Centimeter

Inches

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1 of 1
U.S. Department of Energy
Pittsburgh Energy Technology Center

Refining and End Use of Coal Liquids

Contract No. DE-AC22-93PC91029

Quarterly Report
January - March 1994

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Section 1

Introduction and Summary

This report is Bechtel's second quarterly technical progress report and covers the period of December 20, 1993 through March 27, 1994.

1.1 Introduction

Bechtel, with Southwest Research Institute, Amoco Oil R&D, and the M.W. Kellogg Co. as subcontractors, initiated a study on November 1, 1993, for the U.S. Department of Energy's (DOE's) Pittsburgh Energy Technology Center (PETC) to determine the most cost effective and suitable combination of existing petroleum refinery processes needed to make specification transportation fuels or blending stocks, from direct and indirect coal liquefaction product liquids. This 47-month study, with an approved budget of $4.4 million dollars, is being performed under DOE Contract Number DE-AC22-93PC91029.

A key objective is to determine the most desirable ways of integrating coal liquefaction liquids into existing petroleum refineries to produce transportation fuels meeting current and future, e.g. year 2000, Clean Air Act Amendment (CAAA) standards. An integral part of the above objectives is to test the fuels or blends produced and compare them with established ASTM fuels. The comparison will include engine tests to ascertain compliance of the fuels produced with CAAA and other applicable fuel quality and performance standards.

The final part of the project includes a detailed economic evaluation of the cost of processing the coal liquids to their optimum products. The cost analyses is for the incremental processing cost; in other words, the feed is priced at zero dollars.

The study reflects costs for operations using state of the art refinery technology; no capital costs for building new refineries is considered. Some modifications to the existing refinery may be required. Economy of scale dictates the minimum amount of feedstock that should be processed.

To enhance management of the study, the work has been divided into two parts, the Basic Program and Option 1.

The objectives of the Basic Program are to:

- Characterize the coal liquids
- Develop an optimized refinery configuration for processing indirect and direct coal liquids
- Develop a LP refinery model with the Process Industry Modeling System (PIMS) software.

The work has been divided into six tasks.
Section 1

Introduction and Summary

Task 1 - Development of a detailed project management plan for the Basic Program
Task 2 - Characterization of four coal liquid feeds supplied by DOE
Task 3 - Optimization of refinery processing configurations by linear programming
Task 4 - Pilot plant analysis of critical refinery process units to determine yield, product quality and cost assumptions. Petroleum cuts, neat coal liquids, and coal liquids/petroleum blends will be processed through the following process units: reforming, naphtha and distillate hydrotreating, catalytic cracking and hydrocracking.
Task 5 - Development of the project management plan for Option 1
Task 6 - Project management of the Basic Program and Option 1

The objectives of Option 1 are to:

• Confirm the validity of the optimization work of the Basic Program
• Produce large quantities of liquid transportation fuel blending stocks
• Conduct engine emission tests
• Determine the value and the processing costs of the coal liquids

This will be done by processing the coal liquids as determined by the optimization work, blending and characterizing the product liquids, and running engine emission tests of the blends. Option 1 has been divided into three tasks.

Task 1 - Based on the pilot plant and linear programming optimization work of the Basic Program, production runs of pilot plants (hydrotreating, reforming, catalytic cracking, and hydrocracking) will be conducted to produce sufficient quantities for blending and engine testing.
Task 2 - The pilot plant products will be blended, characterized, and engine tested
Task 3 - An economic analysis will be conducted to determine the costs of processing the coal liquids through the existing refinery

Table 1-1 shows which organization has the primary responsibility for each task.

1.2 Summary

The major efforts conducted during the first quarter of 1994 were in the areas of:

• Subcontract preparation and negotiation
• Linear programming modeling
Section 1

Introduction and Summary

- Project work plan development
- Pilot plant equipment preparation
Introduction and Summary

Table 1-1 Project Task Primary Responsibility Chart

<table>
<thead>
<tr>
<th>Task</th>
<th>Description</th>
<th>Bechtel</th>
<th>SwRI</th>
<th>Amoco</th>
<th>Kellogg</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>Project Management Plan (PMP) development</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Feed characterization</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Linear programming</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Pilot plant analysis -</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Cat cracking of DL liquids</td>
<td></td>
<td></td>
<td>x</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Cat cracking of indirect wax</td>
<td></td>
<td></td>
<td>x</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Hydrocracking of wax</td>
<td></td>
<td></td>
<td>x</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Fractionation, reforming, hydrotreating, etc.</td>
<td></td>
<td></td>
<td></td>
<td>x</td>
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<tr>
<td>5</td>
<td>Option 1 PMP development</td>
<td>x</td>
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<td></td>
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<td>6</td>
<td>Project management</td>
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<td>Option 1</td>
<td>Pilot plant production</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Task 1</td>
<td>Cat cracking of DL liquids and wax</td>
<td></td>
<td></td>
<td></td>
<td>x</td>
</tr>
<tr>
<td></td>
<td>All other production work</td>
<td></td>
<td></td>
<td></td>
<td>x</td>
</tr>
<tr>
<td>Option 1</td>
<td>Fuel blending, characterizing, engine testing</td>
<td></td>
<td></td>
<td></td>
<td>x</td>
</tr>
<tr>
<td>- Task 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Option 1</td>
<td>Economic analysis</td>
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<td></td>
<td></td>
<td>x</td>
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<tr>
<td>- Task 3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

