TITLE: REFINING AND END USE STUDY OF COAL LIQUIDS II - LINEAR PROGRAMMING ANALYSIS

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1.0 Abstract

A DOE-funded study is underway to determine the optimum refinery processing schemes for producing transportation fuels that will meet CAAA regulations from direct and indirect coal liquids. The study consists of three major parts: pilot plant testing of critical upgrading processes, linear programming analysis of different processing schemes, and engine emission testing of final products.

Currently, fractions of a direct coal liquid produced from bituminous coal are being tested in sequence of pilot plant upgrading processes. This work is discussed in a separate paper.

The linear programming model, which is the subject of this paper, has been completed for the petroleum refinery and is being modified to handle coal liquids based on the pilot plant test results. Preliminary coal liquid evaluation studies indicate that, if a refinery expansion scenario is adopted, then the marginal value of the coal liquid (over the base petroleum crude) is $3-4/bbl.

2.0 Project Overview And Objective

Bechtel, with Southwest Research Institute, Amoco Corp., and the M.W. Kellogg Co. as subcontractors, began 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 petroleum refinery processes needed to make specification transportation fuels or blending stocks from direct and indirect coal liquefaction product liquids.

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 and beyond, Clean Air Act Amendment (CAAA) standards. An integral part of the above objective is to test the fuels produced and compare them with appropriate ASTM fuels. The comparison will include engine tests to ascertain compliance of the fuel slate with CAAA and other applicable fuel quality and performance standards.

Three types of coal liquids will be examined in this study: (1) direct coal liquids from a bituminous coal, (2) direct coal liquids from a sub-bituminous coal, and

(3) indirect coal liquids (Fischer-Tropsch). The two direct coal liquids were produced by hydrogenation in the HRI Proof-of-Concept (POC) pilot plant. The indirect coal liquids (distillate and wax portions) were produced in the DOE-AFPDU (Alternate Fuels Process Development Unit) at La Porte, Texas.

The final part of the project includes a detailed economic evaluation of the cost of processing the coal liquids to their optimum products. The study reflects costs for operations using state of the art refinery technology; no capital costs for building new refineries is considered. Some modifications or additions to the existing refinery may be included if they are economically justified. Economy of scale dictates the minimum amount of coal liquid 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.

BASIC PROGRAM

The objectives of the Basic Program are to:

- Characterize the coal liquids
- Develop an optimized refinery configuration for processing indirect and direct coal liquids
- Conduct pilot plant tests on the critical upgrading processes
- Develop a LP refinery model with the Process Industry Modeling System (PIMS) software.

The work has been divided into six tasks.

Task 1 - Development of a detailed project management plan for the Basic Program
Task 2 - Characterization of the three 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

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 and petroleum blends under the optimized conditions indicated by the results obtained in Task 4 , 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 value of processing the coal liquids through the existing refinery

3.0 Linear Programming Model

A model was developed using the Bechtel PIMS (Process Industry Modeling System) linear programming software to simulate a generic Midwest (PADD II) petroleum refinery of the future[1].

This "petroleum-only" version of the model aimed to establish the size and complexity of the refinery after the year 2000 and prior to the introduction of coal liquids. It should be noted that no assumption was made on when a plant will be built to produce coal liquids, except that it will be after the year 2000. The year 2000 was chosen because it is the latest year where fuel property and emission standards have been set by the Environmental Protection Agency. The model assumes the refinery has been modified to accept crudes that are heavier in gravity and higher in sulfur than today's average crude mix. In addition, the refinery has also been modified to produce a product slate of transportation fuels of the future (i.e. 40% reformulated gasolines with advance specifications). This model will in turn be used as a basis for determining the optimum scheme for processing coal liquids in a petroleum refinery.

3.1 Refinery Expansion Scenario

A refinery expansion scenario was chosen as the basis for evaluating the three coal liquids that are being examined in this study. The refinery expansion scenario is a reasonable assumption because:

- No grass roots refineries will be built in the future for economic and environmental reasons.

- As small or uneconomical refineries shutdown, larger and more complex refineries will be expanded to meet consumption.

- Coal liquids will have the highest value when credit is given for capital avoidance. In an expansion, the use of higher quality coal liquids will allow for lower capital expenditures.

