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# DIRECT LIQUEFACTION PROOF-OF-CONCEPT PROGRAM

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Topical Report  
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## ABSTRACT

This report presents the results of the bench-scale work, Bench Run PB-09, HTI Run Number 227-106, conducted under the DOE Proof-of-Concept Option Program in direct coal liquefaction at Hydrocarbon Technologies Inc. in Lawrenceville, New Jersey. Bench Run PB-09 was conducted using two types of Chinese coal, Shenhua #2 and Shenhua #3, and had several goals. One goal was to study the liquefaction performance of Shenhua #2 and Shenhua #3 with respect to coal conversion and distillate production. Another goal of Bench Run PB-09 was to study the effect of different GelCat<sup>™</sup> formulations and loadings. At the same time, the space velocity and the temperature of the first reactor, K-1, were varied to optimize the liquefaction of the two Chinese coals.

The promoter-modified HTI GelCat<sup>™</sup> catalyst was very effective in the direct liquefaction of coal with nearly 92% maf coal conversion with Shenhua #3 and 93% maf coal conversion with Shenhua #2. Distillate yields (C<sub>4</sub>-524°C) varied from 52-68% maf for Shenhua #3 coal to 54-63% maf for Shenhua #2 coal. The primary conclusion from Bench Run PB-09 is that Shenhua #3 coal is superior to Shenhua #2 coal in direct liquefaction due to its greater distillate production, although coal conversion is slightly lower and C<sub>1</sub>-C<sub>3</sub> light gas production is higher for Shenhua #3. The new promoter modified GelCat<sup>™</sup> proved successful in converting the two Chinese coals and, under some conditions, producing good distillate yields for a coal-only bench run. Run PB-09 demonstrated significantly better performance of China Shenhua coal using HTI's coal direct liquefaction technology and GelCat<sup>™</sup> catalyst than that obtained at China Coal Research Institute (CCRI, coal conversion 88% and distillate yield 61%).

## EXECUTIVE SUMMARY

Bench Run PB-09 is part of the Proof-of-Concept Bench Option Contract between the United States Department of Energy and Hydrocarbon Technologies, Inc. (HTI). The primary goal of the run was to evaluate the direct liquefaction of two Chinese coals, Shenhua #2 and Shenhua #3, and to compare them with earlier data on the direct liquefaction of other coals. A further goal of the run was to evaluate a new promoter-modified GelCat™ at different loadings.

The entire bench run was conducted over thirty days and was divided into six operating conditions. PB-09 was initially scheduled to be a twenty-six day long operation, but was increased to thirty days in an attempt to increase the distillate yields. Shenhua coal #3 was used in conditions one through four, while Shenhua #2 coal was used in the final two conditions. A modified GelCat™ was used throughout the run at varying catalyst flow rates. All six conditions used a GelCat™ with a Fe/Promoter atomic ratio of 100/4, except period two, at a ratio of 100/2.

The following points were the highlights of bench run PB-09.

- The promoter-modified GelCat™ catalyst was effective in the direct liquefaction of both Chinese coals. Coal conversion, on a moisture and ash-free (maf) basis, was almost 92% with Shenhua #3 coal and 93% with Shenhua #2 coal.
- The C<sub>4</sub>-524°C distillate yield with Shenhua #3 coal varied from 52 to 68% maf, and 53 to 64% maf with Shenhua #2 coal. The 524°C<sup>+</sup> residuum conversion varied from 70 to 84% maf with Shenhua #3 coal and 71 to 80 % maf with Shenhua #2 coal.
- The C<sub>1</sub>-C<sub>3</sub> light gas yield was slightly higher with Shenhua #3 coal than with Shenhua #2 coal (13% vs. 12% maf, respectively).
- The 524°C residuum yield was lower for Shenhua #3 coal, 7% maf, than for Shenhua #2 coal, 13% maf.
- Overall, both coals had superior direct liquefaction performance, and Shenhua #3 was better than Shenhua #2 coal under the process conditions in PB-09, as shown by the higher distillate yields, with only slightly higher C<sub>1</sub>-C<sub>3</sub> light gas yields and slightly lower coal conversion.
- The promoter-modified GelCat™ with a Fe/Promoter composition of 100/4 (L-942) was superior to the analogous catalyst with a ratio of 100/2 (L-943), as evidenced by product yields. Upon changing from L-942 to L-943 the C<sub>4</sub>-524°C distillate yield derived from Shenhua #3 decreased from 68% maf to 66% maf, the 524°C<sup>+</sup> residuum conversion decreased from 84% maf to 82% maf, the C<sub>1</sub>-C<sub>3</sub> light gas yields increased from 12% maf to 13% maf, and the 524°C<sup>+</sup> residuum yield increased from 7% maf to 9% maf, while the coal conversion stayed the same at 91 % maf.

## BACKGROUND, OBJECTIVES, AND SCOPE OF WORK

The POC Bench Option Project (PB-Series) was started in order to study a wide variety of coal liquefaction and co-processing conditions using various plastics, waste oils, auto shredder material, petroleum residual oils, and lignin-cellulose material. The data collected would be used to develop a continuous multistage liquefaction process using a variety of feeds. Another key concept in the PB-Series runs is the development and testing of a catalytic system that has a high conversion of coal and other feeds with high distillate yields and low C<sub>1</sub>-C<sub>3</sub> gas yields. PB-09 was carried out over thirty days using six process conditions. Two Chinese coals were used in an all-dispersed catalyst mode using promoter-modified GelCat™ with different elemental compositions and under different operating parameters, with the ultimate goal of using data derived from PB-09 in producing economic comparisons with other runs in the DOE database and designing larger scale liquefaction processes to be used in China using one, or both, of these coals.

### Objectives

The main objectives of PB-09 were:

To study the direct liquefaction of two Chinese coals using HTI's modified GelCat™ catalyst and bench unit in an all-dispersed catalyst mode using extinction recycle solvent conditions.

To study the activity of different dispersed catalytic systems and conditions using HTI's modified GelCat™.

To achieve coal conversion greater than 90%, maximize distillate yield and minimize gas yield.



## EXPERIMENTAL

### System Configuration

The direct liquefaction test of the two Shenhua coal samples was carried out in two 2-liter reactors separated by an interstage separator and with an in-line hydrotreater, shown simplified in Figure 1.

The premixed slurry of coal, heated recycle oil and catalyst is charged to the Feed Tank (P-2) every two hours. The feed is pumped and preheated to about 315 to 371°C, depending on the viscosity. Before entering the first-stage reactor (K-1), the heated feed is joined with hydrogen and hydrogen sulfide. The effluent from K-1 is separated in the hot separator (O-1A) into a liquid slurry stream which is fed to the second-stage reactor (K-2), and a vapor which is sent to cold separator (O-2A). From O-2A, the vapor is cooled and condensed, via the Overhead Receiver (O-7A), the Vent Gas Knock Out (O-4A), and the Flare Knock Out (O-5A). Condensates from these vessels are sent to the Hydrotreater Unit (K-3). Gases are vented.

The second-stage reactor feed is joined with hydrogen and TNPS (di-tertiary-nonyl polysulfide). The effluent is sent to the second-stage Hot Separator (O-1). The overhead vapor from O-1 goes to the Hydrotreater Unit (K-3) along with the first-stage liquids previously mentioned. The effluent from K-3 is sent to the Cold Separator (O-2). After going through the Overhead Receiver (O-7), the Vent Gas Knock Out (O-4), and the Flare Knock Out (O-22), the hydrotreater effluent is separated into the separator overhead product, vent gas, and knockouts. The knockouts are returned to K-3 for further processing.