x = key participant
Section 2

SwRI Activities

DL1 Sample Handling

The concerns for coal liquid storage include secure custody of this important liquid, controlled environment to accommodate the inherent chemical reactivity (instability), compilation of and access to a full description of the material, and disbursement of samples. These aspects of the DL1 sample handling are discussed below.

Direct Liquid 1 Sample (DL1) — The material chosen for use in the program was produced by HRI on days 42 through 55 of the Proof of Concept Run Number 1 (POC-1). The product was collected in two compartments of a stainless steel tank trailer and shipped under nitrogen to exclude oxygen of the air. The liquid in the first and second compartments were typical of production during the run, while the third compartment represented a less severe mode of operation.

Sample Storage — Coal liquids can change composition in storage because free radicals remaining from the production process continue to be reactive. Once free radicals present in the coal liquid react with oxygen, polymerization reactions proceed which result in the formation of large molecules. These molecules combine to form precipitates, which come out of solution in storage or when the liquid passes through flow systems. Most such molecules are destroyed or converted during subsequent processing, in effect "resetting" the clock for each new product of processing. This propensity to react and from precipitates is called instability and special storage measures are required to minimize its effects.

Provisions to reduce the reactions of instability include:

- Exclusive oxygen
- Minimize storage temperature
- Eliminate catalytic metals.

The tanks selected for storing the liquids are U.S. DOE Alternative Fuel Center tanks 50A and 50B, each 5000 gallons capacity. They are carbon steel construction without brass or copper anywhere in the piping system. They are shaded from direct sunlight by a canopy designed to prevent solar heat gain and thereby minimize daily temperatures. The tanks have vacuum and pressure vents for ullage pressure control and a nitrogen purge regulator to supply inert gas when required for diurnal pressures changes or "breathing". These measures are taken to minimize oxygen contact with the samples.

The tank truck from HRI arrived March 15, 1994, with the two DL1 products. Compartments 1 and 2 contained product from POC-1 production run and these materials were composited in T50A. Compartment 3 product was from later in POC-1 than the product in compartments 1 or 2 and was stored in T50B. Both tanks were inerted and have nitrogen blanketing in operation. The identification numbers and preliminary analyses are presented in Table 2-1. No losses were reported upon delivery and after the
SwRI Activities

Effluent connections of the tanks were secured, a measurement of the tank contents showed 1800 gallons each.

DL1 Composition — A full suite of analyses required for input to PIMS is in progress and will be added to the collection of data for DL1. The samples for these tests were separated by boiling ranges specified in the model via vacuum distillation. The volumes for the various samples were determined as shown in Figure 2-1.

The preliminary DL1 (FL-2219) was used to evaluate the method for phenolics measurement. A determination for the whole sample showed 1.43% phenols and 0.004% thiophenols by mass. Another portion was distilled before measuring phenolics. The results are shown in Table 2-2.

DL1 Sample Disbursements — The sample requests awaiting fulfillment include:

<table>
<thead>
<tr>
<th>Requestor</th>
<th>Contact</th>
<th>Volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>PETC</td>
<td>R.G. Lett</td>
<td>2 @ 30 gals</td>
</tr>
<tr>
<td>University of Kentucky</td>
<td>B.H. Davis</td>
<td>TBD*</td>
</tr>
<tr>
<td>Sandia</td>
<td>F. Stohl</td>
<td>TBD</td>
</tr>
<tr>
<td>Consol R &amp; D</td>
<td>R. Winschel</td>
<td>6 gals</td>
</tr>
</tbody>
</table>

* To be determined

An MSDS was prepared to accompany the containers for these shipments. It appears in Exhibit 1.

FUTURE PRODUCT SLATE SPECIFICATIONS

The Clean Air Act (CAA) amendments of 1990 created a challenge for the refining industry to produce environmentally cleaner transportation fuel. Improvements have already been realized in the CO nonattainment areas. The mandated use of weight 2.7% minimum oxygen has reduced the number of high CO "exceedences". Also, mandated vapor pressure reduction has improved the ambient hydrocarbon levels.