The first step in developing this expansion scenario was to establish a base refinery configuration. This configuration, which is called Case 1, represents how the refinery would look prior to expansion.

The Case 1 refinery has the following characteristics:

- Nominal crude feed rate is 150,000 BPD .
- Crude is heavier and higher in sulfur than current average PADD II crudes.
- Unit capacities are adjusted from 1993 PADD II average capacities.
- All process units are running at capacity.
- Product slate and specifications are based on year 2000 estimates and the EPA Complex Model.

Case 2 or the expansion scenario, involves expanding the Case 1 refinery based on the following assumptions:

- Nominal feed rate is increased to 200,000 BPD by increasing product demand by 33.3% (over Case 1). The increase in feed consists of either additional crude or coal liquids.
- Process units are added or expanded as economically warranted. Capital costs are charged for expansion costs above Case 1 capacities.
- The product slate is the same as for Case 1.
- The crude feedstock is the same as for Case 1.

Figure 1 shows the differences between the two cases. Except as noted, the coal liquids will be evaluated under the Case 2 - expansion allowed scenario.

3.2 Initial coal liquid pilot plant data

The Direct Coal Liquid 1 (DL1) heavy distillate hydrotreating pilot plant tests conducted by SwRI provided treated samples produced under a number of different conditions. Three of these samples (treated under mild, medium and high severity conditions) and an untreated sample were sent to M.W. Kellogg for catalytic cracking tests. This section of the report describes how the results from the SwRI and Kellogg tests were used in the LP model to decide on the optimum processing sequence.

The procedure used was to take the raw test data and develop yields, consumptions, and product properties for hydrotreating and catalytic cracking the DL1 heavy distillate. These yields, consumptions, and properties were then entered into the LP model and the refinery operations were optimized.

Heavy Distillate Hydrotreating

Input to the model for the three samples that were sent to Kellogg was developed as follows:

- Hydrogen consumptions were estimated for the three samples based on hydrogen uptake and heteroatom removal.
- Volumetric yields were adjusted to achieve a weight balance for each condition.
- Distinct liquid product streams were created for each severity level.
- Capital costs and utilities (per barrel) were assumed to be the same for each severity level, thus giving an advantage to the high severity case.

Catalytic Cracking

Data for the model for the three treated and one untreated samples were developed as follows:

- Volumetric yields were calculated for the four coal liquids based on Kellogg weight based yield data.
- For each product cut range (naphtha, diesel, etc.) the properties were assumed to be the same regardless of the feed type.
- Fuel usage was adjusted based on coke yield for each feed type to achieve a heat balanced operation.

The results from the above work are summarized in the table below. It shows that, as expected, as hydrotreating severity increases, the hydrogen consumption and distillate yield increase, and the specific gravity decreases. The gasoline yields from catalytic cracking increase as the hydrogen content of the hydrotreater product increases.

Distillate Hydrotreating				
Severity		Low	Medium	High
Pressure, psig		700	1350	1800
Temperature, °F		653	687	730
LHSV		2.2	0.8	0.9
Hydrogen Consumption, SCF/bbl		212	286	565
Distillate yield, volume %		100.15	100.49	101.69
Product specific gravity		0.914	0.909	0.887
Catalytic Cracking				
Feed hydrotreating severity	Neat	Low	Medium	High
C5-430, volume % of feed	63.6	63.8	66.9	73.7
Fuel usage, MMBtu/bbl	0.200	0.200	0.203	0.264

Operating fuel usage is an adjustment to achieve a heat balanced yield.

3.3 Preliminary coal liquid evaluation studies

3.3.1 Distillate hydrotreating/catalytic cracking

A diagram showing the possible processing options for the DL1 heavy distillate is shown in Figure 2. This shows that the program is allowed to choose the most economical path for processing the heavy distillate. Each path has advantages and disadvantages.

1. Sending the neat heavy distillate to diesel/fuel oil blending avoids the capital and operating costs of hydrotreating and cat cracking, but the product has a lower value than gasoline. In addition, the neat liquid may not meet diesel specifications even after blending with higher quality material.

2. Hydrotreating the heavy distillate before sending it to blending may allow it to meet specifications, but there are significant costs and, again, the blended product has a low value.