The bottoms from the Hot Separator (O-1) are sent to the Flash Vessel (O-3), the Overhead Receiver (O-17), and the Bottoms Receiver (O-6). In O-6, this stream is separated into the separator bottoms, knock outs (also sent back to the hydrotreater unit), and the bottoms vent gas. Water is added to the feed line of the cold separators O-2 and O-2A.

The products from the operations shown in Figure 1 are three gases (O-5A, O-22 and O-14), separator overhead (O-7), and O-6 bottoms. Not shown in Figure 1 are three downstream batch processing steps: pressure filtration, vacuum distillation and extraction. Pressure filtration separates the O-6 bottoms into a Pressure Filter Liquid (PFL) and a Pressure Filter Cake (PFC). Vacuum distillation, at a nominal 454°C cut point, separates the PFL into Vacuum Still Bottoms (VSB) and Vacuum Still Overhead (VSOH). Finally the PFC is extracted with toluene to recover toluene-soluble oils from toluene-insoluble solid.

### Materials

Two coals were received from China, designated Shenhua Coal #2 (HTI-6769) and Shenhua Coal #3 (HTI-6770). Table 1 shows the properties of the two coal samples, as analyzed by HTI.

Three iron-based catalysts of different formulations with two promoters were prepared for the run, using proprietary procedures. These catalysts were designated L-942, L-943, and L-945. L-942 and L-945 had similar promoters content (Fe/Promoter atomic ratio of 100/4) which was higher than that of L-943 (100/2).

The Hydrotreater used Criterion C-411 Trilobe catalyst.

## SUMMARY OF OPERATIONS

PB-09 was operated over a thirty-day time span (30 operating periods each 24 hours long) and included six different conditions which was four days longer and one condition more than originally scheduled. Shenhua #3 coal was used in conditions 1 through 4 and Shenhua #2 coal was used in conditions 5 and 6. The L-943 catalyst was used in condition 2, while the other five conditions used either L-942 or L-945. Other variables were feed space velocity, catalyst flow rate and K-1 temperature. The K-2 temperature was kept at 450°C, the in-line hydrotreater temperature was 379°C, and the O-1A hot separator temperature was 343°C throughout the entire run.

Operating parameters in condition 1 were based on previous experience with Shenhua coal, which was obtained at CCRI and HTI. Conditions 2 and 3 studied the impact of catalyst loading and promoter levels. In condition 4, space velocity was increased by 20% to assess its impact. In condition 5, the first-stage reactor temperature was lowered by 5°C, in an attempt to reduce the gas yield. Finally, in condition 6 operating parameters were the same as in condition 1, with Shenhua #2 coal.

Operation of the unit during the run was very smooth. Feed was continuously maintained to the unit for 713 hours (just short of thirty days), except for two minor interruptions totaling four hours. In the first interruption, during Period 5, the first-stage backpressure control valve plugged, necessitating about a three-hour oil wash at lower reactor temperature. In the second instance during Period 25, a problem with the charge pump packing caused feed to be interrupted for about one hour. The run was voluntarily terminated after the completion of Period 29, as scheduled. The unit was found clean upon inspection after shutdown, except for a plug in the recycle line of the first-stage reactor.

The average daily material balance for this run was 98.4 W%. A chart of the daily material balance is shown in Figure 2. Table 2 shows the Operating Summary and the Process Performance for the run, while Figure 3 shows the reactor temperatures and feed space velocity for each period. The operational problems mentioned above are evident in Figures 2 and 3. The K-1 temperature dip in Periods 16 and 17 were a response to the increased velocity specified in the run plan.

### Run Conditions

PB-09 (227-106) included six different conditions. Shenhua #3 coal was used in conditions 1 through 4 and Shenhua #2 coal was used in conditions 5 and 6. The low promoter-level GelCat™, L-943, was used in condition 2, but in the other five conditions either L-942 or L-945 was used, both having the same composition. Other variables were feed space velocity, catalyst flow rate, and K-1 temperature. The K-2 temperature was kept at 450°C, the in-line hydrotreater

temperature was kept at 379°C, and the O-1A hot separator temperature was kept at 343°C throughout the entire run.

### **Startup & Condition 1 (periods 1-5)**

Startup consisted of insulating the unit, establishing the proper flow of oils and gases, setting the correct temperatures, pressurizing the system, and adding the catalyst to the HTU. Filtered heavy gas oil was used as the startup oil. Period 1 started with the introduction of coal feed at 0400 hours on October 15, 1997. Each twenty-four-hour period started and ended at 0400 hours. During condition 1 the Shenhua #3 coal feed rate was 1069 g/h, the O-6 bottoms feed rate was 960 g/h, and both the VSB and the toluene-extracted oil (TEO) feed rates were 240 g/h. the reactor feed space velocity was 449 kg/h/m<sup>3</sup>. The reactor temperatures were 440°C in K-1 and 450°C in K-2. The promoter-modified GelCat™ catalyst (L-942) was fed at the relatively low rate of 54 g/h.

In Period 2 the vacuum still cut point was increased from 427°C to 454°C and the O-1 temperature was increased to 357°C from 343°C in an attempted residual oil extinction recycle. There was a feed interruption during period 5-A when the backpressure control valve plugged. The unit was put on wash for 4 hours. All gases were routed through the second stage vent, the temperature was lowered and all water, H<sub>2</sub>S, and TNPS injections were halted. The plug broke on its own, but the feed interruption necessitated the use of period 4 as the work-up for condition 1.

### **Condition 2 (periods 6-10)**

In period 7-A the overhead line became plugged and acetic acid (1%) was added to the water injection rate of 300 g/h, to dissolve the ammonium sulfide salt. Near the end of period 7-B excess VSOH was added to P-2 to decrease the viscosity, which had been slowly increasing. The VSOH additions were stopped in period 8-A and the VSB additions were increased to 480 g/h to make up for the loss of TEO in the feed. Starting in period 9 the TEO feed rate was 100 g/h, VSB feed rate was 290 g/h, and the O-6 bottoms flow rate was 1050 g/h. period 10 was the work up period for condition 2.

Condition 2 differed from the first condition only in that the GelCat™ catalyst (L-943) had a lower loading of promoter. There was a concurrent increase in the catalyst flow rate to 71 g/h during period 8 with a further increase to 95 g/h for periods 9 and 10. Coal and oil feed rates, along with all temperatures and pressures, were the same as in Condition 1.

### **Condition 3 (periods 11-15)**

Condition 3 returned to the original catalyst (L-942) and the catalyst flow rate was lowered to 80 g/h. periods 11 through 13 saw an increase in the VSB and O-6 bottoms feed rates to 390 g/h and

1050 g/h, respectively, as TEO was removed. TEO was added back to the feed in periods 14 and 15 with a feed rate of 100 g/h and the VSB feed rate was decreased to 290 g/h.

There was a sudden increase in viscosity during period 13-A, possibly due to a piece of semi-dry material in the charge can that was added to P-2. Period 15 was the work up period for condition 3.

#### **Condition 4 (periods 16-19)**

Operating parameters in this condition 4 were set so as to reduce the gas yield. Starting with period 16-A, the space velocity was increased 20%. The feed rate of Shenhua #3 coal and O-6 bottoms increased to 1283 g/h and 1260 g/h, respectively. The TEO was completely removed from the feed slurry for the rest of the run while the VSB feed rate was increased to 468 g/h. the GelCat™ (L-942) catalyst flow rate was increased to 96 g/h. a new catalyst, L-945, that had the same elemental composition as L-942 was introduced in period 17-A with a flow rate of 113 g/h. due to decreased distillate formation, the K-1 temperature was raised to 440°C in period 17. Period 19 was the work up period for condition 4.