Future increased use of oxygenates will help replace high octane aromatics. The increased use of oxygenates will free up reactive C5 olefins for conversion to ether, and the other C5 olefins may become economically attractive alkylation feedstocks. California, with its more stringent specifications for transportation fuels, may set the standard which the entire U.S. will use as a pattern. It is with these trends in mind, that the following specifications were developed for the slate of PADD-II transportation fuels.
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in the study. The specifications described here are intended to apply to the 2000 – 2015 time frame.

The structure of the tables of specifications and the paragraphs which describe the line items in the tables is a summary of information from Southwest Research Institute, Bechtel's PIMS library, and Amoco. The regulations and trends described in the paragraphs were collected and presented in the first column, while the second column gives the values for reformulated fuel in use by the PIMS model. Amoco maintains watch over the requirements and conditions for its refineries and recommends the values in the last column for future reformulated fuel. These are the best projections available now and will be updated as more information and improved understanding are available.

GASOLINE

The factors influencing gasoline composition and specification are the most complex of the products in the End Use Study. Table 2-3 presents the key properties to be controlled to meet future performance and environmental constraints. The following paragraphs discuss each property as it is considered for its future levels in the gasoline specification.

RVP — The basic concern with Reid Vapor Pressure (RVP) is evaporative emissions from gasoline, which contribute to ozone formation principally in the summer. RVP has a large impact on evaporative emissions. The removal of lead from gasoline resulted in changes in the properties of gasoline, one of which was increased RVP. The EPA volatility requirements for gasoline require gasoline sold May 1 through September 15 cannot be above 9.0 psi.\(^1\) For ozone nonattainment areas, the RVP maximum is 7.8 psi.\(^1\) The butanes normally used to control vapor pressure of gasoline have been severely reduced. Further reductions in the vapor pressure could impact the utilization of the C\(_3\) hydrocarbons. The California Phase 2 regulations require a 7.0 psi maximum summer RVP.\(^2\) The EPA simple model sets the RVP at 7.2 psi.\(^3\) Wintertime RVP is important for cold start and driveability and will remain at prevailing values.

Sulfur — Reducing sulfur reduces gasoline tailpipe hydrocarbon emissions. The catalyst in the automobiles' catalytic converter is temporarily poisoned by sulfur. Reducing/removing sulfur increases the activity of the converter, thereby reducing emissions. The California Phase 2 regulations limit sulfur to 40 ppm maximum.\(^2\) The EPA simple model caps the sulfur concentration in gasoline at the refiners' 1990 average gasoline sulfur concentration. The 1990 industry average gasoline sulfur content is reported at 338 ppm.\(^4\)

Benzene — Benzene, classified as a carcinogen, is undesirable from the standpoint of human health. The EPA simple model and California Phase 2 gasoline limit the benzene concentration to 1.0 volume percent.\(^2\)\(^3\) Reduction in the benzene content of gasoline has a significant impact on the toxic emissions.
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Oxygenates — Use of oxygenates is mandated. The EPA simple model requires a minimum oxygen content of 2.0 weight %. \(^{(3)}\) The California Phase 2 gasoline requires 1.8-2.2 weight % oxygen. \(^{(2)}\) The winter gasoline program requires the use of 2.7 weight % oxygen minimum for 39 carbon monoxide nonattainment areas. Use of high octane aromatics has been reduced through the use of oxygenates.

Aromatics — The mandated elimination of lead resulted in increased reformate quantity. The increased reformer severity resulted in additional aromatics. Increased use of oxygenates dilute in part the aromatic content of gasoline. Not all aromatics are bad. Benzene with its low vapor pressure, high octane, and low photochemical reactivity is being reduced for human health reasons. The heavier aromatics have greater reactivity and are more difficult to combust, directionally increasing tailpipe hydrocarbon emissions. California Phase 2 regulations limit aromatics to 25 volume % maximum. \(^{(2)}\)

Olefins — The C\(_5\) olefins have been considered major contributors to ground level ozone formation. The heavier olefins present in the back end of fluid catalytic cracking unit gasoline will be reduced by lowering the distillation 50% and 90% points of finished gasoline. California Phase 2 gasoline limits olefins to 6 volume % maximum. \(^{(2)}\) The EPA simple model caps the olefins at the 1990 average. \(^{(3)}\) The 1990 industry average olefin content is reported at 9.2 and 11.9 volume % for summer and winter, respectively. \(^{(4)}\)

Distillation — Reducing the T50 and T90 temperatures reduces hydrocarbon and air toxics emissions. The California Phase 2 regulations specify a T50 of 210°F maximum and T90 of 300°F maximum. \(^{(2)}\) The EPA simple model caps the T90 at the 1990 average. The 1990 industry average gasoline is reported at 330°F. \(^{(4)}\)

**DIESEL**

Considerable research has shown that sulfur content, aromatic level, and cetane number can have a significant impact on exhaust emissions. Table 2-4 lists the key properties to be controlled for diesel fuel. The following paragraphs discuss the properties.

