.% blend of virgin gas oil and light coker gas oil at 650 °F, 750 psig, 1.43 LHSV and 3100 SCFB (avg of 2 runs.)
- (4) Fluid catalytic cracking of a blend of 57.4/42.6 vol.% heavy virgin gas oil and DL-2 heavy distillate. Conditions were 983.5 °F avg riser temperature, 35 psig riser outlet, 10.5 catalyst/oil ratio, 76 wt.% conversion.

Other production runs were made during Basic Program phase of the study. The test data for all production runs are given in Reports 6A and 6B, and results from many of these tests have been incorporated into the correlation work discussed above in Section 2.1.

## Product Blending

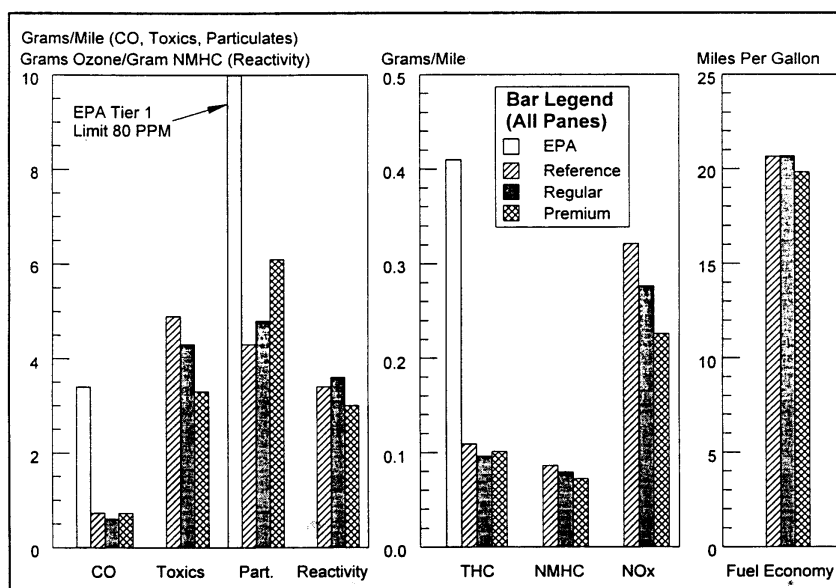
The following slate of emission testing fuels were used:

- Highway Diesel (42.8 cetane number) containing 15.9 vol.% of unhydrotreated DL-2 light distillate.
- Highway Diesel (42.5 cetane number) containing 16.0 vol.% of unhydrotreated DL-1 light distillate.
- Off-Road Diesel (41.1 cetane number) containing 7.1 vol.% of unhydrotreated DL-2 light distillate and 15.5 vol.% of unhydrotreated DL-2 heavy distillate.
- Jet Fuel A (17.8 vol.% aromatics) containing 27.8 vol.% of unhydrotreated DL-2 light distillate
- Regular Gasoline (91.2 RON, 83.9 MON) containing 20.9 vol.% of Run (1) reformat and 26.6 vol.% of Run (4) FCC depentanizer bottoms.
- Reformulated Premium Gasoline (94 RON, 87.9 MON) containing 4.1 vol.% of Run (1) reformat and 23.2 vol.% of Run (4) FCC depentanizer bottoms.

Detailed compositions and inspections are given in **Report 6**, Section 6 Tables 6-1 through 6-12. Reference fuels used for comparison are listed in Table 6-13.

## Emissions Testing

Gasoline testing was done in a 1997 Buick LeSabre with a 3.8L V-6 engine and an automatic transmission, which showed 21614 odometer miles at the start of testing. The principle results are given in Figure 7.2 of **Report 6** (reproduced below.) Taken as a whole these results indicate that the partially coal-derived gasolines compare favorably with the reference fuels in terms of grams/mile emissions of CO, toxics, THC, NMHC and NO<sub>x</sub> but are slightly higher in particulates. Results are well within EPA standards.



