U.S. Department of Energy
Federal Energy Technology Center

Refining and End Use Study of Coal Liquids

Contract No. DE-AC22-93PC91029--17

Topical Report - Option 1
Economic Evaluation

Disclaimer

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1. Executive Summary

Two direct coal liquids were evaluated by linear programming analysis to determine their value as petroleum refinery feedstock. The first liquid, DL1, was produced from bitiuminous coal using the Hydrocarbon Technologies, Inc.(HTI) two-stage hydrogenation process in Proof of Concept Run No.1, POC-1. The second liquid, DL2,was produced from sub-bituminous coal using a three-stage HTI process in Proof of Concept Run No. 2, POC-2; the third stage being a severe hydrogenation process.

A linear programming (LP) model was developed which simulates a generic 150,000 barrel per day refinery in the Midwest U.S. Data from upgrading tests conducted on the coal liquids and related petroleum fractions in the pilot plant testing phase of the Refining and End Use Study was inputed into the model.

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 DL1 material had essentially the same value as the generic crude. Due to its higher quality, the DL2 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 under this scenario, but the values are dependent on the prices of the alternative crudes.

2. Background

This report summarizes the work conducted in the Option 1 section of the Refining and End Use Study of Coal Liquids which is funded by the U.S. Department of Energy's Federal Energy Technology Center under contract no. DE-AC22-93PC91029.

The overall objective of the study was to determine the most cost effective combination of upgrading processes needed to make high quality, liquid transportation fuels from petroleum crude and direct and indirect coal liquefaction products in an existing petroleum refinery. In addition, transportation fuels were produced from blends of coal liquids and petroleum, and used in engine performance and emission tests.

The Basic Program consisted of three primary tasks. The first task involved fractionating and characterizing two direct and one indirect coal liquids. The second task involved conducting pilot plant tests on various upgrading processes. The third task involved developing a linear programming model for the petroleum refinery. This model will be used to determine the optimum processing scheme for the coal liquids and for economic evaluation analysis.

The second half of the End Use study, Option 1, involves the production and testing coal derived fuels, and the economic evaluation. The results of the economic evaluation section of Option 1 will be summarized in this report.

It should be noted that the work on the indirect liquid was curtailed due to budget problems and concerns over the quality of the liquid. For this reason, the economic evaluation was conducted only on the two direct coal liquids.

The two direct coal liquids, DL1 and DL2, were produced at the Hydrocarbon Technologies, Inc. (HTI) facility in New Jersey. The first liquid, DL1, was produced from bitiuminous coal using HTI's two-stage hydrogenation process in Proof of Concept Run No.1, POC-1. The second liquid, DL2,was produced from sub-bituminous coal using a three-stage process in Proof of Concept Run No.2, POC-2; the third stage being a severe hydrogenation process.

3. Introduction

The primary objective of the economic evaluation work is to determine the value of the coal liquids as a refinery feedstock; that is, how much would a refinery be willing to pay for these liquids.

The primary tool used to conduct the evaluation work was a PIMS (Process Industry Modeling System) linear programming (LP) model which was developed specifically for the Refining and End Use Study.

The model simulates a generic petroleum refinery situated in the PADD II (Midwest U.S.) district. The nominal capacity of the refinery is 150,000 barrels per day (bpd). A detailed description of this petroleum model was provided in a topical report issued in March of 1995[1]

The key features of this model are:

1. Each of the individual processing units in the refinery operates at the maximium capacity.

2. 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.

3. 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[2]

4. 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

[1] Topical report, "LP Model Design Basis Base Petroleum Refinery" Refining and End Use Study of Coal Liquids, March 20, 1995

[2] "Supplement to the Annual Energy Outlook 1995", Department of Energy/Energy Information Agency, February, 1995, DOE/EIA-0554(95)

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 the Basic Program section of this study. This work provided yields and property data on the upgrading of the two direct coal liquids[3]. Separate submodels were added to the model to handle each of the direct liquids. The coal liquid portion of the model is described in a topical report[4].