Aromatics — Aromatics are the primary environmental issue because they can lead to the emission of particulates, unburned hydrocarbons, and nitrogen oxides in the exhaust. EPA regulations as of October 1, 1993 require a 500 ppm sulfur maximum with a 40 minimum cetane index or 35 volume % aromatics. \(^{(5)}\) California regulations are more stringent. Effective October 1, 1993, diesel fuel aromatics are set at 10 volume % maximum with 500 ppm sulfur maximum. \(^{(6)}\) An alternative emission fuel is acceptable if the emissions from a specified engine are less than a specified reference fuel. Several
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diesel fuels have been certified with aromatic contents ranging from 19 to 25 volume %. (7X8X9X10)

Cetane Number — As the aromatic content is reduced, cetane number increases. California reference fuel used for the alternative emissions process specifies a 48 natural cetane number. Fuels that have been certified reported cetane numbers of 55-59. (7X8X9X10) EPA requirements for diesel fuel is a minimum 40 cetane index.

Sulfur — The maximum sulfur permitted in diesel fuel is 500 ppm. Fuels that have been certified in California have reported sulfur contents of 33 to 196 ppm. (7X8X9X10) Reduced sulfur would directly reduce the soluble portion of particulate emissions.

JET FUEL

Processing changes required to meet the reformulated gasoline and diesel performance and environmental constrains may impact the jet fuel quality. Table 2-5 lists the key properties for jet fuel. The following paragraphs discuss the properties.

Sulfur — The current sulfur limit for Jet A and JP8 is 3000 ppm maximum, and no change is anticipated.

Aromatics — Of the major hydrocarbons types, aromatics have the poorest combustion performance. Additionally, the excellent solvency of aromatics may affect the fuel system elastomers. Current specifications for Jet A and JP8 aromatic content are 20 and 25 volume % maximum, respectively. (11X12) The appropriate limit should be applied to each grade of jet fuel produced.

Freezing Point — The freezing point of jet fuel must be below the coldest temperature reached within the fuel system. The current specification for freezing point of Jet A is -40°C, while JP8 requires -47°C. (11) The appropriate limit should be applied to each grade of jet fuel produced.

References


(2) Proposed CARB Phase 2, Reformulated Gasoline Regulations, Title 13, California Code of Regulations, August 24, 1992.

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(5) ASTM D975-92a, "Standard Specifications for Diesel Fuel Oils".


### TABLE 2-1. ANALYSIS OF DL1

<table>
<thead>
<tr>
<th>Test</th>
<th>Method</th>
<th>Compartments 1&amp;2 in T50A</th>
<th>Compartments 3 in T50B</th>
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<tr>
<td>Sample ID No.</td>
<td></td>
<td>FL-2236</td>
<td>FL-2237</td>
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<tr>
<td>Specific Gravity</td>
<td>D1298</td>
<td>0.8628</td>
<td>0.8681</td>
</tr>
<tr>
<td>Distillation, °F</td>
<td>D86</td>
<td></td>
<td></td>
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<tr>
<td>IBP/5 Vol%</td>
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<td>141/194</td>
<td>138/184</td>
</tr>
<tr>
<td>10/20</td>
<td></td>
<td>223/282</td>
<td>218/277</td>
</tr>
<tr>
<td>30/40</td>
<td></td>
<td>348/410</td>
<td>336/391</td>
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<tr>
<td>50</td>
<td></td>
<td>462</td>
<td>441</td>
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<td>60/70</td>
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<td>502/534</td>
<td>483/522</td>
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<td>80/90</td>
<td></td>
<td>566/603</td>
<td>558/599</td>
</tr>
<tr>
<td>95/EP</td>
<td></td>
<td>631/661</td>
<td>631/658</td>
</tr>
<tr>
<td>Sulfur</td>
<td>Antek</td>
<td>405</td>
<td>817</td>
</tr>
<tr>
<td>Nitrogen</td>
<td></td>
<td>529</td>
<td>891</td>
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<td>Viscosity, 40°C, cSt</td>
<td>D445</td>
<td>1.75</td>
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</table>

### TABLE 2-2. PHENOLIC DISTRIBUTION

<table>
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<tr>
<th>Range, °F</th>
<th>Volume %</th>
<th>Phenolics, M%</th>
<th>Thiophenols, M%</th>
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<tr>
<td>Whole sample</td>
<td>100</td>
<td>1.43</td>
<td>0.004</td>
</tr>
<tr>
<td>IBP - 350</td>
<td>30</td>
<td>1.35</td>
<td>0.004</td>
</tr>
<tr>
<td>350 - 450</td>
<td>10</td>
<td>3.18</td>
<td>0.016</td>
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<tr>
<td>450 - EP</td>
<td>60</td>
<td>1.54</td>
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### TABLE 2-3. FUTURE GASOLINE SPECIFICATION