**Figure 7-2 Coal and Petroleum Derived Gasoline Exhaust Emissions Comparison**  
(Axis Titles at Top)

Jet fuels were tested in a combustor rig based on hardware from an Allison T63 gas turbine engine, a small helicopter engine. Summarized results at idle and full load are given in Table 8-7 of **Report 6** (reproduced below.) Comparisons of CO, HC and smoke emissions and liner temperature are virtually identical. If anything, NO<sub>x</sub> emissions are lower than for the reference fuel. The conclusion is that the jet fuel derived from direct liquid DL-2 has the same combustion characteristics as standard jet fuel. Other properties such as lubricity and thermal stability would have to be evaluated for a more detailed comparison.

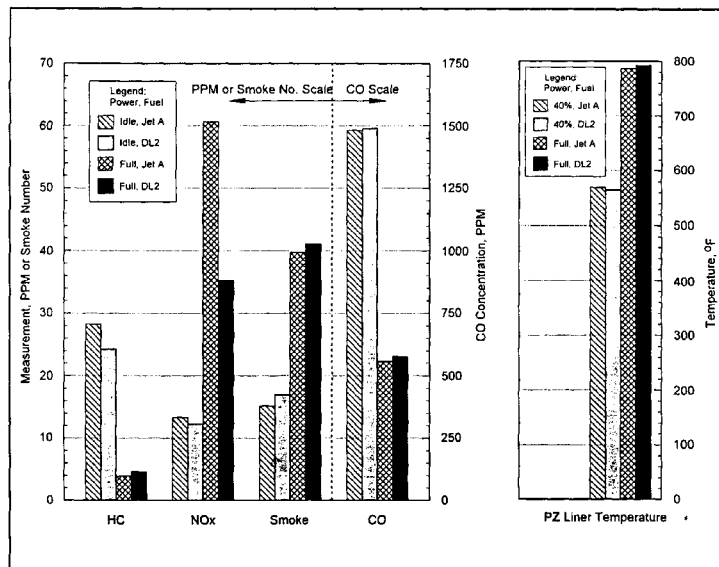


Figure 8-7 Summary Combustion Characterizations of DL2 Jet Fuel

Diesel fuels were tested in Caterpillar 3176 engine using exhaust gas recirculation. This engine is believed to provide an excellent test bed for fuel sensitivity studies for the next generation of heavy-duty diesel engines. Test results for highway diesel are given in Table 9-4 and, for off-road diesel, in Table 9.5 of **Report 6**. Comparison with the reference fuels shows a virtual

Table 9-4 Weighted Highway Emissions Results

Emissions Rate [ g/(hp-hr) ]	Highway Fuels		
	Reference (sample deviation)	DL1 Test Fuel	DL2 Test Fuel
NO <sub>x</sub>	2.68 (± 0.0473)	2.64	* 2.63
CO	0.80 (± 0.0153)	0.79	* 0.76
HC	0.152 (± 0.0047)	0.156	0.149
Particulate	0.068 (± 0.0049)	* 0.061	* 0.063

\*Indicates a significant change (i.e. difference is greater than one standard deviation of the reference fuel results).

**Table 9-5 Weighted Emissions Results for Off-Road Fuels**

<b>Emissions Rate [ G/(Hp-hr) ]</b>	<b>Off-road Fuels</b>		
	<b>Reference</b>	<b>D12 Test Fuel</b>	<b>Change</b>
NO <sub>x</sub>	2.71	2.64	- 2.4%
CO	0.85	0.92	+ 5.0%
HC	0.169	0.178	+ 8.4%
Particulate	0.118	0.121	+ 2.4%

standoff in NO<sub>x</sub>, CO, HC and Particulate emissions, though SwRI has stated in a few cases that the differences are statistically significant.

### 3. Emissions Testing of Fischer-Tropsch Diesel

Indirect coal liquid would have completely different handling characteristics in a refinery than the direct liquids discussed in Section 2. Fischer-Tropsch naphtha would make a very poor cat reformer feed but an excellent feed to a naphtha cracker for producing ethylene. The distillates are very high quality and additional high quality distillate can be produced by hydrocracking the wax. Quite possibly, an excellent lube oil could be produced by hydroisomerization. The molecular weight distribution can be varied by changing operating conditions and catalysts and the licensors of Fischer-Tropsch technology have generally taken advantage of this to produce mainly a high quality middle distillate fraction which makes an excellent diesel fuel.