3. Cat cracking the neat heavy distillate avoids the costs of hydrotreating and results in higher value gasoline blendstock, but the cat cracking yields are lower than the yields with hydrotreated feeds.

4. Cat cracking the hydrotreated heavy distillate is the most expensive option from a capital and operating standpoint. The higher gasoline yields, however, may compensate for these costs.

A run was made in which 50,000 bbl/day of DL1 were fed into refinery under the Case 2 - refinery expansion scenario. An analysis showed that 90 percent of the neat heavy distillate bypassed the distillate hydrotreater and was sent to the catalytic cracker (option 3 above). This is because the improved cat cracker yields from the hydrotreated feeds are not enough to compensate for the additional hydro-treating capital costs. Seven percent of the neat heavy distillate was sent directly to diesel blending. The remaining three percent was hydrotreated (at medium severity) and then blended into the diesel pool.

3.3.2 Feedstock value determination

In determining the value of different feedstocks such as coal liquids, it is important to understand the term *objective function*. *Objective function* is a linear programming term defined as follows:

Objective Function = Revenues - Purchases - Utilities - Capital charges

The linear program maximizes the objective function based on the constraints set by the model.

Using a method similar to the one used for the alternate crude feedstocks, the value of the coal liquids was determined by using the linear programming model. The first step was to run the model without any coal liquid feed. This was followed by forcing a given amount of the coal liquid into the model at zero value. The coal liquid value is the change in objective function divided by the amount of coal liquid feed. The end result is such that when this value for the coal liquid is used in the model , the objective function will be the same as for the zero coal liquid case.

3.3.3 Preliminary coal liquid value determination

Figure 3 shows the results of the coal liquid evaluation work. With the base petroleum crude set at $18/bbl, the DL1 coal liquid had a value varying from 21 to 22 $/bbl, depending on the amount of coal liquid fed into the refinery. Under closer inspection, this coal liquid margin of $3-4/bbl is due to a combination of capital avoidance and lower feedstock (crude, butanes, methanol, etc.) volumes.

The capital avoidance portion of the margin is distributed into a number of areas. In comparison with the Case 2 run with zero coal liquid, there is:

- Less cat cracking (less resid to process)
- Less alkylation (less olefins from cat cracking)
- Less kerosene/distillate treating (higher quality CL distillate allows bypassing)
- More naphtha HDT/reforming (more light material in CL)
- Less low value product

At 50,000 BPD of coal liquid, the $3.25/bbl margin over the base petroleum crude is broken down as follows:

	$/bbl	
Capital avoidance -	1.48	
Utility charge	(0.10)	
Additional feedstock avoidance	2.79	(less total feedstock is required with coal liquids)
Additional product	(0.92)	
Total	3.25	

Figure 4 shows the significance of capital avoidance. For the Case 2 - expansion allowed scenario, the daily capital charges are plotted versus increasing amounts of coal liquid. This shows that at zero coal liquid, the daily capital charges would be approximately $274,000. This falls steadily to $193,000 when 60,000 BPD of coal liquids are processed. This $81,000 savings is directly due to the characteristics of the DL1 coal liquid.

3.3.4 Expansion vs. no expansion allowed

The DL1 coal liquid was also evaluated under the Case 1 - no expansion scenario. Here, the coal liquid displaced a portion of the 150,000 BPD of crude. The results are shown in Figure 5. The coal liquid margin is significantly lower, 0.50 to 1.20

$/bbl. This is because the model is much more restricted in the number of ways it can process the coal liquid. In particular, there is no credit for capital avoidance.

3.3.5 Effect of new pilot plant data

Prior to the experimental work detailed in section 3.2, direct coal liquid yields, properties, etc. were estimated based on preliminary DL1 characterization work and yields and properties from previous coal liquid upgrading studies. These studies in turn were based on using coal liquid feedstocks from early liquefaction processes such as Solvent Refined Coal (SRC) and Exxon Donor Solvent (EDS). These liquids are significantly inferior in quality to DL1 and, thus, require more extensive upgrading than DL1 requires.

These yield and property estimates were used in the model and several runs were made to determine the coal liquid values at several feed rates.