4. Case Studies

The direct coal liquids were evaluated under the following scenarios:

- Refinery expansion vs. no expansion allowed
- Alternative crude

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. On simple terms, the objective function is the daily profit for the refinery and is defined as follows:

Objective Function = Revenues - Purchases - Utilities - Capital charges

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

An example of this calculation is as follows:

Petroleum crude cost, $/bbl =	18.00
Objective Function for an all petroleum feed, $/day =	868,000
Direct coal liquid feed rate, bbl/day =	50,000
Objective Function for above coal liquid feed rate, $/day =	1,950,000
Coal liquid value @ 50,000 bpd feed rate, $/bbl =	21.64

[3] Final report, "Basic Program - Refining and End Use Study of Coal Liquids", due to be published November, 1997

[4] Topical report, "Addendum to the Linear Programming Refinery Model Design Basis" Refining and End Use Study of Coal Liquids, due to be issued November 1997

(1,950,000 - 868,000)/50,000
Incremental coal liquid value @ 50,000 bpd feed rate, $/bbl= 3.64
(21.64 - 18.00)

Note that the coal liquid values are based on calculating the difference between the two Objective Functions. When the coal liquid flows are low (<5,000 bpd), the difference in the Objective Functions are also low. Convergence tolerances in the linear programming are magnified in this area and the calculated coal liquid values should be carefully examined.

4.1 No expansion vs. expansion allowed

4.1.1 Description

As mentioned in Section 3, the base refinery linear programming model is configured for a nominal 150,000 bpd throughput of the base petroleum crude. All of the individual process units operate at capacity with this crude.

The direct coal liquids were evaluated under two scenarios: Case 1 - No Expansion and Case 2 - Expansion Allowed.

4.1.1.1 Case 1 - No Expansion

As the name implies, there is no expansion allowed in any of the individual process units in the refinery. The product slate is fixed (see Table 1). Under this scenario, an all petroleum feed resulted in an Objective Function value of $868,500/day.

The DL1 coal liquid was then introduced into the model at various flowrates to replace approximately the same amount of petroleum crude. The coal liquid value was then calculated at each of these flow rates. The results shown in Figure 2 indicate that the DL1 liquid has approximately the same value as the base petroleum crude ($18.00/bbl).

The same method was used to evaluate the DL2 liquid. The results shown in Figure 3 shows that the DL2 liquid has a slightly higher value than the DL1 material. This is primarily due to the higher yields in the reformer and catalytic cracking units. A secondary reason is that the blending quality of the neat DL2 light distillate is higher than the neat DL1 light distillate.

4.1.1.2 Case 2 - Expansion Allowed

In Case 2 - Expansion Allowed, an assumption was made that a market opportunity exists to increase refinery production by one-third. The basis for this assumption was that as smaller refineries shut down because of economics, environmental regulations, market changes; larger and more complex refineries will have to expand to fill the void.

The difference between Cases 1 and 2 are shown in Figure 1. The top section of the figure shows the base refinery producing approximately 150,000 bpd of refined products. The bottom section of the figure shows that in Case 2, the refinery is expanded to increase production by one-third.

The capital cost estimation feature of the LP model was used to determine the cost of the expansion on a daily capital charge basis. The increase in operating costs for each process unit was based on the increase in unit throughput.

The capital cost for the expansion is highly dependent on the type of refinery feed used to increase production. This is one area where the direct coal liquids show a significant advantage over the petroleum crude. Because they have essentially no bottoms, both coal liquids are lower boiling than the "typical" PADD II crude oil used in the base expansion scenario case, and less cracking and resid processing capacity has to be added for expansion with coal liquids. The avoidance of the additional capital expenditures for the two coal liquids cases compared to the petroleum case is the predominant reason that these coal liquids are more valuable that the "typical" PADD II crude oil mix.

Example - 50,000 bpd of direct coal liquids

Each coal liquid was evaluated by bringing in exactly 50,000 bbls/day of the coal liquid and removing an appropriate amount of petroleum so that the refinery will make exactly the same amount of the primary products (gasoline, diesel, jet fuel and fuel oil) as the base expansion scenario case (all petroleum feed). The amount of the LPG and small volumes of miscellaneous heavy products were allowed to fluctuate. Table 2 shows the total refinery input flows for the three cases in thousand barrels per day (KBPD). Differing amounts of methanol, MTBE, normal butane, isobutane, and natural gas (for feed to the hydrogen plant) are purchased in each case. These materials are used for alkylation, ether production, and blending, and vary depending on the refinery feed composition and process unit yields.