#### **Condition 5 (periods 20-23)**

Shenhua #2 coal was introduced to the reactor at the beginning of Condition 5, at a rate of 1069 g/h as the space velocity was reduced back to 455 kg/h/m<sup>3</sup>. The O-6 bottoms and VSB feed rates were decreased at the same time to 1050 g/h and 390 g/h, respectively. The L-945 catalyst flow rate was lowered to 93 g/h. the K-1 temperature was also decreased at the beginning of period 20 to 435°C in another attempt to lower the gas yield. PFL, which had been used as the buffer oil, was replaced with a mixture of VSOH and PFL in the ratio of 1:3, in period 21-B. the K-1 buffer line plugged in period 22, and therefore the H<sub>2</sub> pressure in K-1 was increased by 10% in period 23. Period 23 is the work up period for condition 5.

### Condition 6 (periods 24-29)

The goal of the last condition was to increase distillate yield while minimizing the light gas yield. Condition 6 used the same catalyst loading, space velocity, feed rates, O-6 bottoms rate, VSB rate and L-945 catalyst, for Shenhua #2 coal as in Condition 1 with Shenhua #3 coal. The K-1 temperature was increased to 440°C in period 24-A (taking 2 hours to reach the new temperature) and was further increased to 443°C in period 24-B, again taking 2 hours to reach the final temperature. The O-6 bottoms flow rate was reduced to 858 g/h starting in period 24. The hot separator (O-1A) temperature was increased to 399°C (originally 343°C) in period 24-A.

There was an interruption in the feed pumping in period 25-B due to problems with the charge pumps. The unit was put on heavy oil wash for less than one hour, until the problem was rectified. The feed pump problem necessitated an extension of condition 6. A new feed blend in period 26-A consisted of 1069 g/h of Shenhua #2 coal, 720 g/h of O-6 bottoms, 720 g/h of VSB and 62 g/h of L-945. The vacuum cut point was raised from 427°C to 454°C and higher during period 28 and the VSB flow rate was raised in period 29-A from 720 g/h to 820 g/h in order to recycle the VSB to extinction. Period 29 was the work up period for condition 6.

## PROCESS PERFORMANCE RESULTS

A discussion on the feed conversion and of the yields of different products follows. The overall process performance is summarized in Table 2 and is depicted in Figures 4 through 7. The data presented in these tables and figures represent the performance during the last period in each condition, after steady-state operation had presumably been achieved for that condition.

### Coal and 524°C<sup>+</sup> Residuum Conversions

Coal and 524°C<sup>+</sup> residuum conversions obtained for each condition are shown in Figure 4. Coal conversion is defined as the conversion to quinoline-soluble products, and is calculated on an SO<sub>3</sub><sup>-</sup> free basis. Coal conversion for the entire run varied from 90 to 93% on a moisture-and-ash-free (maf) basis, with an average of about 91%. Overall, there is no significant difference in coal conversion between the two Chinese coals. Shenhua #2 coal (operating conditions 5 and 6) had coal conversions of 90.5 and 93.1% maf, while Shenhua #3 coal (operation conditions 1 through 4) had conversion in the range of 90 to 91.8%. There is, however, a large variation in the 524°C<sup>+</sup> residuum conversion, varying from 69 to 84% maf, as seen in Figure 4. The highest conversion occurs in condition 1, while the lowest occurs in condition 4 (highest space velocity) both with Shenhua #3 coal. The exact process conditions (reactor temperatures, space velocity, catalyst composition and loading), rather than the type of coal, exerted the most influence on the overall 524°C<sup>+</sup> residuum conversion.

### C<sub>4</sub>- 524°C Distillate and 524°C<sup>+</sup> Residuum Yields

The C<sub>4</sub>- 524°C distillate and 524°C<sup>+</sup> residuum yields are shown in Figure 5. Distillate yields over the run varied from 52 to 68% maf and 524°C<sup>+</sup> residuum yields varied from 7 to 22% maf. With Shenhua #3 coal (condition 1 through condition 4), the distillate yield decreased from 68 to 52% maf, while the 524°C<sup>+</sup> residuum increased from 7 to 22% maf. The distillate yield with Shenhua #2 coal (conditions 5 and 6), was 54 and 63% maf, while the respective 524°C<sup>+</sup> residuum yields were 20 and 13% maf. As shown in Figure 5, there is an inverse relationship between C<sub>4</sub> - 524°C distillate and 524°C<sup>+</sup> residuum yields.

The distillate yield in condition 1 was 68% maf. In condition 2, the Fe catalyst loading was increased 50 percent, but the promoters were reduced by 25%, compared to condition 1. The light naphtha yield increased by 2 wt. % and the dry gas yield increased slightly at the expense of heavier liquid products, but the total C<sub>4</sub> - 524°C distillate yield dropped by 3 w%, to 65 w%. condition 3 used the same Fe loading as in condition 2, but both catalyst promoters were doubled. This resulted in a further slight increase in light products (dry gas and naphtha), but a further reduction in total distillate yield, to 59 w%. In condition 4, the space velocity was increased by 20% over previous conditions, in an attempt to reduce the C<sub>1</sub> - C<sub>3</sub> gases yield. A drastic decrease in distillate yield, to 52 w% was observed. When coal was switched (#3 to #2) in

Condition 5, the first-stage reactor temperature was lowered, while the space velocity was reduced to the previous level. Apparently the lower (5°C) temperature produced the same result as increased space velocity, and resulted in a total distillate yield of 54 w%. Operating parameters in condition 6 were nearly the same as in condition 1, with slightly higher space velocity and slightly higher first-stage reactor temperature. The distillate yield was found to increase to 63 w%, a few percentage points lower than in condition 1, possibly due to performance differences in the two coals. There was a change in recycle strategy in this last condition, namely to recycle as much resid as possible. This resulted in a recycle containing 64 w% resid, compared to 49-59 w% in previous conditions. Due to the complexity of the parameter matrix, the effect of recycle composition is not yet conclusive.

### **Distillate Selectivity**

The selectivity of each distillate fraction, namely naphtha (IBP-177°C), middle distillate (177-343°C), and heavy distillate (343-524°C) is shown in Figure 6. As discussed in the previous section, the increased catalyst usage in conditions 2 and 3 enhanced the light-ends distribution and correspondingly reduced the relative portion of the heavier distillates. Despite use of different coal types and despite variations in space velocity and first-stage reactor temperature, the liquid products obtained in conditions 4 and 5 showed the same trend of low total distillate yield with high yields of middle and heavy distillates. Liquid products from condition 6 showed high selectivity to heavy-distillate formation. This difference in performance, compared to condition 1, may be partly attributable to the differences in properties of the two coal samples and partly to the difference in the recycle composition.

### **Hydrogen Consumption and Light Gas (C<sub>1</sub>-C<sub>3</sub>) Yield**

As shown in Figure 7, the hydrogen consumption for conditions 1 through 4 (Shenhua #3 coal) decreased from 8.8 to 6.8% maf, varying with the amount of C<sub>4</sub>-524°C distillate produced. The final two conditions (Shenhua #2 coal) had a hydrogen consumption of 7.1 – 7.3 % maf. The C<sub>1</sub>-C<sub>3</sub> light gas yield for the first four conditions using Shenhua #3 coal is 12-13 %, slightly higher than that in Conditions 5 and 6 using Shenhua #2 coal (about 11% maf). The relatively low space velocities, coupled with the chemical nature of the two coal samples, probably contributed to the relatively high gas yields produced by #3 coal in conditions 1 to 3.