Figure 6 compares the results from these LP runs to the results from the runs made with the new pilot plant data. The lower curve is the coal liquid values with the original estimates for yields, properties, etc. The upper curve is the values based on the new data. This shows that using the pilot plant data results in about a $1/bbl increase in coal liquid value. This increased value emphasizes the higher quality of DL1 over the coal liquids of earlier generations. In particular, DL1 does not require costly heavy distillate hydrotreating.

4.0 Summary

The linear programming model of a generic PADD II refinery was used to make preliminary evaluations of the DL1 coal liquid. The evaluations were made using the assumption that the coal liquids could fulfill the incremental feedstock requirements in a refinery expansion scenario. The results showed that:

- The DL1 coal liquid margin ranged from $3-4/bbl depending on the amount of coal liquid fed into the refinery. A significant portion of this margin is due to the avoidance of capital expenditures when coal liquids are used.
- In a case scenario where no expansion is allowed and all refinery process unit capacities are fixed, the margin falls to 0.5-1.2 $/bbl.
- Incorporation of the recent pilot plant test data into the model resulted in 1.0 $/bbl increase in the coal liquid margin over the value using literature data. This increase reflects the higher quality of the DL1 coal liquid over previous coal liquids.

5.0 References

1. "Petroleum Refinery Linear Programming Model Design Basis", DOE Contract No. DE-AC22-93PC91029, Topical Report, March, 1995.

6.0 Acknowledgments

Bechtel, along with the Southwest Research Institute, Amoco Corp. and the M.W. Kellogg Co., would like to express their appreciation to the Department of Energy for their financial support and technical assistance.