For the throughputs in this example, the DL1 coal liquid is about 2.89 $/bbl more valuable than the petroleum crude, and the DL2 coal liquid is 3.44 $/bbl more valuable. The 0.55 $/bbl difference between the DL2 and DL1 coal liquid is primarily because the DL2 contains more hydrogen, contains less heteroatoms, and produces better fluid catalytic cracking and reforming yields. About half of the difference between the DL2 and DL1 coal liquids is attributable to the better properties of the "neat" coal liquid, and the remainder is attributable to the aforementioned improved process unit yields.

The values for the DL1 and DL2 coal liquids at various feed rates under the Case 2 - Expansion Allowed scenario are shown in Figures 2 and 3, respectively. Note that the decline in the liquid values as the usage increases is characteristic of price determination via LP analysis. The decline is due to more and more restrictions (capacities, specifications, etc.) as the flow increases.

4.2 Alternative Crudes

4.2.1 Background

The studies described above were based on a petroleum crude, PD2, which was a generic blend of Light and Heavy Arabian crudes. The blend ratio was adjusted to simulate a representative feedstock to the PADD II region in the year 2000. Key properties of this crude are shown in Table 3.

Another scenario which was considered was to allow for co-processing the direct coal liquids with two alternative crudes.

- An Arabian Heavy crude, ARH.

- A high metal, heavy crude with asphalt qualities, HMH.

The properties of these two crudes are also shown in Table 3. It should be noted that substantial modifications to the model were required to simulate the processing of these two crudes properly[5].

This crude slate represents a wide range of crude types that should be available in the year 2000. It will help determine the value of the coal liquids in relation to a wide variation in crude properties.

4.2.2 Alternative crude price determination

A detailed description of the method for determining the value/price of the alternatives crudes is given in the topical report on the LP model design basis[5]. The key point that should be noted is that the price of these alternative crudes reflect the capital costs of processing these crudes in the Case 2 - Expansion Allowed scenario. In other words, the prices have a “built-in” discount factor for the capital portion of processing. The prices of these crudes are shown in Table 3.

4.2.3 Direct coal liquid value

The direct coal liquids were evaluated using the same methods described in Section 4.1 except that instead of a single petroleum crude available for co-processing, PD2, two additional crudes could be utilized, HMH and ARH. The results for DL1 and DL2 are shown in Figures 4 and 5, respectively.

For Case 1 - No Expansion scenario, coprocessing with the alternative crudes increases the values of both of the direct coal liquids; over $1/bbl for DL1 and around $0.35/bbl for DL2. This increase is primarily the effect of the low prices of the alternative crudes. (As mentioned previously, these prices are depressed because of the built-in capital cost component.) There is also a synergistic effect between processing the coal liquids which have a very small resid component and the alternative crudes which have high resid components.

For Case 2 - Expansion Allowed scenario, the value of the DL1 is lower than it is in the base scenario (PD2 only). This is because of the high Objective Function of the no-coal liquid base case. In this base case, only low cost alternative crudes are used. As more DL1 is forced into the model, less low-cost crude is used. This is in contrast to the base crude scenario (PD2 only) where as more DL1 is forced into the model, less high-cost crude (PD2) is used.

The value of DL2 in the alternative crude scenario is basically the same as the PD2-only scenario.

5. Conclusions

The value of the direct coal liquids as a petroleum refinery feedstock is very dependent on the scenario chosen for the evaluation.

For a generic refinery which has no plans or ability to expand capacity, the direct coal liquids have essentially the same value as the petroleum crude currently running in the refinery. The DL2 liquid has a

[5] Topical report, “LP Model Design Basis Base Petroleum Refinery” Refining and End Use Study of Coal Liquids, March 20, 1995

slightly higher value due to its higher quality. The coal liquids could potentially have a higher value if low-cost, high resid crudes are available for co-processing.

For a refinery where expansion is allowed and an increased market is availabe, the coal liquids have a significant higher value, $3-4 per barrel, over petroleum crude. This is primarily because the capital expansion costs would be significantly less if coal liquids are used instead of the petroleum crude.