### **Hydrogen Utilization**

There are two major indicators that characterize hydrogen utilization: hydrogen efficiency and C<sub>1</sub>-C<sub>3</sub> gas selectivity. Hydrogen efficiency is the amount of distillate produced for a given amount of hydrogen consumed, while C<sub>1</sub>-C<sub>3</sub> gas selectivity is the amount of C<sub>1</sub>-C<sub>3</sub> gas obtained for a given amount of distillate produced. Figure 8 shows that the hydrogen efficiency is not significantly different for the first five conditions, 7.3 to 7.8%, but then increased sharply to 8.8% for condition 6 which is the most hydrogen efficient condition. The C<sub>1</sub>-C<sub>3</sub> gas selectivity ranges



from 0.18 to 0.22 with the best efficiency (lowest  $C_1$ - $C_3$  gas selectivity) occurring in conditions 1 and 6, which correspond to the conditions with the greatest distillate yields. The least attractive conditions (highest  $C_1$ - $C_3$  gas selectivity) are conditions 3 and 4 with had the lowest distillate yields and the highest light-gas yields.

## PRODUCT QUALITY

Analytical results are presented for the liquid product fractions, namely the separator overhead product and the vacuum still overhead product, as well as for the vacuum still bottoms and the pressure filter solids. The separator overhead and the vacuum still overhead constitute the total distillate product.

### Separator Overhead (SOH)

Table 3 shows the properties for the SOH oil. The SOH oil is the hydrotreated product from the combined HTU feed composed of the light materials generated in the first and second stage liquefaction reactors. It is the major product of coal liquefaction, and has a fairly high H/C atomic ratio, close to the petroleum counterpart. The boiling range (50-350°C) shows that it is mainly gasoline and diesel fuel. The API gravities varied from 35 to 37°C and the H/C atomic ratios were about 1.85, except for 1.92 in condition 1, possibly due to the high initial activity of the HTU catalyst. The heteroatom content of the SOH is low, especially the nitrogen content, which decreased from 0.23 to 0.0% as the run proceeded. The relatively high sulfur level (0.17 to 0.27%) is mainly due to H<sub>2</sub>S and elemental sulfur dissolved in the oil, which can be eliminated by steam stripping in commercial operation.

### Vacuum Still Overhead (VSOH)

The properties of the VSOH are shown in Table 4. Distillation results show that about half of the VSOH is light distillate, which is a diesel fuel fraction, while the remaining half is a heavy distillate, which is a good FCC feedstock. The API gravity ranged from 5.5 to 11.0°, and the initial boiling point was about 220°C. The H/C atomic ratio varied from a high of 1.29 during condition 1 to a low of 1.14 during condition 6. The nitrogen levels were around 0.85%, except during condition 1, when it had a value of 0.49%. The sulfur levels varied from 0.08% to 0.49%.

### Vacuum Still Bottoms (VSB)

The properties of the VSB are shown in Table 5. VSB is the major component of the recycle solvent. The gravity was very low (-15 to -17 °API) and the initial boiling point was at least 340°C, except for condition 6 which has an initial boiling point of 401°C when the vacuum distillation cut point was raised from 426°C to 454°C. The H/C atomic ratio ranged from 0.75 to 0.87. The nitrogen level ranged from 0.95 to 1.07%, except for condition 1 which was 0.83%. The sulfur levels varied from 0.17 to 0.36%.

Pre-asphaltenes and asphaltenes concentrated in the VSB. As the vacuum distillation cut point was increased by 28°C, the pre-asphaltenes and asphaltenes content of VSB was highest in condition 6.

### **Pressure Filter Solids (PFS)**

The solids derived from filtration are oil containing solids, which are extracted with toluene to recover the oils. The oil-free solid is then analyzed to determine the extent of coal conversion, based upon the solubility of the PFS in quinoline. The properties of the PFS are shown in Table 6. The H/C atomic ratios of PFS ranged from 0.58 to 0.73, and the quinoline insolubles, including ash, ranged from 58 to 73%.

### **Characterization of Total Distillate Product**

The total distillate product, composed of SOH and VSOH proportionally, was subjected to the True-Boiling-Point (TBP) distillation, followed by analysis of the TBP fractions. The analytical results for the total distillate products from conditions 1 and 6 are summarized in Tables 7 and 8. These two conditions were chosen because they gave the best results for the two coals tested in this run.

## DISCUSSION OF PROCESS PERFORMANCE RESULTS

### Effect of Coal Feed Type

The data shows that under the optimum condition chosen for each coal during the run, both coals performed well, while Shenhua #3 Coal had a superior performance over Shenhua #2, as depicted in Figures 9 and 10. While the coal conversions were essentially the same with the two coals, the 524°C<sup>+</sup> residuum conversion was substantially higher with Shenhua #3 coal than with Shenhua #2 coal. The superiority of the Shenhua #3 coal was further evidenced by the higher C<sub>4</sub>-524°C distillate yield and the lower 524°C<sup>+</sup> residuum yield, even though the C<sub>1</sub>-C<sub>3</sub> light gas yields were slightly lower when Shenhua #2 coal was used. The differences between Shenhua #2 and Shenhua #3 coals are not excessive though, and could be largely attributed to the process conditions employed, since the two coals were not tested under the same exact conditions.

Product yield, however, should not be the only criterion in comparing the liquefaction performance of the two coals. As shown in Figure 8, using the Shenhua #2 coal improved the hydrogen efficiency over the Shenhua #3 coal, which may compensate for the lower distillate yield in the economic analysis.

### Effect of GelCat™ Formulation and Loading

As mentioned previously, two catalyst formations were used in PB-09. L-942 and L-945 had Fe/promoter atomic ratios of 100/4, while L-943 has a Fe/promoter atomic ratio of 100/2. Comparisons of the two types of GelCat™ catalysts employed in this run are depicted in Figures 11 and 12. L-942 gave higher coal and 524°C<sup>+</sup> residuum conversions than L-943. L-942 also produced higher yields of C<sub>4</sub>-524°C<sup>+</sup> distillate and lower yields of C<sub>1</sub>-C<sub>3</sub> light gas and 524°C<sup>+</sup> residuum yields. Therefore, the L-942 catalyst with the higher promoter loading was superior in converting the residuum and in producing a distillate product.

Catalyst loadings tested in this run show that increasing catalyst usage beyond 5,000 ppm would increase light ends (gas and naphtha) yields, but would reduce the total liquids yield.

## Operational Parameters

Results from conditions 4 and 5 clearly indicate that the total distillate (C4-524°C) yield is sensitive to the change in reactor temperature and space velocity. Since the operating parameters in condition 1 were selected based on experimental results previously obtained by CCRI and HTI, they appeared to be close to optimal, at least for the Shenhua #3 coal, as demonstrated in PB-09. An increase in space velocity or a decrease in the first-stage reactor temperature resulted in a substantial reduction in residuum conversion and in lower distillate yield. Shenhua coal liquefaction tests conducted at CCRI gave coal conversion of 88% and distillate yield of 60.7%\*, lower than those achieved in Run PB-09 using HTI coal liquefaction technology and HTI's proprietary GelCat™ catalyst.

Test results clearly indicate that for both coals, conversion above 90% was not difficult to achieve. However, attempts to raise coal conversion beyond 92-93% were not successful. This is obviously restricted by the high content of inert components in Shenhua coals. Residuum conversion as well as distillate yields, however, are fairly high, relative to coals of similar rank. Operating conditions and catalyst loading/ formulations can be further adjusted to improve liquefaction performance of Shenhua coals, #2 coal in particular.