This study was designed to test the relative emissions characteristics of commercial grade indirect diesel fuels, not necessarily from coal but known to be similar, since the Fischer-Tropsch operating conditions can be made similar. The work is reported in two SwRI reports: (1) **Report 9** covers the Phase I screening study, comparing Fischer-Tropsch diesels against diesels from petroleum sources, using an EPA developed, transient emissions testing procedure. (2) **Report 10** covers Phases II and III, which looked at engine modifications to take advantage of the special properties of F-T diesel. Phase II examined the effect of timing retard on emissions and Phase III looked at the effect of adding aftertreatment to the engine exhaust, which is possible when running on F-T diesel.

Typical diesel cuts were obtained from three licensors of Fischer-Tropsch technology and these were tested in an advanced technology, heavy-duty diesel engine in comparison with a typical and an advanced-design petroleum refinery diesel fuel. The licensors requested anonymity so that all that can be disclosed are typical ASTM inspections. All three Fischer-Tropsch diesels were superior products, with cetane numbers above 74, and gave significant reductions in emissions as compared to the reference fuels. When full advantage was taken of the special properties of F-T diesel in Phase III, an order of magnitude reduction in particulates and hydrocarbon emissions was achieved, CO was cut by 80% and NO<sub>x</sub> by close to 50% as compared to a standard diesel fuel.