Figure 1 - Base and Expansion Scenarios

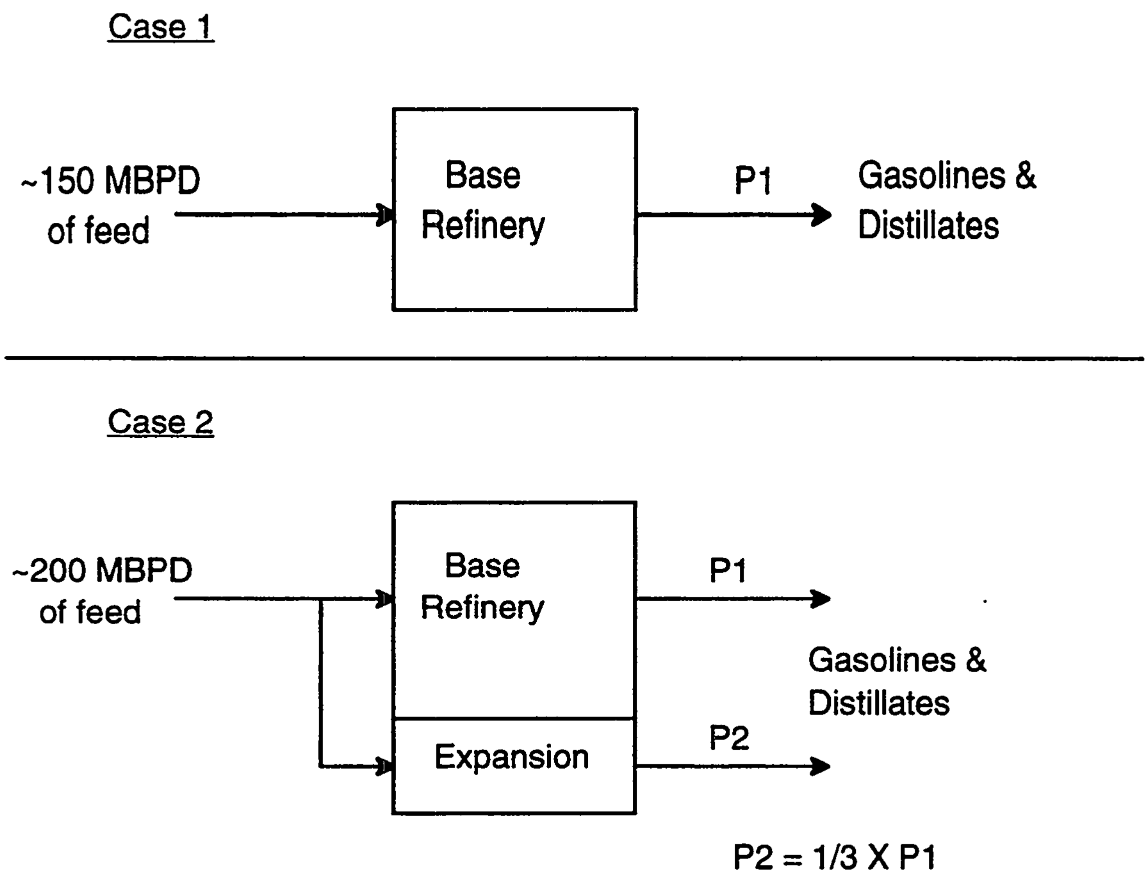

Figure 2
Heavy Distillate Hydrotreating/Catalytic Cracking

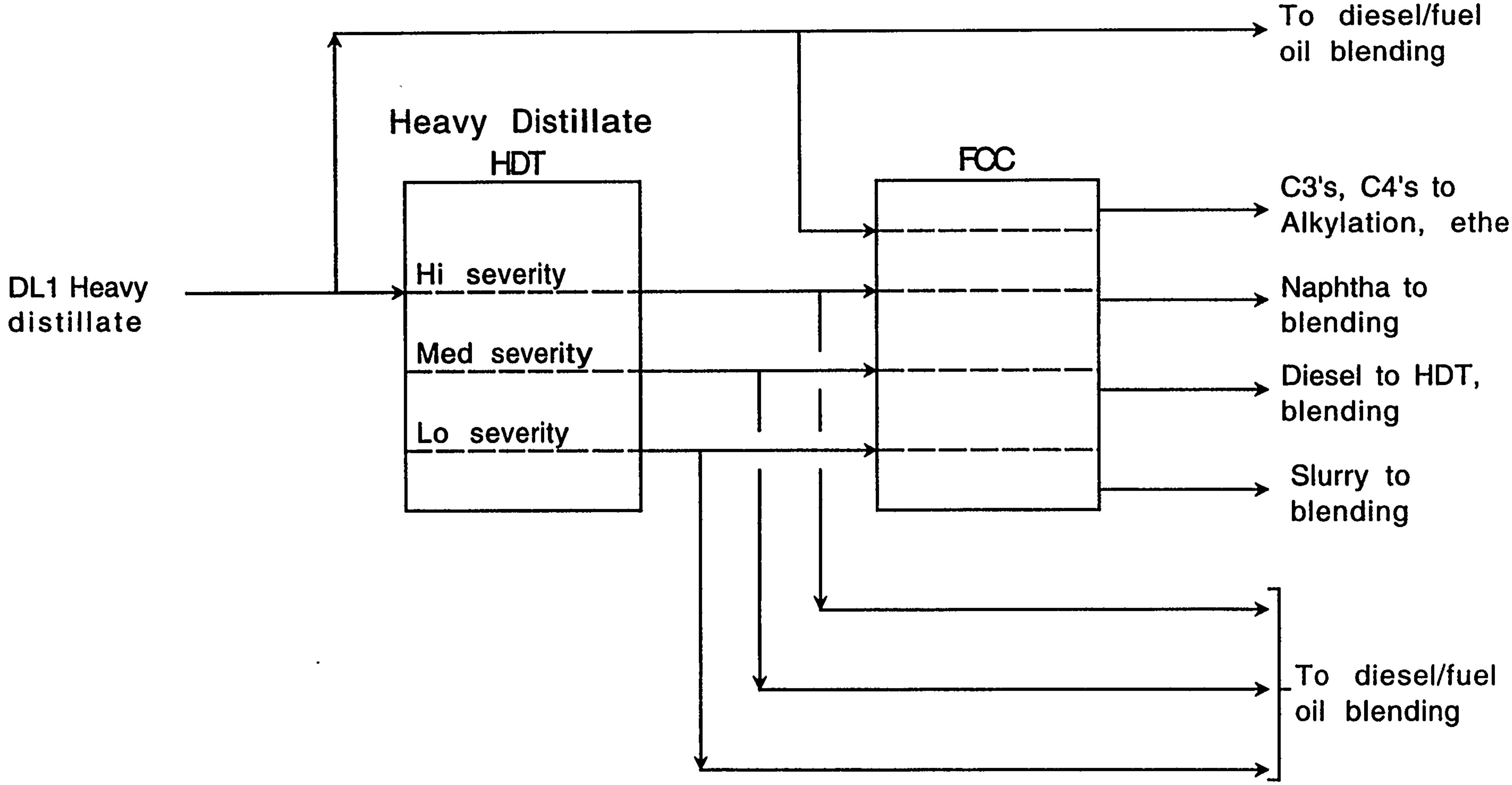

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Figure 3
DL1 Coal Liquid Value