Since the number of conditions studied in the test is limited, conditions 1 and 6 represent only the best results achieved in this run, and may not be optimum conditions for the two coals. Other parameters, such as recycle ratio and composition have not yet been carefully studied. This means that there is considerable room for improvement of liquefaction performance of the Shenhua coals, in further studies.

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\* Jin Jialu et al. Proceedings of International Symposium on Clean Coal Technology, Nov. 1997, Xiamen, China, pp777-781.

## TECHNO-ECONOMIC ASSESSMENT

Economics were assessed for six conditions of PB-09, using the yields and operating conditions previously presented. The basis was a grass-roots liquefaction complex, feeding 12,000 tons/day of coal, at a US Gulf Coast location.

Table 9 presents the material balances for the conditions assessed. Product yields are seen relatively high in conditions 1, 2, and 6 and notably poorer in conditions 3 through 5. Byproduct propane and butane are high in all conditions but especially in conditions 2 and 3.

Table 10 shows hydrogen balances, utility requirements, and thermal efficiencies for the conditions. Conditions 4 and 5 show an appreciably lower total hydrogen consumption, but because of the decreased product yield the hydrogen used per barrel of product is higher than the other conditions.

The capacities of the process units and off-sites are summarized in Table 11.

The details of the liquefaction plant investment estimates are shown in Table 12. Due to the higher space velocity, condition 4 has a lower reactor cost than the other cases but outside of this condition, the investment costs are within  $\pm 1\%$  of each other.

The total plant investment costs are summarized in Table 13. Conditions 3 and 4 show about a 4 percent lower total plant investment than the others, because of reduced hydrogen plant cost. Again, however the decreased product yield increases the cost per daily barrel of product. The lowest cost per BPSD is found for condition 1.

Table 14 is a summary of the product costs and Table 15 itemizes the equivalent crude price by categories. By far the best economics are obtained in condition 1, with condition 6 in second place. Conditions 4 and 5 show the poorest economics because of lower product yield and higher hydrogen consumption per barrel of product.

Outside of capital-related costs, coal cost and natural gas cost account for the biggest contribution to equivalent crude price. The coal price used in this analysis was set by China authorities. Figure 13 shows the sensitivity of the coal cost, and Figure 14 shows the effect of the natural gas price on the equivalent crude price.

## CONCLUSIONS

The following conclusions were found from Bench Run PB-09:

- The promoter-modified GelCat™ catalyst proved to be successful direct liquefaction catalyst. Coal conversion was as high as 93% maf and 524°C<sup>+</sup> residuum conversion went as high as 85% maf.
- The promoter-modified GelCat™ also enhanced product yield as evidenced by C<sub>4</sub>- 524°C distillate yields as high as 67% maf.
- Both Shenhua #3 and #2 coals had good liquefaction performance, with coal conversion in the range of 91-93% maf. However, 524°C<sup>+</sup> residuum conversions were higher for Shenhua #3 coal than for Shenhua #2 coal, 85% maf versus 80% maf.
- The selectivity of products derived from the direct liquefaction of Shenhua #3 coal proved to be more superior than products derived from Shenhua #2 coal: C<sub>4</sub>-524°C distillate yields were higher, 67% maf vs. 60% maf, 524°C<sup>+</sup> residuum yields were lower, 7% maf vs. 13% maf, while C<sub>1</sub>-C<sub>3</sub> light gas yields were slightly higher, 13% maf vs. 11% maf.
- Shenhua #3 coal appeared more economically attractive than Shenhua #2 coal. The most favorable economic results were obtained using commercial projections from Condition 1.
- Coal conversion and distillate yield achieved in Bench run PB-09 on Shenhua coal using HTI coal liquefaction technology and GelCat™ catalyst exceeded those obtained at CCRI.

**Table 1. Feed Coal Analysis**

Shenhua Coal Number	2		3	
HTI Designation	6769		6770	
Moisture Content, W%	8.31		9.4	
	W% dry	W% daf	W% dry	W% daf
<i>PROXIMATE ANALYSIS</i>				
Fixed Carbon	57.95	61.79	59.28	61.91
Volatile matter	35.84	38.21	36.47	38.09
Ash	6.21	—	4.25	—
<i>ULTIMATE ANALYSIS</i>				
Carbon	75.87	80.90	79.47	83.00
Hydrogen	4.24	4.52	4.13	4.31
Nitrogen	0.98	1.04	1.05	1.10
Sulfur	0.42	0.45	0.42	0.44
Oxygen	12.28	13.09	10.68	11.15
Ash	6.21	—	4.25	—
<b>TOTAL</b>	<b>100.00</b>	<b>100.00</b>	<b>100.00</b>	<b>100.00</b>
<i>H/C atomic Ratio</i>	0.67		0.62	



**Table 2. Process Performance Summary**

Condition	1	2	3	4	5	6
Periods	1-4	5-10	11-15	16-19	20-23	24-29
Work-up Period	4	10	15	19	23	29
<b>Process Conditions</b>						
Coal type (Shenhua #)	3	3	3	3	2	2
Space velocity, kg/hr/m <sup>3</sup>	449	444	446	529	455	455
Temperature, K-1, °C	440	440	440	440	435	443
Temperature, K-2, °C	450	450	450	450	450	450
Catalyst type	L-942	L-943	L-942	L-942	L-945	L-945
Catalyst loading, Fe, ppm	5000	7500	7500	7500	7500	5000
Recycle/MF coal	1.5	1.5	1.5	1.5	1.5	1.5
Solids/MF coal	0.15	0.15	0.17	0.15	0.17	0.10
<b>Normalized yields, w% maf feed</b>						
C <sub>1</sub>	4.40	4.52	4.53	4.15	.77	3.89
C <sub>2</sub>	3.72	3.89	3.81	3.45	3.06	3.26
C <sub>3</sub>	4.48	4.75	4.94	4.34	3.94	4.34
C <sub>4</sub>	2.80	2.80	3.05	2.65	2.42	2.70
C <sub>5</sub>	1.51	1.58	1.59	1.02	1.06	0.68
C <sub>6</sub> & C <sub>7</sub> gases	1.10	1.31	1.34	1.35	0.99	1.13
C <sub>1</sub> - C <sub>3</sub>	12.60	13.16	13.28	11.94	10.77	11.49
C <sub>4</sub> - C <sub>7</sub> gases	5.41	5.73	5.98	5.02	4.47	4.51
IBP - 177°C	9.75	12.33	12.45	8.55	10.54	10.14
177 - 260°C	11.97	11.76	10.98	8.26	9.10	9.35
260 - 343°C	21.93	16.57	15.02	13.06	12.52	14.47
343 - 399°C	12.98	10.38	6.86	7.63	8.38	15.44
399 - 454°C	4.48	5.09	4.09	4.97	4.58	6.42
454 - 524°C	1.45	3.20	3.09	4.52	4.57	3.08
524°C	7.39	8.63	13.41	21.58	19.84	12.84
Unconverted coal	8.06	8.39	9.21	8.81	9.36	6.81
Water	10.63	10.73	11.25	10.51	11.13	10.88
CO	0.28	0.23	0.25	0.20	0.23	0.26
CO <sub>2</sub>	1.12	1.07	1.22	0.96	0.98	0.84
NH <sub>3</sub>	1.03	0.95	0.88	0.67	0.74	0.76
H <sub>2</sub> S	-0.27	0.07	-0.01	0.11	-0.11	-0.04
<b>Process performance, W% maf feed</b>						
Coal conversion	91.8	91.4	90.0	91.0	90.5	93.1
524°C <sup>+</sup> residuum conversion	84.5	82.7	77.3	69.5	70.7	80.3
C <sub>4</sub> - 524°C distillate yield	68.0	65.1	58.5	52.0	54.2	63.4
C <sub>4</sub> - 399°C distillate yield	59.2	53.9	48.2	39.9	42.6	51.2
H <sub>2</sub> consumption	8.80	8.31	7.95	6.81	7.11	7.25
Material recovery balance, %	100.8	100.1	102.4	101.4	101.5	101.0