<table>
<thead>
<tr>
<th>Parameter</th>
<th>SwRI&lt;sup&gt;(1)&lt;/sup&gt;</th>
<th>Bechtel&lt;sup&gt;(2)&lt;/sup&gt;</th>
<th>Amoco&lt;sup&gt;(3)&lt;/sup&gt;</th>
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<tr>
<td>Summer RVP, psi Max</td>
<td>6.0</td>
<td>9.75</td>
<td>10.5</td>
</tr>
<tr>
<td>Benzene, V% Max</td>
<td>1.0</td>
<td>1.0</td>
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</tr>
<tr>
<td>Aromatics, V% Max</td>
<td>20</td>
<td>25</td>
<td>21.3</td>
</tr>
<tr>
<td>Olefins, V% Max</td>
<td>6</td>
<td>10.8</td>
<td>11.5</td>
</tr>
<tr>
<td>T50 °F Max</td>
<td>210</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>T90 °F Max</td>
<td>300</td>
<td>300</td>
<td>-</td>
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<tr>
<td>Sulfur, ppmw Max</td>
<td>200</td>
<td>338</td>
<td>198</td>
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<tr>
<td>(R+M)/2</td>
<td>Market 87 - 92</td>
<td>87 - 92</td>
<td>-</td>
</tr>
<tr>
<td>Oxygen, Wt%</td>
<td>2.0 - 2.7</td>
<td>2.1 - 2.7</td>
<td>-</td>
</tr>
</tbody>
</table>

<sup>(1)</sup> Projection through 2015 by extrapolation from current trends and regulations.

<sup>(2)</sup> Letter from Cliff Lowe to J. Erwin, 2/24/94, current PIMS values.

<sup>(3)</sup> J.J. Nichols, Jr., Amoco, no date.
### TABLE 2-4. FUTURE DIESEL SPECIFICATION

<table>
<thead>
<tr>
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<tbody>
<tr>
<td></td>
<td>SwRI(1)</td>
</tr>
<tr>
<td>Aromatics, V% Max</td>
<td>30</td>
</tr>
<tr>
<td>Cetane No. Min</td>
<td>50</td>
</tr>
<tr>
<td>Sulfur, ppmw Max</td>
<td>500</td>
</tr>
<tr>
<td>Specific Gravity @ 60°F</td>
<td>0.816 - 0.876</td>
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<tr>
<td>Pour Point, °F Max</td>
<td>15.8</td>
</tr>
<tr>
<td>% Off @ 400°F Min</td>
<td>10</td>
</tr>
<tr>
<td>Flash Point, °F Min</td>
<td>125</td>
</tr>
</tbody>
</table>

(1) Projection through 2015 by extrapolation from current trends and regulations.
(2) Letter from Cliff Lowe to J. Erwin, 2/24/94, current PIMS values.
(3) J.J. Nichols, Jr., Amoco, no date.

### TABLE 2-5. FUTURE JET FUEL SPECIFICATION

<table>
<thead>
<tr>
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<tr>
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<td>SwRI(1)</td>
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<tr>
<td>Sulfur, ppmw Max</td>
<td>3000</td>
</tr>
<tr>
<td>Aromatics, V% Max</td>
<td>Jet A 20/JP8 25</td>
</tr>
<tr>
<td>T10 °F Max</td>
<td>400</td>
</tr>
<tr>
<td>T100 °F MAX</td>
<td>570</td>
</tr>
<tr>
<td>Freezing Point, °C Max</td>
<td>Jet A -40/JP8 -47</td>
</tr>
<tr>
<td>Specific Gravity @ 60°F</td>
<td>0.775 - 0.823</td>
</tr>
<tr>
<td>Smoke Point, mm Max</td>
<td>25</td>
</tr>
<tr>
<td>Flash Point, °F Min</td>
<td>100</td>
</tr>
</tbody>
</table>

(1) Projection through 2015 by extrapolation from current trends and regulations.
(2) Letter from Cliff Lowe to J. Erwin, 2/24/94, current PIMS values.
(3) J.J. Nichols, Jr., Amoco, no date.
Figure 2-1.