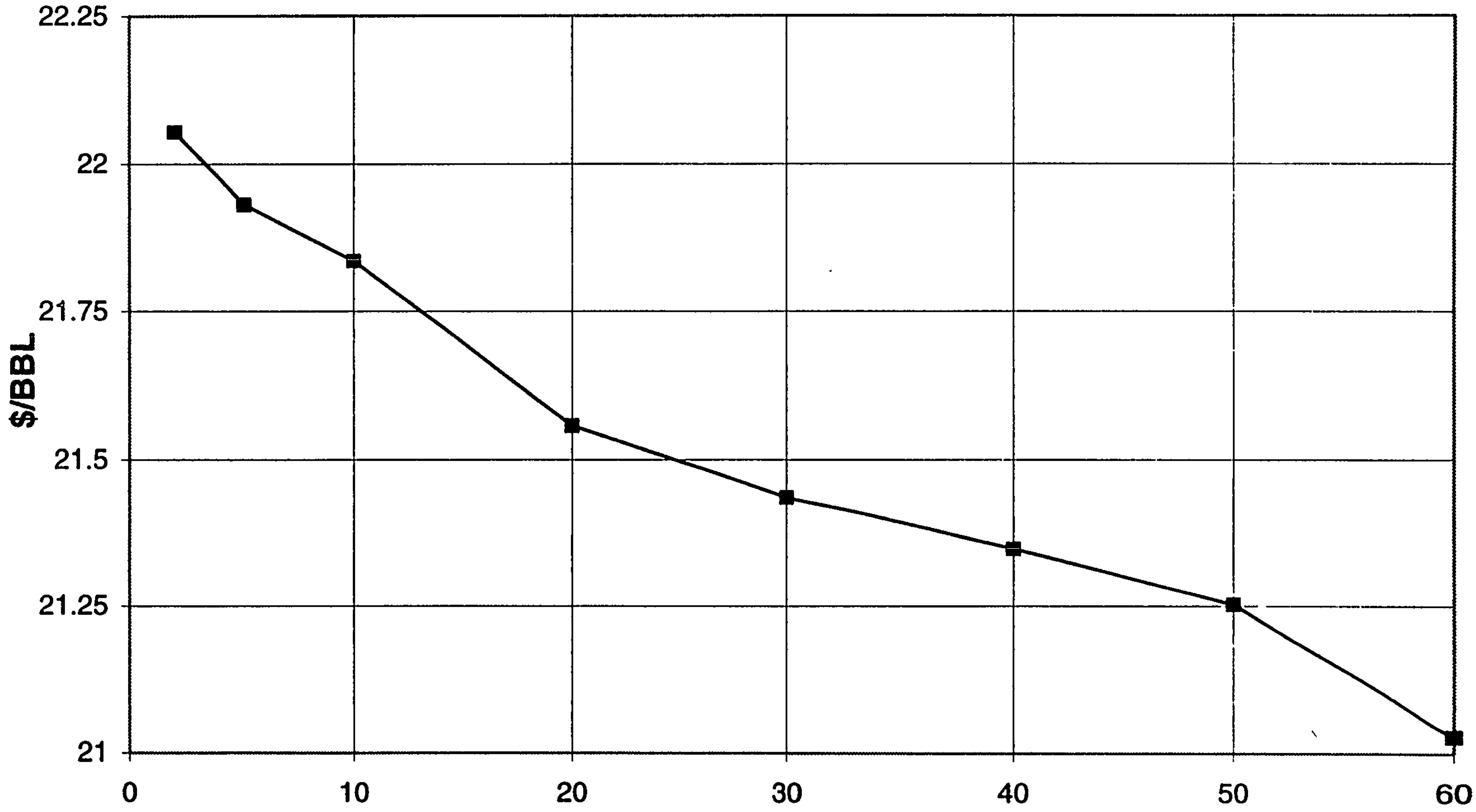

Figure 4
Capital Expenditures