All conditions utilized a hydrotreater (379°C), an interstage separator, and solid recycle

**Table 3. Separator Overhead (SOH) Properties**

Condition	1	2	3	4	5	6
Period	4	10	15	19	23	29
Gravity, °API	36.9	35.0	36.2	36.4	36.6	37.0
IBP, °C	58	50	60	52	51	56
FBP, °C	340	339	330	339	349	349
<i>Elemental Analysis, W%</i>						
C	86.15	86.62	85.92	85.81	86.16	86.39
H	13.87	13.49	13.35	13.29	13.41	13.39
N	0.23	0.20	0.04	0.04	0.04	0.00
S	0.17	0.19	0.23	0.55	0.25	0.27
H/C atomic ratio	1.92	1.86	1.85	1.85	1.85	1.85
<i>ASTM Distillation, W%</i>						
IBP – 177 °C	26.7	32.2	35.5	34.6	33.3	34.4
177 – 260 °C	28.7	27.9	28.0	28.2	26.5	26.1
260 – 343 °C	36.4	30.7	29.0	28.0	28..56	27.9
343 °C+	8.2	9.2	7.5	9.2	11.7	11.7
<b>TOTAL</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>

**Table 4. Vacuum Still Overheads (VSOH) Properties**

Condition	1	2	3	4	5	6
Period	4*	10	15	19	23	29
Gravity, °API	11.0	8.3	7.0	7.5	8.9	5.5
IBP, °C	226	215	222	225	213	233
<i>Elemental Analysis, W%</i>						
C	88.32	88.22	88.20	87.13	87.84	88.53
H	9.55	8.80	8.62	8.77	9.09	8.48
N	0.49	0.77	0.80	0.92	0.87	0.88
S	0.49	0.09	0.42	0.08	0.12	0.32
H/C atomic ratio	1.29	1.19	1.16	1.20	1.23	1.14
<i>ASTM Distillation, W%</i>						
IBP – 343°C	45.5	55.3	44.5	52.7	59.9	28.7
343 – 454°C	45.8	43.4	43.6	45.4	33.7	49.4
454 – 524°C	8.7	1.4	11.8	1.9	6.4	20.2
524°C+	0.0	0.0	0.0	0.0	0.0	1.7
<b>TOTAL</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>

\*Sub-period "A" only

**Table 5. Vacuum Still Bottoms (VSB) Properties**

Condition	1	2	3	4	5	6
Period	4	10	15	19	23	29
Gravity, °API	-14.8	-14.5	-15.4	-14.9	-14.8	-16.7
IBP, °C	356	340	350	345	347	401
<i>Elemental Analysis, W%</i>						
C	89.75	90.28	90.74	89.59	90.58	90.53
H	6.56	6.23	5.95	6.06	6.29	5.68
N	0.83	0.97	0.95	1.01	1.07	1.06
S	0.29	0.26	0.19	0.19	0.25	0.26
H/C atomic ratio	0.87	0.82	0.78	0.81	0.83	0.75
<i>ASTM Distillation, W%</i>						
IBP – 3.85°C	8.1	11.5	8.5	9.3	8.2	0.0
343 – 454°C	21.9	15.7	14.5	23.4	12.8	10.0
454 – 524°C	10.1	14.4	14.8	**	13.8	15.9
524°C+	59.9	58.4	62.2	67.3	65.2	74.1
<b>TOTAL</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>
<i>Solvent Extraction, W%</i>						
Toluene Insolubles	19.0	28.0	29.5	26.98*	28.47*	32.2
Cyclohexane Insolubles	55.9	78.6	77.1	79.27*	82.91*	93.7

\*Sub-period "A" only

\*\* Combined 385-454°C and 454-524°C fractions for period 19

**Table 6. Pressure Filter Solids (PFS) Properties**

Condition	1	2	3	4	5	6
Period	4	10	15	19	23	29
<b><i>Elemental Analysis, W%</i></b>						
C	66.34	61.35	64.05	62.32	53.47	51.4
H	4.08	3.37	3.42	3.39	2.84	2.49
N	0.49	0.55	0.56	0.62	0.00	0.48
S	3.50	4.74	3.97	3.79	4.93	3.94
H/C atomic ratio	0.73	0.65	0.63	0.64	0.63	0.58
<b><i>Composition, W%</i></b>						
Quinoline solubles	41.7	36.6	38.8	38.8	32.1	27.0
Ash-free quinoline insolubles	34.9	36.1	33.8	32.8	29.8	33.3
Ash	23.4	27.3	27.4	28.4	38.1	39.7
<b><i>TOTAL</i></b>	<b><i>100.0</i></b>	<b><i>100.0</i></b>	<b><i>100.0</i></b>	<b><i>100.0</i></b>	<b><i>100.0</i></b>	<b><i>100.0</i></b>
Sulfur content of ash, W%	2.8	4.1	3.2	3.6	9.9	9.3
<b><i>Solvent Extraction, W%</i></b>						
Toluene Insolubles	47.3	70.8	67.0	68.0	72.4	82.9
Cyclohexane Insolubles	73.4	80.9	78.3	—	—	—

**Table 7. Characterization of Total Distillate Product for Condition 1**

	<i>IBP-82</i>	<i>82-204</i>	<i>204-288</i>	<i>288-343</i>	<i>343-524</i>	<i>WHOLE</i>
Cut, °C						
Weight % of Total	1.60	22.05	32.45	26.15	17.75	100.00
Gravity, °API	60.8	46.4	29.1	23.5	15.0	29.7
Specific Gravity (18°C)	0.7358	0.7954	0.8811	0.9129	0.959	0.8778
Carbon, W%	84.51	85.17	87.30	87.96	88.01	87.62
Hydrogen, W%	14.86	14.02	12.88	12.35	10.70	12.68
Nitrogen, ppm	4	145	264	1,236	5,145	1,387
Sulfur, ppm	<1	11	475	1,061	4,798	989
CCR, W%					0.610	0.007
Ash (ASTM), W%						0.00
Heptane Insolubles, W%						0.06
Basic Nitrogen, ppm						663
Pour Point, °C				-13.1		
Freezing Point, °C			-57	-21	13	-32
Aniline Point, °C		47.2	50.8	51.7	too dark	53.1
Viscosity, cst @ 38°C			2.63	7.10		2.90
Viscosity, cst @ 23.3°C			3.69			
Smoke Point, mm			12.6			
Copper Corrosion, ASTM D130					1A	
Existent Gum, mg/100 mL		11.4				
<b>Metals, ppm</b>						
Vanadium						<1
Nickel						<1
Copper						<1
Iron						<1
<b>PONA Analysis, V%</b>						
Paraffins		23.9	14.4			
Olefins		1.4	0.0			
Naphthenes		71.6	66.8			
Aromatics		3.1	15.8			
Naphthalenes		0.0	3.0			
<b>Total</b>		<b>100.0</b>	<b>100.0</b>			