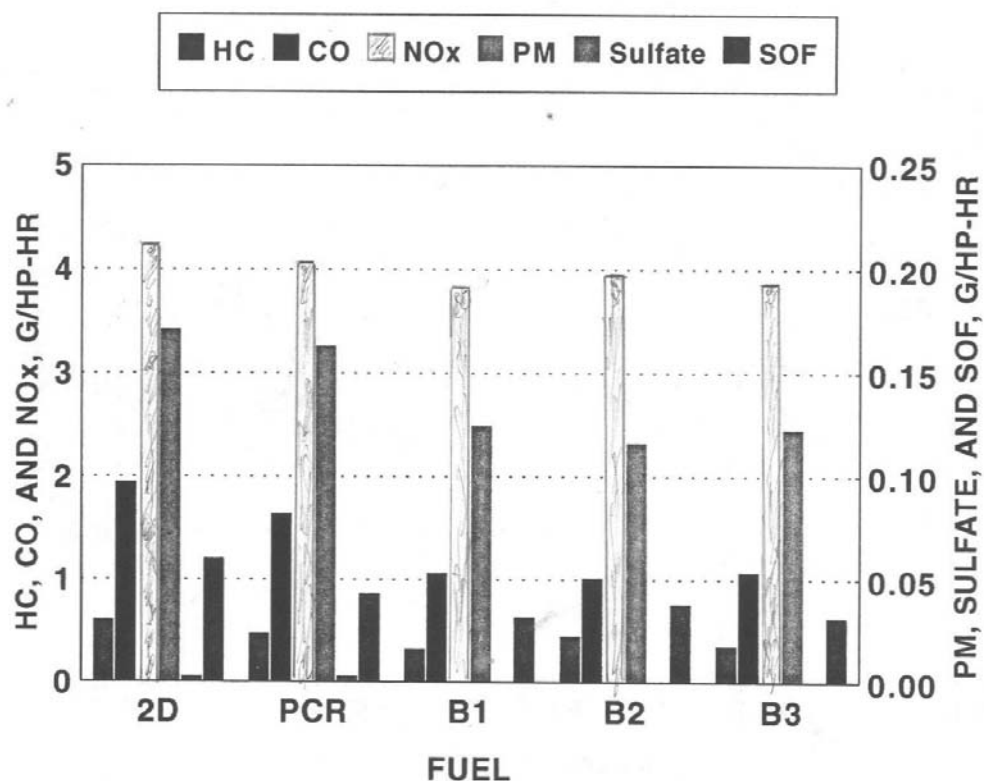
#### 3.1 Phase I – Screening

The screening test procedure used was a transient emissions measurement procedure developed by the EPA for emissions regulatory purposes. A prototype, 1991 Detroit Diesel Corporation Series 60 heavy-duty diesel engine was used. The procedure utilized several hot-start transient tests run in a specific sequence using five diesel fuels. The fuels included a low-sulfur-emissions, grade 2D reference fuel, identified as Fuel 2D; three F-T licensor-supplied diesel fuels identified as Fuels B1, B2 and B3; and a “pseudo” California reference fuel, designated Fuel PCR. Fuel properties were given in Report 9, Table A-4, reproduced below. Transient cycle emissions of HC, CO, NO<sub>x</sub>, total particulate (PM), sulfate, soluble organic fraction (SOF) of PM, and volatile organic fraction (VOF) of PM were obtained over repeat hot-start test.

Table A-4  
DIESEL SAMPLE ANALYSIS

<u>TEST</u>	<u>METHOD</u>	<u>2D</u>	<u>PCR</u>	B1	<u>B2</u>	<u>B3</u>
Distillation	D86					
IBP, °F		376	410	338	348	382
10%		438	446	427	394	448
50%		501	488	590	458	546
90%		587	556	646	536	620
EP%		651	652	672	562	640
Cetane No.	D613	45.5	50.2	>74.0	>74.0	74.0
Cetane Index	D976	47.5	46.7	80.5	72.9	77.2
	D4737			94.1	77.9	87.6
API@600F		36.0	36.6	49.1	52.5	49.1
Density B/ML@15°C				0.7832	0.7688	0.7830
Specific Gravity@60/60		0.8447	0.8419	0.7835	0.7690	0.7833
Cloud PT., °C	D2500	-16.6	-15.5	8	-23	-12
PourPT., °C	D97	-26		11	-20	-16
Viscosity@40°C,cSt	D445	2.75	2.79	3.85	1.58	2.66
Bocle Scuff, Grams				1850	1700	2300

Screening results are presented in **Report 9**, Figure 2, reproduced on the next page. Emissions in all categories are less for the three indirect F-T diesels than for either the standard or the “low emissions” California diesel fuel, both derived from petroleum. The results are in line with other work showing that emissions of CO, HC and PM decrease as the Cetane number of the diesel increases. According to these screening tests, Fischer-Tropsch diesel is a demonstrably superior product.



**FIGURE 2. AVERAGE HOT-START TRANSIENT EMISSIONS USING BECHTEL FUELS IN 1991 PROTOTYPE DDC SERIES 60 ENGINES**

### 3.2 Phase II and III Equipment Modifications

The engine used for Phases II was a 1993 model, 11.1 liter, DDC Series 60 heavy-duty diesel engine fitted with a DDEC II electronic control system. In Phase III, a passive, continuously regenerating trap aftertreatment device was added to the exhaust system. A new transient command cycle was generated for each configuration based on a torque map run.

The nine different engine configurations tested are presented in **Report 10**, Table 1, reproduced below. Type 2D diesel and one Fischer-Tropsch fuel were each evaluated at the engine's original "as received" injection timing, and with the timing modified to four, six, and eight degrees retard relative to the original factory timing. The ninth configuration consisted of using the Fischer-Tropsch fuel, with the engine's fuel injection timing set to eight degrees retard, and using the continuously regenerating trap (CRT) as an aftertreatment device. The aftertreatment device was not evaluated with the Type 2D fuel because the sulfur content in that fuel, although low, was too high to permit proper operation of the device

**TABLE 1. CONFIGURATIONS TESTED**

Fuel	Exhaust Aftertreatment <sup>a</sup>	Fuel Injection Timing Retard <sup>b</sup>			
		0°	4°	6°	8°
Type 2D Diesel	None	✓	✓	✓	✓
Fischer-Tropsch	None	✓	✓	✓	✓
Fischer-Tropsch	CRT	No Test	No Test	No Test	✓
Notes: <sup>a</sup> Aftertreatment device was a continuously regenerating trap developed by Johnson Matthey. <sup>b</sup> Timing changes were relative to the "as received" engine setting.					