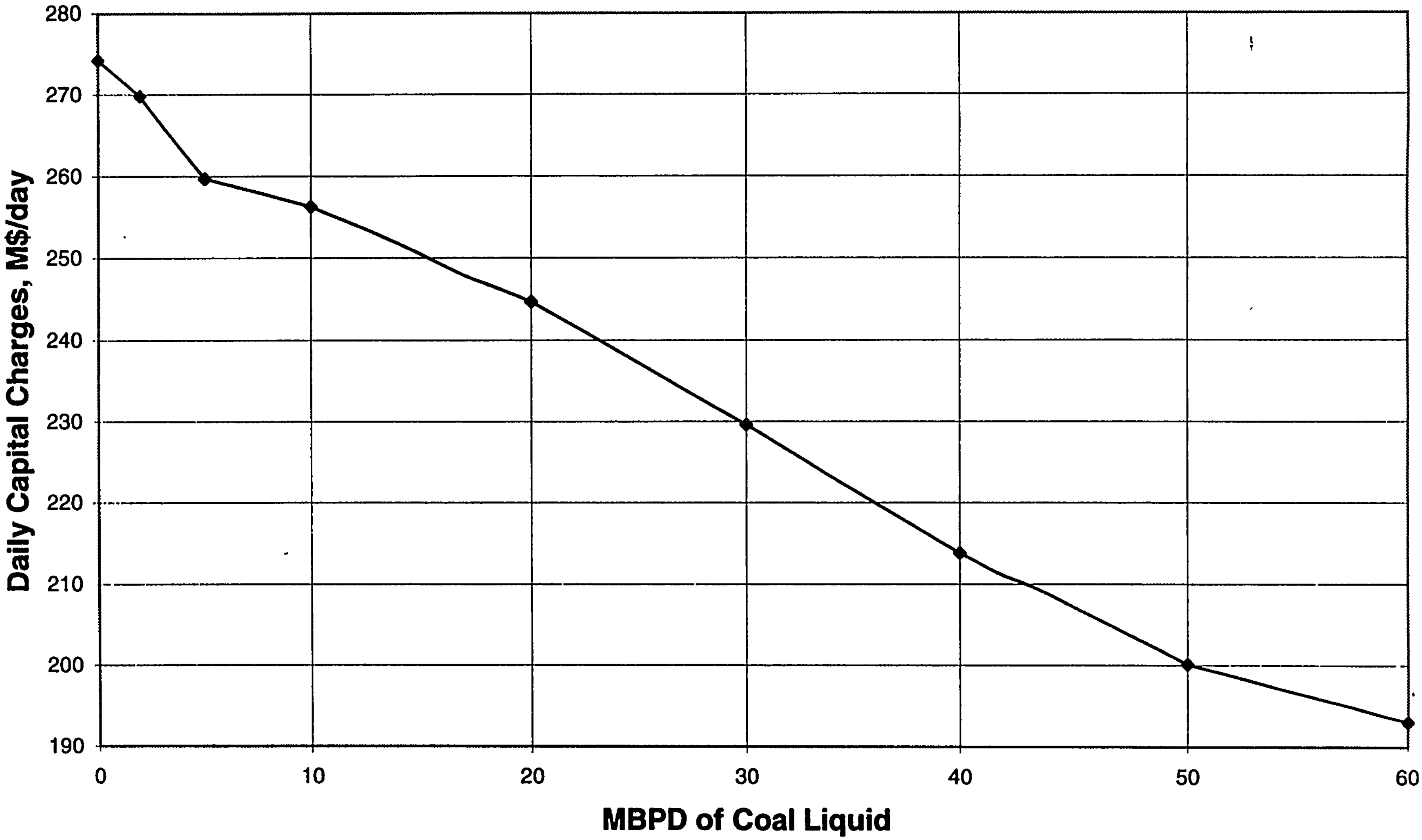

Figure 5
DL1 Coal Liquid Value
Expansion vs. No Expansion