**Table 8. Characterization of Total Distillate Product for Condition 2**

	<i>IBP-82</i>	<i>82-204</i>	<i>204-288</i>	<i>288-343</i>	<i>343-524</i>	<i>WHOLE</i>
Cut, °C						
Weight % of Total	2.15	23.75	22.50	17.20	34.40	100.00
Gravity, °API	61.2	45.6	24.2	14.8	5.8	22.5
Specific Gravity (18°C)	0.7343	0.7990	0.9088	0.9672	1.0306	0.9188
Carbon, W%	84.76	85.25	87.42	87.98	89.06	87.90
Hydrogen, W%	14.97	13.84	11.91	10.65	9.04	11.28
Nitrogen, ppm	<1	183	354	3,316	8,745	3,003
Sulfur, ppm	<1	14	156	891	4,824	870
CCR, W%					0.626	0.116
Ash (ASTM), W%						0.00
Heptane Insolubles, W%						0.65
Basic Nitrogen, ppm						2,388
Pour Point, °C				-12.0		
Freezing Point, °C			-59	-18	-21	-42
Aniline Point, °C		43	51	59	too dark	46
Viscosity, cst @ 38°C			2.99	12.09		4.34
Viscosity, cst @ 23.3°C			4.17			
Smoke Point, mm			10.3			
Copper Corrosion, ASTM D130					1A	
Existent Gum, mg/100 mL		12.4				
<b>Metals, ppm</b>						
Vanadium						<1
Nickel						<1
Copper						<1
Iron						1.4
<b>PONA Analysis, V%</b>						
Paraffins		21.5	5.8			
Olefins		1.1	0.0			
Naphthenes		71.0	61.4			
Aromatics		6.4	28.8			
Naphthalenes		0.0	4.0			
<b>Total</b>		<b>100.0</b>	<b>100.0</b>			

**Table 9. Material Balance for Economic Assessment**

<i>Condition</i>	<i>Coal type, Shenhua #</i>					
	<u>1</u>	<u>2</u>	<u>3</u>	<u>4</u>	<u>5</u>	<u>6</u>
<i>Feed to Liquefaction</i>						
Coal, T/D	12,000	12,000	12,000	12,000	12,000	12,000
<i>Liquid Products, B/D</i>						
Gasoline	15,059	14,077	12,486	10,801	10,980	13,524
Diesel Fuel	35,582	33,260	29,501	25,521	25,944	31,953
Total	50,641	47,337	41,987	36,322	36,924	45,477
Bbl Product/Ton Feed	4.22	3.94	3.50	3.03	3.08	3.79
<i>By-Products</i>						
Propane, B/D	5,713	6,046	6,264	5,494	4,900	5,417
Butane, B/D	3,365	3,407	3,607	3,132	2,823	3,166
Sulfur, T/D	35	36	38	38	37	32
Ammonia, T/D	118	109	101	77	83	86
Waste to Disposal, T/D	527	530	537	546	777	766



**Table 10. Hydrogen Balance, Utilities & Thermal Efficiency**

Condition	<u>1</u>	<u>2</u>	<u>3</u>	<u>4</u>	<u>5</u>	<u>6</u>
<b>Hydrogen Balance</b>						
<i>Hydrogen Consumption, 10<sup>6</sup> SCFD</i>						
Liquefaction	381.5	360.2	344.6	295.2	302.0	307.9
Product Upgrading	44.8	53.3	49.7	57.3	36.4	65.1
Solution & Purge Losses	15.7	15.9	15.9	13.1	12.0	12.6
Total	442.0	429.4	410.2	365.6	350.4	385.6
Hydrogen used, SCF/Bbl	8,730	9,070	9,770	10,070	9,490	8,480
<i>Hydrogen Production, 10<sup>6</sup> SCFD</i>						
Partial Oxidation	154.9	186.1	245.2	322.1	291.5	183.4
Steam Reforming	287.1	243.3	165.0	43.5	58.9	202.2
Total	442.0	429.4	410.2	365.6	350.4	385.6
<b>Hydrogen Balance</b>						
Power, MW	268	275	290	298	283	254
Steam, 600 Psig, 10 <sup>3</sup> lb/hr	220	215	165	189	143	151
Cooling water, 10 <sup>3</sup> GPM	187	186	177	168	154	162
Natural Gas, 10 <sup>9</sup> BTU/D	141.6	127.2	99.7	62.7	70.8	120.6
Raw water, 10 <sup>3</sup> Gal/D	7,229	7,766	8,291	9,521	8,442	6,868
<b>Thermal Efficiency</b>						
<i>Inputs, 10<sup>9</sup> BTU/Day</i>						
Feed	322.4	322.4	322.4	322.4	308.3	308.3
Natural Gas	157.1	141.2	110.6	69.6	78.6	133.8
Total	479.5	463.6	433.0	392.0	386.9	442.1
<i>Outputs, 10<sup>9</sup> BTU/Day</i>						
Gasoline	82.5	77.1	68.3	59.1	60.1	74.1
Diesel Fuel	206.7	193.1	171.2	148.0	150.5	185.5
Propane & Butane	36.7	38.1	39.8	34.8	31.1	34.6
Sulfur & Ammonia	2.6	2.4	2.3	1.8	1.9	2.0
Total	328.5	310.7	281.6	243.7	243.6	296.2
Thermal Efficiency, HHV	68.5	67.0	65.0	62.2	63.0	67.0

**Table 11. Capacities of Process Units & Offsites**

<b>Condition</b>		<b><u>1</u></b>	<b><u>2</u></b>	<b><u>3</u></b>	<b><u>4</u></b>	<b><u>5</u></b>	<b><u>6</u></b>
<b><i>Area or Item</i></b>	<b><i>Sizing Basis</i></b>						
Coal Preparation	T/D dry coal	12,000	12,000	12,000	12,000	12,000	12,000
Liquefaction	T/D total feed	12,000	12,000	12,000	12,000	12,000	12,000
<b><i>H<sub>2</sub> Manufacture</i></b>							
Steam Reforming	10 <sup>6</sup> SCFD H <sub>2</sub>	287.1	243.3	165.0	43.5	58.9	202.2
Partial Oxidation	10 <sup>6</sup> SCFD H <sub>2</sub>	154.9	186.1	245.2	322.1	291.5	183.4
Oxygen Plant	T/D Oxygen	1,922	2,312	3,048	4,009	3,624	2,280
<b><i>Treating</i></b>							
Sour water treating	gpm sour water	1,921	1,857	1,779	1,601	1,575	1,665
Sulfur recovery	T/D Sulfur						
Gas plant	lb/hr C <sub>1</sub> -C <sub>3</sub>	120,650	126,010	127,160	114,320	101,010	107,770
<b><i>Product Upgrading</i></b>							
Catalytic Reforming	B/D gasoline	15,059	14,077	12,486	10,801	10,980	13,524
Hydrotreating	B/D liquids	35,582	33,260	29,501	25,521	25,944	31,953
<b><i>Utilities</i></b>							
Steam generation	10 <sup>3</sup> lb/hr	220	215	165	189	143	151
Power generation	MW	268	275	290	298	283	254
Cooling water	10 <sup>3</sup> GPM	187	186	177	168	154	162
<b><i>Tankage</i></b>							
Product Liquids	B/D liquids	50,641	47,337	41,987	36,322	36,924	45,477
Propane & Butane	B/D	9,078	9,453	9,871	8,626	7,723	8,583
Solids handling	T/D	527	530	537	546	777	766
General Offsites	T/D total feed	12,000	12,000	12,000	12,000	12,000	12,000