POC-1 T50A FL-2236
Comparison of D 88 Plot with TBP Calc'n
MATERIAL SAFETY DATA SHEET

COAL DISTILLATE, POC-1

A. IDENTIFICATION AND EMERGENCY INFORMATION

PRODUCT NAME
NSB (Typical) - (Direct Coal Liquid Distillate)

DOT PROPER SHIPPING NAME
Petroleum Distillate, No. 5

PRODUCT APPEARANCE AND ODOR
Dark amber liquid with strong coal tar odor

EMERGENCY TELEPHONE NUMBER
(713) 654-1701 Poison Control Center

B. COMPONENTS AND HAZARD INFORMATION

<table>
<thead>
<tr>
<th>Components</th>
<th>CAS Number</th>
<th>Approx. Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal Liquid</td>
<td>6474 1599</td>
<td>Bulk</td>
</tr>
</tbody>
</table>

HAZARDOUS MATERIALS IDENTIFICATION SYSTEM (HMIS)
Combustible Liquid/may contain hydrogen sulfide

NATIONAL FIRE PROTECTION ASSOCIATION (NFPA) - HAZARD IDENTIFICATION

<table>
<thead>
<tr>
<th>Health</th>
<th>Flammability</th>
<th>Reactivity</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

C. EMERGENCY AND FIRST AID PROCEDURES

EYE CONTACT
If splashed into the eyes, flush with clear water for 15 minutes or until irritation subsides. If irritation persists, call a physician.

SKIN CONTACT
In case of skin contact, remove any contaminated clothing and wash skin thoroughly with waterless handsoap and flush with water.

INHALATION
If overcome by vapor, remove from exposure and call a physician immediately. If breathing is irregular or has stopped, start resuscitation, administer oxygen, if available.

INGESTION
If ingested, DO NOT induce vomiting: call a physician immediately.

D. FIRE AND EXPLOSION HAZARD INFORMATION

Irritating vapors may form in fire situations. Flash Point <60°F, Flammable Limits N/D. May contain hydrogen sulfide gas.
Section 2

SwRI Activities

Flash Point (Minimum)
<60°F

HANDLING PRECAUTIONS
Keep product away from heat, sparks, pilot lights, static electricity, and open flame.

FLAMMABLE OR EXPLOSIVE LIMITS (Approx. Percent by Volume in Air)
Estimated values: Lower flammable limit _______ Upper flammable limit _______ Not determined

EXTINGUISHING MEDIA AND FIRE FIGHTING PROCEDURES
Water spray, dry chemical, foam or carbon dioxide.

Water or foam may cause frothing. Use water to cool fire-exposed containers. If a leak or spill has not ignited, use water spray to disperse the vapors and to provide protection for persons attempting to stop the leak.

DECOMPOSITION PRODUCTS UNDER FIRE CONDITIONS
Sulfur dioxide and various hydrocarbon gases.

"EMPTY" CONTAINER WARNING
"Empty containers retain residue (liquid and/or vapor) and can be dangerous. DO NOT PRESSURIZE, CUT, WELD, BRAZE, SOLDER, DRILL, GRIND OR EXPOSE SUCH CONTAINERS TO HEAT. FLAME, SPARKS OR OTHER SOURCES OF IGNITION: THEY MAY EXPLODE AND CAUSE INJURY OR DEATH. Do not attempt to clean since residue is difficult to remove. "Empty" drums should be completely drained, properly bunged and promptly returned to a drum reconditioner. All other containers should be disposed of in an environmentally safe manner and in accordance with governmental regulations. For work on tanks refer to Occupational Safety and Health Administration regulations, ANSI Z49.1, and other governmental and industrial references pertaining to cleaning, repairing, welding, or other contemplated operations.

E. HEALTH AND HAZARD INFORMATION
Combustible liquid.

VARIABILITY AMONG INDIVIDUALS
Health studies have shown that many petroleum hydrocarbon and synthetic lubricants pose potential human health risks which may vary from person to person. As a precaution, exposure to liquids, vapors, mists or fumes should be minimized. Coal liquids have been shown to have teratogenic activity in laboratory tests. Females of child bearing circumstance should use extreme caution.

EFFECTS OF OVEREXPOSURE (SIGNS AND SYMPTOMS OF EXPOSURE)
High vapor concentrations (greater than approximately 1000 ppm) are irritating to the eyes and the respiratory tract, may cause headaches and dizziness, are anesthetic, and may have other central nervous system effects.

NATURE OF HAZARD AND TOXICITY INFORMATION
Respiratory - MSHA approved positive pressure air supplied respirators if hydrogen sulfide level exceeds 20 ppm.

Ventilation - Adequate to meet permissible concentrations H₂S TLB/TWA 10.0 ppm, ceiling limit 20.0 ppm.

Protective Clothing - Gloves resistant to chemicals and petroleum distillates recommended.