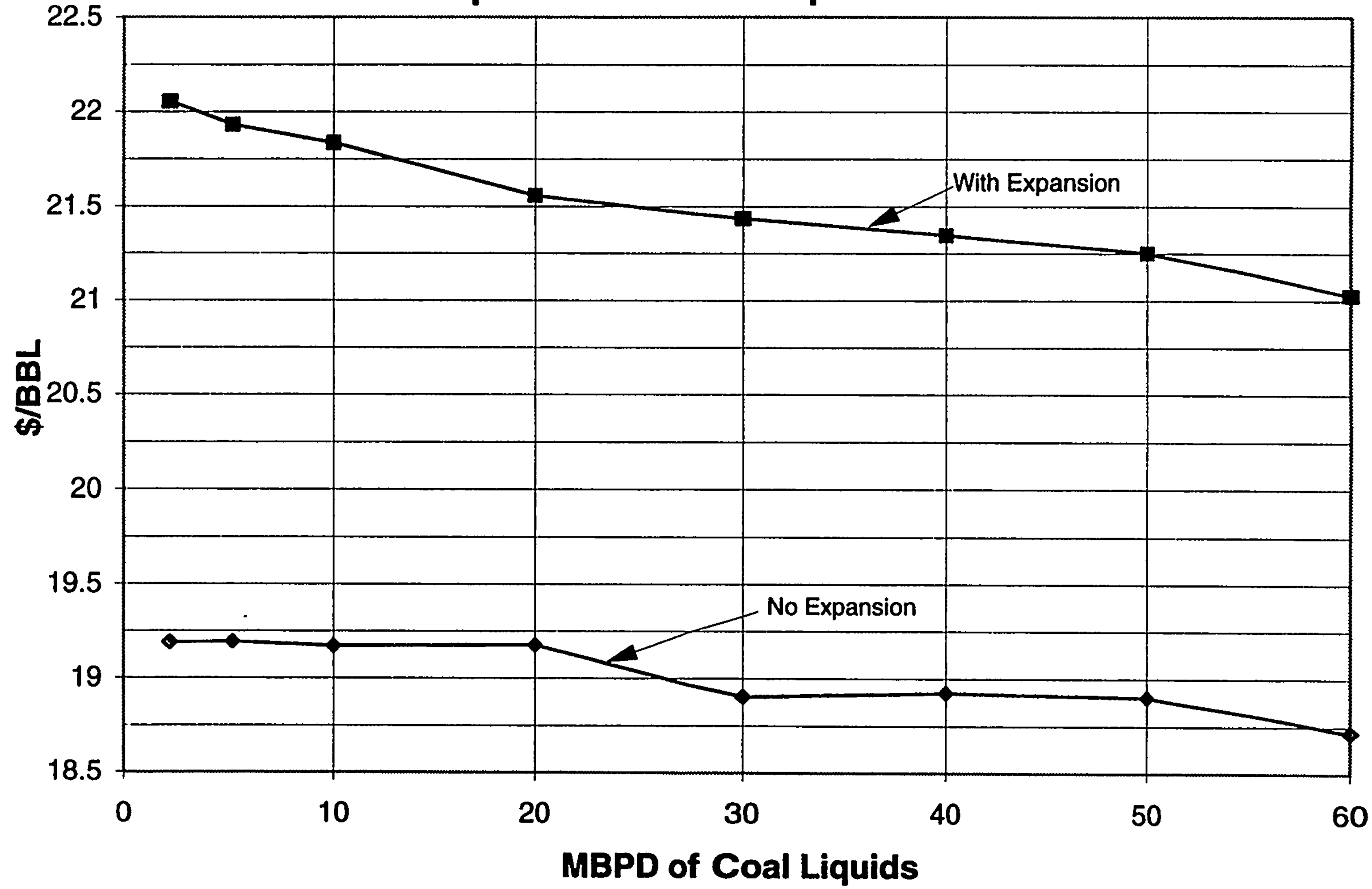

Figure 6
DL1 Coal Liquid Value
Effect of Pilot Plant Data