Levels of NO<sub>x</sub> were reduced by increasing the amount of timing retard, but PM levels increased. Table 10, from **Report 10**, reproduced below, presents the cold-hot composite emission results for the four configurations tested over a cold- and hot-start testing sequence. In general, composite cold-hot emission levels, using the Type 2D fuel with injection at the original timing, were about 4.99 g/hp-hr for NO<sub>x</sub> and about 0.20 g/hp-hr for PM. By simply changing to Fuel FT, all composite emission levels dropped by approximately 25 percent. With Fuel FT and timing retarded by eight degrees, the NO<sub>x</sub> level was minimized, but HC, CO, and PM levels were substantially increased. The aftertreatment device was added to this configuration to compensate for the increased emissions, and the result was a slightly lower NO<sub>x</sub> level, and dramatically reduced HC, CO, and PM levels. The PM level was reduced an order of magnitude using the aftertreatment device, and it is believed that the small amount of particulate collected was largely sulfate salts being released from the catalyst, and sulfate-bound water.

Table 10  
SUMMARY OF COLD-HOT COMPOSITE EMISSIONS RESULTS USING  
A 1993 DDC SERIES 60 ENGINE IN SEVERAL CONFIGURATIONS\*

Timing Retard <sup>b,c</sup>	Exhaust Config. <sup>d</sup>	Fuel Type <sup>e</sup>	Transient Emissions, g/hp-hr <sup>a</sup>					BSFC, lb/hp-hr	Cycle Work, hp-hr	Ref. Work, hp-hr
			HC	CO	NO <sub>x</sub>	PM	CO <sub>2</sub>			
0°	Stock	2D	0.064	2.462	4.997	0.197	596	0.416	23.59	24.47
0°	Stock	FT	0.038	1.794	4.039	0.149	557	0.393	22.26	23.16
8°	Stock	FT	0.083	2.014	2.860	0.166	643	0.450	20.76	22.94
8°	Cat-Trap	FT	0.000	0.494	2.763	0.022	629	0.443	21.09	22.94

<sup>a</sup> Composite is computed by adding one-seventh (1/7) cold-start value to six-sevenths (6/7) hot-start value.  
<sup>b</sup> Fuel injection timing denoted as 0° was the engine setting at which the engine was received for testing.  
<sup>c</sup> Injection timing denoted as 8° retard was relative to the "as received" setting.  
<sup>d</sup> The "Cat-Trap" exhaust aftertreatment device was an oxidizing catalyst and particulate trap.  
<sup>e</sup> Fuel FT was Fischer-Tropsch designated by SwRI as EM-2257-F.

#### 4. Biomass Gasification F-T Modeling

This was a self-contained add-on study in which Bechtel employed the Coal Gasification and Fischer-Tropsch Liquefaction ASPEN Model to develop a similar type of modeling capacity using biomass as the feed. This study was done to support the research and development program of the National Renewable Energy Laboratory (NREL) in the thermochemical conversion of biomass to liquid transportation fuels. The original ASPEN Model was developed under the Baseline Design/Economics for Advanced Fischer-Tropsch Technology study of DOE Contract DE-AC-91PC90027.

The ASPEN Model was developed for a Battelle biomass-based gasification process, of which the design detail was an extension of the work developed by Mitretek for the Battelle biomass gasification plant in 1996. The Mitretek study investigated the use of two biomass gasifiers; the RENGAS gasifier being developed by the Institute of Gas Technology, and the indirectly heated gasifier being developed by Battelle Columbus. The Battelle Memorial Institute of Columbus, Ohio indirectly heated biomass gasifier was selected for this model development because the syngas produced by it is better suited for Fischer-Tropsch synthesis with an iron-based catalyst for which a large amount of experimental data are available.