Eyes - Chemical type safety glasses or goggles, face shield optional.
Section 2

SwRI Activities

F. PHYSICAL DATA

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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<tbody>
<tr>
<td>Boiling Point</td>
<td>176 to 705°F</td>
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<tr>
<td>Vapor Pressure</td>
<td>N/D</td>
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<tr>
<td>Solubility</td>
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<tr>
<td>Viscosity @ 122°F 30.0&quot;</td>
<td></td>
</tr>
<tr>
<td>Specific Gravity</td>
<td>0.8378</td>
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<tr>
<td>pH</td>
<td>N/D</td>
</tr>
<tr>
<td>Volatility</td>
<td>N/D</td>
</tr>
</tbody>
</table>

G. REACTIVITY

This product is stable and will not react violently with water. Hazardous polymerization will not occur. Compatible with other products. Avoid contact with strong oxidants such as liquid chlorine, concentrated oxygen, sodium hypochlorite or calcium hypochlorite.

H. SPILL OR LEAK PROCEDURES

**SPILL INFORMATION:** (800) 424-9300 [Chemtrec]

**STEPS TO BE TAKEN IN CASE MATERIAL IS RELEASED OR SPILLED**

Shut off and eliminate all ignition sources. Keep people away. Recover free product. Add sand, earth or other suitable absorbent to spill area. Minimize breathing vapors. Use self-contained breathing apparatus or supplied-air mask for large spills in confined area. Minimize skin contact. Ventilate confined spaces. Open all windows and doors. Keep product out of sewers and watercourses by diking or impounding. Advise authorities if product has entered or may enter sewers, watercourses, or extensive land areas.

Assure conformity with applicable governmental regulations. Continue to observe precautions for volatile, combustible vapors from absorbed material.

I. PROTECTION AND PRECAUTIONS
Section 2

SwRI Activities

VENTILATION
Adequate to meet permissible concentrations H₂S TLB/TWA 10.0 ppm, ceiling limit 20.0 ppm. Use only ventilation sufficient to prevent exceeding recommended exposure limit or buildup of explosive concentration of vapor in air. Use explosion-proof equipment. No smoking or open lights.

RESPIRATORY PROTECTION
Use MHSA approved positive pressure air supplied respirators if hydrogen sulfide level exceeds 20 ppm.

PROTECTIVE GLOVES
Use gloves resistant to chemicals and petroleum distillates recommended. Use chemical type safety splash goggles or face shield where eye contact may occur.

OTHER PROTECTIVE EQUIPMENT
Use chemical-resistant apron or other impervious clothing, if needed, to avoid contaminating regular clothing on which could result in prolonged or repeated skin contact.

WORK PRACTICES/ENGINEERING CONTROLS
Keep containers and storage containers closed when not in use. Do not store near heat, sparks, flame or strong oxidants. To prevent fire or explosion risks from static accumulation and discharge, effectively ground product transfer system in accordance with the National Fire Protection Association standard for petroleum products.

PERSONAL HYGIENE
Minimize breathing vapor or mist. Avoid prolonged or repeated contact with skin. Remove contaminated clothing: launder or dry-clean before reuse. Remove contaminated shoes and clean thoroughly after contact, wash well before breaks and meals, and at end of work period. Product is readily removed from skin by waterless hand cleaners followed by washing thoroughly with soap and water.

J. TRANSPORTATION INFORMATION
Transport, handle and store in accordance with OSHA Regulation 1910.106 and applicable DOT Regulations.

Store away from heat and open flame.

TRANSPORTATION INCIDENT INFORMATION
For further information relative to spills resulting from transportation incidents, refer to latest Department of Transportation Emergency Response Guidebook for Hazardous Materials Incidents, DOT P 5800.3

DOT IDENTIFICATION NUMBER
UN#1268

The information and recommendations contained herein are the best known at this time and belief, accurate and reliable as of the date issued. The MSDS does not warrant or guarantee their accuracy of reliability, and cannot be liable for any loss or damage arising out of the use thereof.

The information and recommendations are offered for the user's consideration and examination, and it is the user's responsibility to satisfy itself that they are suitable and complete for its particular use.

The Hazardous Materials Identification System (HMIS) and National Fire Protection Association (NFPA) ratings have been included in order to provide additional health and hazard classification information. The ratings recommended are based upon the criteria supplied by the developers of these rating system.

/asm 4/94
Section 3

Bechtel Activities

3.1 Linear Programming model - Task 3

The primary objective of Task 3 is to develop a linear programming model which will assist in determining the optimum refinery configuration for processing coal liquids.

3.1.0 Development work

The primary focus of the work was to develop a flexible refinery processing configuration for the PIMS linear programming model. Major accomplishments were:

1. A basic petroleum refinery model was developed by combining certain aspects of the following models:
   - The model from the Direct Liquid Baseline study
   - A model developed to meet California Air Resources Board specifications
   - A model developed to produce reformulated gasoline blends.