Table 1 - Product slate and pricing

	BPSD	$/BBL
LPG		12.66
Unleaded regular gasoline	54,600	28.25
Unleaded premium gasoline	18,200	29.16
Reformulated regular gasoline	18,200	29.03
Reformulated premium gasoline	6,070	29.76
Kerosene/Jet fuel	12,840	19.36
No. 2 fuel oil	13,100	19.08
Low sulfur diesel	15,770	19.46
High sulfur diesel	13,990	19.08
Low sulfur fuel oil	-	17.70
Asphalt	-	15.6
Anode-grade coke, short tons		75.00
Fuel-grade coke, short tons		3.00
Cat slurry		10.00
Sulfur, long tons		89.60

Table 2 - Total Refinery Input

	Petroleum, KBPD	DL1, KBPD	DL2, KBPD
Coal Liquid	0.0	50.0	50.0
Crude Oil	199.7	146.7	150.7
Methanol	1.6	1.4	1.4
MTBE	5.1	5.1	2.4
Normal butane	1.6	3.0	2.9
Isobutane	4.4	4.0	3.8
Natural gas in FOEs	1.9	1.5	1.5
Total Purchases	214.5	211.7	212.7

Table 3 - Petroleum Crude Properties

	Crude PD2	Crude ARH	Crude HMH
API gravity	32.8	28.1	17.5
Sulfur content, wt%	1.31	2.73	2.21
Resid content, volume%	13.3	27.0	35.0
Price, $/bbl	18.00	14.61	14.75