The development of Aspen model for a Battelle-based gasification, Fischer-Tropsch (F-T) liquefaction and combined-cycle power plant is described in **Report 11** titled “*ASPEN Process Flowsheet Simulation Model of a Battelle Biomass-Based Gasification, F-T Liquefaction and Combined Cycle Power Plant*”.

The Biomass Gasification Model was developed in the same spirit as the original model. It is intended to be a research guidance tool, and not for detailed process design. However, it does contain some unique process design features, such as sizing of F-T slurry bed reactor, whereby the effects of varying some process and operating conditions on the overall plant heat and material balances can be predicted. It also predicts the effect of operations on the capital cost and operating labor requirements.

## 5. Updated Gas-to-Liquids Baseline Design/Economic Study

### Background

In 1995, Nexant (successor to Bechtel Technology and Consulting Company) developed, on behalf of DOE under Contract DE-AC22-91PC90027, a *Baseline Design for Natural Gas Conversion* using advanced Fischer-Tropsch (F-T) technology to produce high-quality, ultra clean, transportation fuels. This 1995 study has assisted DOE in providing direction for its research and development, focusing on technologies that have the largest impact on the overall gas conversion economics.

The 1995 Baseline study uses natural gas (i.e., 95% C<sub>1</sub>) as the feed, and the design was intentionally conservative, using a combination of commercially proven technologies of non-catalytic partial oxidation (POX) and steam methane reforming (SMR) for syngas generation. F-T plant design was based on the 1991 cobalt catalyst performance data of Satterfield. A total of 24 slurry-bed reactors were used for F-T synthesis producing 45,000 barrels per day (BPD) of FT liquids, at a total estimated plant cost of 1.8 billion U. S. dollars. It concluded that in order for the F-T gas conversion process to be economical, a low-cost (e.g., \$0.50 per million Btu) gas has to be used as the feedstock. Even then, the gas feed cost accounts for over 22% of the total cost of F-T production.

A follow-up study showed that power co-production can reduce the FT plant cost at the expense of a small sacrifice in overall thermal efficiency. The plant also uses 95% C<sub>1</sub> natural gas as the feed, but was designed for a smaller (10,000 BPD) capacity. Syngas generation was based on enriched-air blown autothermal reforming technology. Despite the loss of economies of scale, gas conversion economics can be improved via power co-production providing there is a demand for the co-produced electricity.

### The Updated GTL Design/Economics Study

The updated study is designed for a natural gas feed containing 13% CO<sub>2</sub>. This composition is more representative of a low-cost associated (or sub-quality and/or flared) gas feedstock. In addition, the design incorporates the latest FT synthesis performance, and slurry-bed reactor design and size. The FT product upgrading section also has been simplified to include only wax hydrocracking, thereby producing an upgraded FT diesel and a raw FT naphtha as the main products. This resulted in a significant reduction in the overall plant cost. Detail of this work was described in **Report 12** which forms the basis of a peer-reviewed technical paper entitled “Design/Economics of an Associated Gas (or Sub-Quality Gas) Fischer-Tropsch Plant” presented at the 6<sup>th</sup> Natural Gas Conversion Symposium, June 17-22, 2001, at Girdwood, Alaska. The paper was published in a Conference Proceedings by Elsevier Science.

## **6. Updated The Rentech FT Liquids**

Rentech has produced Fischer-Tropsch (FT) liquids and wax from their Bubble Column Reactor pilot plant at Denver, Colorado. Through a competitive bidding process, PARC of Pittsburgh, PA was selected to upgrade the FT liquids and wax. The properties of the different fractions of the upgraded FT liquids were analyzed according to the standard procedures employed for conventional petroleum products. These data will be used in the LP Models developed for other DOE Liquid Fuels programs.

## APPENDIX A

### KEY PROJECT REPORTS

This appendix lists a series of key project reports, collectively, document most, if not all of the significant technical information that were prepared during the course of this DOE contract, DE-AC22-93PC91029. Quarterly reports that were issued for the project also document these information but only included the technical progress of the study to that point. Monthly summary reports were prepared for the project, but they normally did not contain any significant technical information.