   In addition, a new version of the PIMS linear program is being used which will calculate road emissions based on the EPA Complex equation.

2. A telephone conference call was held between SwRI, Amoco, Burns and Roe, and Bechtel to discuss various aspects of the design basis for the model. The following topics were discussed:
   - Proximity of the coal liquefaction plant to the refinery
   - Refinery configuration/complexity
   - Crude slate and crude pricing
   - Product slate and specifications
   - Ethanol/ETBE usage

   Based on this meeting and subsequent discussions with the project participants, the following changes were made to the model.

   a. The C₄ isomerization and dehydrogenation and the BTX extraction plants were removed from the model. The second reformer ahead of the BTX extraction plant was also eliminated.

   b. Gasoline specifications were changed to the national statutory baseline values.

   c. A submodel was added to simulate an ETBE/TAEE plant.
Section 3

Bechtel Activities

d. The amount of reformulated gasoline was reduced from 70% to 40%. The amount of low sulfur diesel was reduced from 85% to 53%.

e. Recursion rows were added to provide the Conradson carbon content of the FCC feed. This may be used later to estimate the coke burnoff at different Conradson carbon feed contents.

f. The LCO hydrotreater was removed. The cat diesel can be hydrotreated in the distillate hydrotreater instead.

g. The vacuum gas oils were added to the hydrocracker feed.

h. The formula for asphalt was changed from a mixture of atmospheric resid and heavy distillate to a mixture of vacuum resid and heavy vacuum gas oil.
Amoco Activities

Amoco provided Bechtel with comments on the LP design basis sent to them on February 24. In addition to participating in the above meeting, they also provided subsequent consultation on a number of subjects.

During this reporting period, the hydrocracking pilot plant was retrofitted to handle the viscous FT wax. Test runs were made with the remaining FT wax from a previous FCC program.
Section 5

**M. W. Kellogg Activities**

There were no activities reported by M.W. Kellogg reported during this quarter.
Project Management

6.1 KICKOFF MEETING

The primary activity that took place during this period was the kickoff meeting at Southwest Research Institute in San Antonio, Texas on January 26-27, 1994. At this meeting various project participants spoke on past and ongoing activities and on their roles and plans for the project. The key areas that were discussed were:

- Direct coal liquids characterization efforts
- Direct coal liquids production at HRI
- Catalyst/wax separation efforts at SwRI
- PIMS linear programming model
- Pilot plant testing and production
- Engine testing
- Emission testing

Meeting minutes were submitted to DOE/PETC and approved.

6.2 Contracts

Subcontracts with SwRI, Amoco, and M.W. Kellogg were negotiated and signed.

6.3 Plans

The Project Work Plan for the Basic Program was approved and issued.

6.4 Reports and Schedules

The milestone schedule and status for the Basic Program and Option 1 is shown in Figure 6-1.
**Figure 6-1**

Milestone Schedule for Basic Program & Option 1

| 1. TITLE | Refining and End Use Study of Coal Liquids |
| 2. REPORTING PERIOD | 12/20/93 TO 3/27/94 |
| 3. IDENTIFICATION NUMBER | DE-RP22-93PC91029 |
| 4. PARTICIPANT NAME AND ADDRESS | Bechtel Corporation |
| | 50 Beale Street |
| | San Francisco, CA 94105 |
| 5. START DATE | 11/1/93 |
| 6. COMPLETION DATE | 9/30/97 |

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<th>7. ELEMENT CODE</th>
<th>8. REPORTING ELEMENT</th>
<th>93</th>
<th>FY 94</th>
<th>FY 95</th>
<th>FY 96</th>
<th>FY 97</th>
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<tr>
<td>Task 1</td>
<td>Project Work Plan</td>
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<tr>
<td>Task 2</td>
<td>Feed Characterization</td>
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<td>Task 4</td>
<td>Pilot Plant Analysis</td>
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<td>Option 1 Task 3</td>
<td>Economic Study</td>
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</table>

1. Submit final Project Work Plan
2. Characterize DL1 liquid
3. Characterize IL liquid
4. Characterize DL2 liquid
5. Develop LP model
6. Conduct final DL1 LP runs
7. Conduct final IL, LP runs
8. Conduct final DL2 runs
9. Conduct DL1 pilot plant tests
10. Conduct IL pilot plant tests
11. Conduct DL2 pilot plant tests
12. Production runs for DL1
13. Production runs for IL
14. Production runs for DL2
15. ASTM tests for DL1
16. ASTM tests for IL
17. ASTM tests for DL2

11. SIGNATURE OF PARTICIPANTS PROJECT MANAGER AND DATE

[Signature]

5/25/94
DATE
FILMED
9/14/94

END