Figure 1 - No Expansion vs. Expansion Allowed

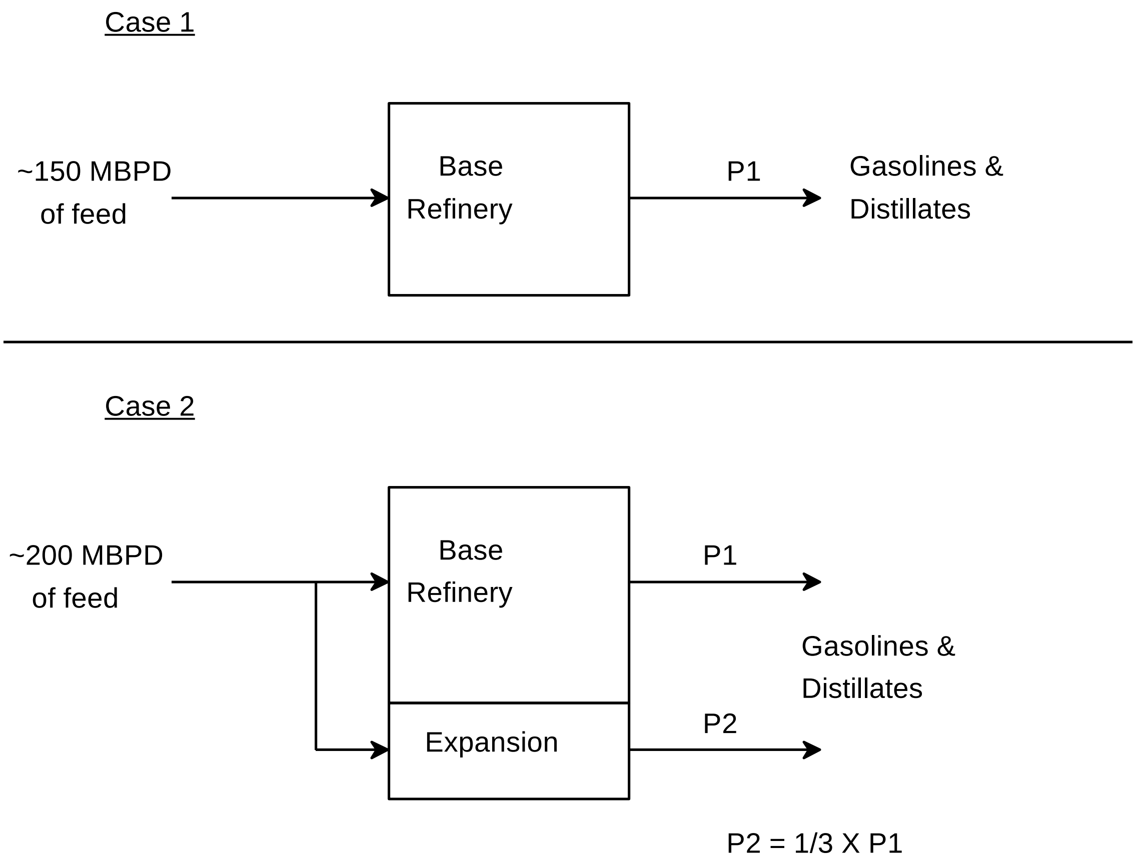

Figure 2 - DL1 Value with Base Crude

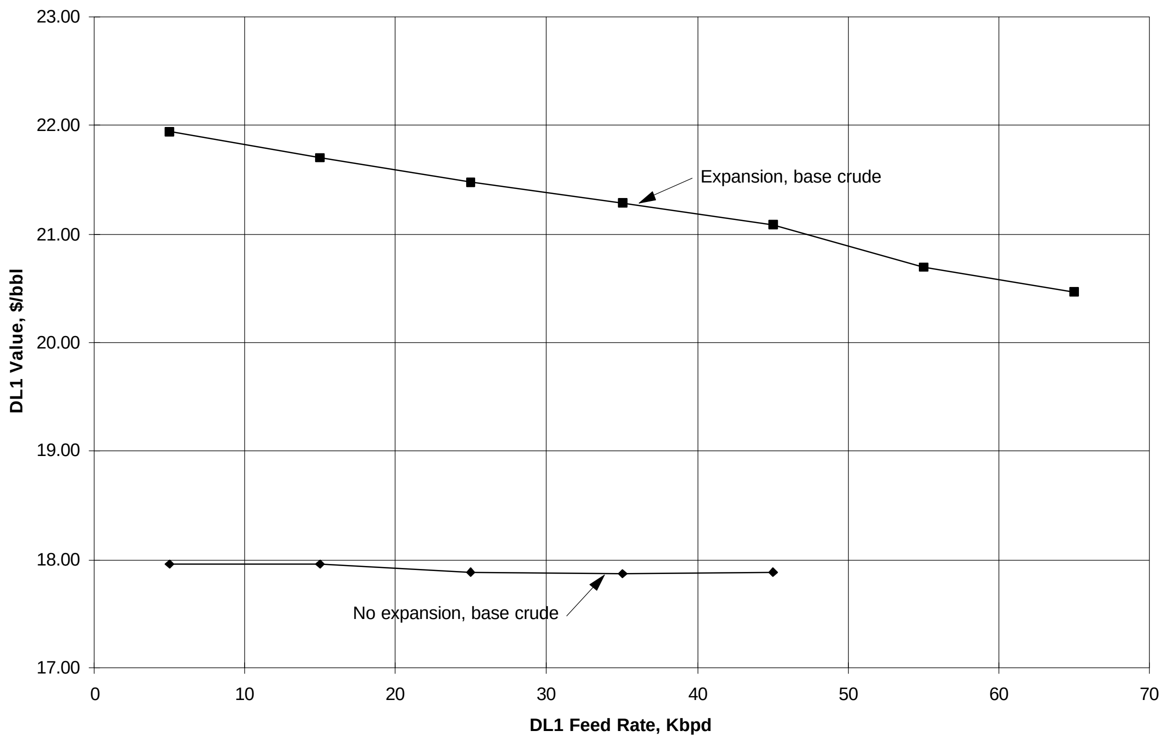

Figure 3 - DL2 Value with Base Crude