The list of these reports, cited also in INTRODUCTION section, are:

**Report 1** - The current volume.

**Report 2** - Refining and End Use Study of Coal Liquids Final Report – *Basic Program* (Topical Report issued March 1999 by Bechtel.)

**Report 3** - Refining and End Use Study of Coal Liquids Topical Report – *Petroleum Refinery Linear Programming Model Design Basis* (Topical Report issued March 1995 by Bechtel and discussed in **Report 2**, the *Basic Program Report*.)

**Report 4** - Refining and End Use Study of Coal Liquids Topical Report – *Addendum to the Linear Programming Refinery Model Design Basis* (Topical Report issued October 1997 by Bechtel and discussed in **Report 2**, the *Basic Program Report*.)

**Report 5** - Refining and End Use Study of Coal Liquids Topical Report – *Option 1 Economic Evaluation* (Topical Report issued in July 1998 by Bechtel.)

**Reports 6 and 7** - Refining and End Use Study of Coal Liquids Final Report - *Option 1 Fuel Production and Engine Testing* (Final Report and Appendix issued in May 1999 by SwRI.) Production runs are correlated along with small scale test data in **Report 2**, the *Basic Program Report*.

**Report 8** - Refining and End Use Study of Coal Liquids Topical Report – *In-line Hydrotreater Simulation Study* (Topical Report issued in June 2001 by SwRI)

**Report 9** - *Engine Evaluation of Fischer-Tropsch Diesel, Phase I* (Final Report prepared for Bechtel by SwRI and issued in October 1995)

**Report 10**- *Heavy-Duty Transient Emissions at Various Engine Timings using Fischer-Tropsch Diesel* (Final Report prepared for Bechtel by SwRI and issued in April 1997)

**Report 11** - *ASPEN Process Flowsheet Simulation .Model of a Battelle Biomass-Based Gasification, F-T Liquefaction and Combined Cycle Power Plant* (Topical Report issued by Bechtel in May, 1998.)

**Report 12** - *Updated Baseline Design/Economics of Indirect Gas Conversion* (Topical Report issued by Nexant in December, 2000.)

A single volume of each of the above are attached and sent along with the current Final Report.

## APPENDIX B

### PUBLICATIONS AND PRESENTATION

Following is a list of conference publications and presentations that were prepared during the course of this DOE Contract.

- C. Lowe, J. Erwin and S. Moulton “Refining and End Use Study of Coal Liquids Test Fuel Production and Testing – Part I” Proceedings of Coal Liquefaction and Gas Conversion Contractors Review Conference, Sept. 7-8, 1994.
- C. Lowe, J. Erwin and S. Moulton “Refining and End Use Study of Coal Liquids Test Fuel Production and Testing – Part II” Proceedings of Coal Liquefaction and Gas Conversion Contractors Review Conference, Sept. 7-8, 1994.
- C. Lowe and S. Tam “Refining and End Use Study of Coal Liquids II – Linear Programming Analysis” Proceedings of Coal Liquefaction and Gas Conversion Contractors Review Conference, August 29-31, 1995.
- C. Lowe, A. Lee, S. Tam, J. Erwin and S. Moulton “Refining and End Use Study of Coal Liquids – Effect of Direct Coal Liquefaction Severity on Upgrading Operations” Joint Power and Fuel Systems Contractors Conference, 1996.
- C. Lowe and S. Tam “Refining and End Use Study of Coal Liquids” Proceedings of Coal Liquefaction and Gas Conversion Contractors Review Conference, August 29-31, 1995.
- G. Choi, A. Helgeson, A. Lee, S. Tam, V. Venkataraman and S. Rogers “Design/Economics of an Associated Gas (or Sub-Quality Gas) Fischer-Tropsch Plant” 6<sup>th</sup> Natural Gas Conversion Symposium, June 17-22, 2001 at Girdwood, Alaska.