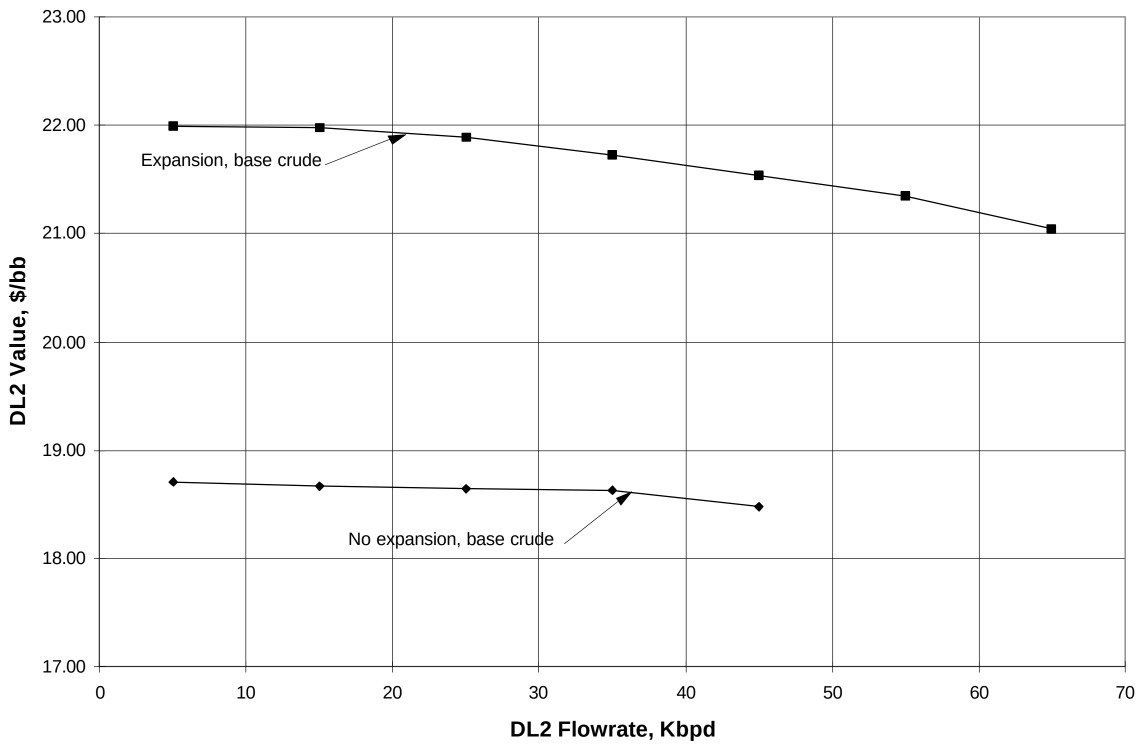

Figure 4 - DL1 Value with Full Crude Slate

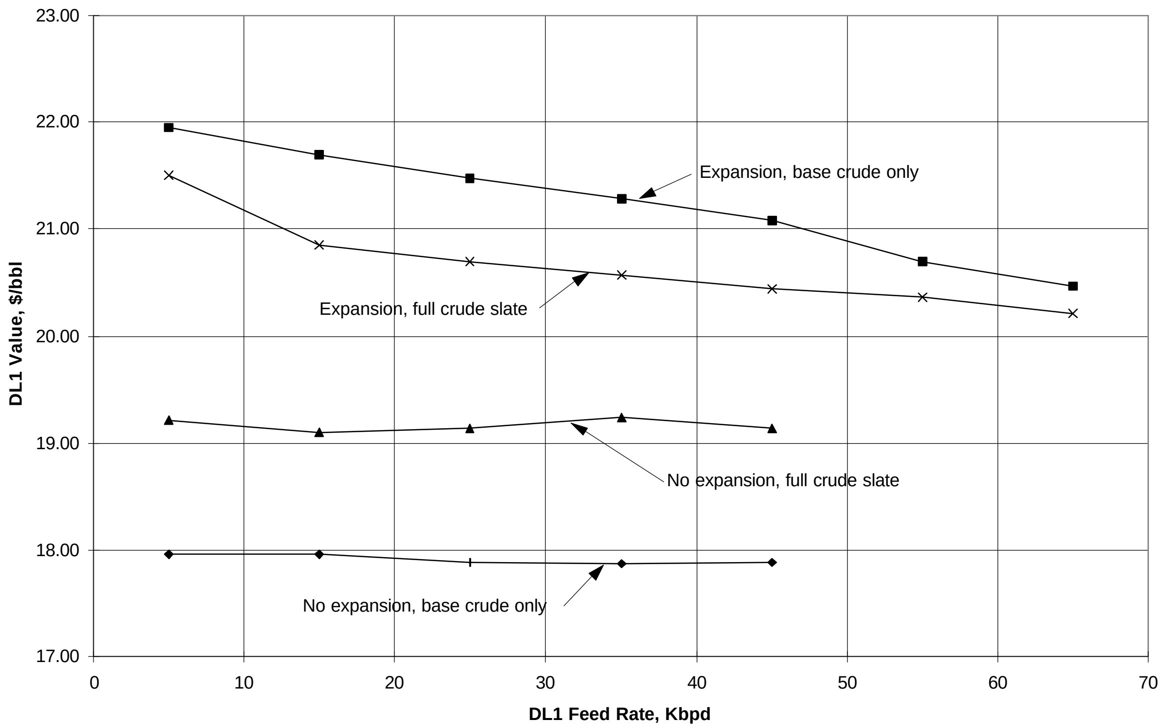

Figure 5 - DL2 Value with Full Crude Slate