**Table 12. Liquefaction Plant Investment Details**

<b>Condition</b>	<b><u>1</u></b>	<b><u>2</u></b>	<b><u>3</u></b>	<b><u>4</u></b>	<b><u>5</u></b>	<b><u>6</u></b>
<b><i>Major Equipment Cost, 10<sup>3</sup> \$</i></b>						
Pumps	22,319	22,447	22,420	22,215	22,379	22,725
Reactor	52,237	52,657	52,657	47,085	51,798	51,798
Fired heaters	14,544	15,201	15,511	15,998	16,190	16,491
Exchangers	20,615	20,470	20,327	20,172	20,139	20,340
Drums	30,681	30,617	30,625	30,808	30,849	30,594
Towers	8,468	8,581	8,652	8,831	8,900	8,961
Compressors	35,084	34,315	33,720	31,762	32,007	32,298
HPU	20,568	20,810	20,828	18,250	17,086	17,631
Total	204,516	205,098	204,740	195,121	199,348	200,838
<b><i>Plant Investment, 10<sup>6</sup> \$</i></b>						
Materials & Equipment	370.6	371.6	371.0	353.5	361.2	363.8
Labor & Subcontracts	160.3	160.8	160.5	153.0	156.3	157.5
Indirects	133.4	133.8	133.5	127.3	130.0	131.0
Total	66.43	666.2	66.50	633.8	647.5	652.3

**Table 13. Total Plant Investment**  
(Plant Investment in 10<sup>6</sup> \$, 1994 US Gulf Coast Basis)

<b>Condition</b>	<b><u>1</u></b>	<b><u>2</u></b>	<b><u>3</u></b>	<b><u>4</u></b>	<b><u>5</u></b>	<b><u>6</u></b>
Coal Preparation	57.6	57.6	57.6	57.6	57.6	57.6
Liquefaction	664.3	666.2	665.0	633.8	647.5	652.3
Hydrogen Manufacture	363.5	355.8	338.9	287.6	284.7	327.6
Oxygen Plant	74.2	84.5	102.5	124.2	115.7	83.6
Treating	346.4	355.6	357.1	332.4	307.1	320.1
Product Upgrading	115.9	114.5	112.1	110.7	111.6	115.1
Utilities	318.4	325.1	337.8	343.1	330.4	307.1
Tankage, Waste Handling	158.0	149.8	136.1	121.6	125.9	147.8
General Offsites	211.0	211.0	211.0	211.0	211.0	211.0
Subtotal	2,309.3	2,320.1	2,318.1	2,222.0	2191.5	2,222.2
Contingency & Fee	461.3	463.4	463.2	443.7	437.9	444.1
Total Plant Investment	2,770.6	2,783.5	2,781.3	2,665.7	2,629.4	2,666.3
\$/BPSD of Product	54,710	58,800	66,240	73,390	71,210	58,630

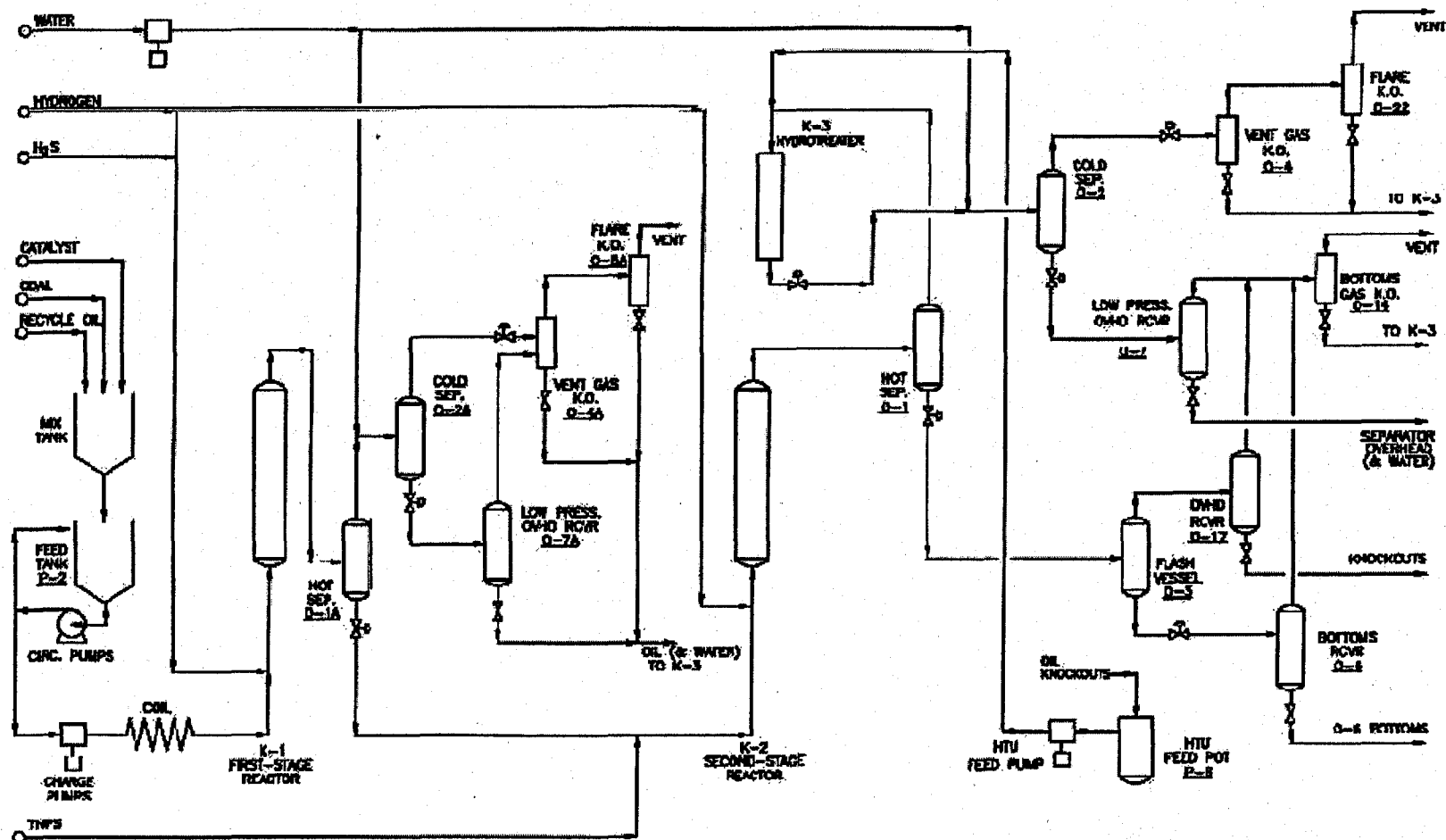
**Table 14. Product Cost**

<b>Condition</b>	<b><u>1</u></b>	<b><u>2</u></b>	<b><u>3</u></b>	<b><u>4</u></b>	<b><u>5</u></b>	<b><u>6</u></b>
<i>Operating Costs, 10<sup>6</sup> \$/yr</i>						
Coal, as received (\$13.25/Ton)	58.03	58.03	58.03	58.03	58.03	58.03
Natural Gas (\$2.00/10 <sup>6</sup> BTU)	93.01	83.54	65.48	41.17	46.49	79.23
River Waste (\$0.10/10 <sup>3</sup> gal)	0.24	.026	0.27	0.31	0.28	0.23
Waste Disposal (\$5.00/Ton)	0.87	0.87	0.88	0.90	1.28	1.26
Catalysts & Chemicals	20.03	17.79	13.73	7.46	7.90	15.19
Dispersed Catalyst	33.94	49.11	33.94	33.94	33.94	33.94
Labor	22.99	22.99	22.99	22.99	22.99	22.99
Maintenance	20.59	20.59	20.59	20.59	20.59	20.59
Capital-related costs	415.41	415.57	412.65	393.61	388.82	398.25
Total	665.11	668.75	628.56	579.00	580.32	629.71
<i>By-product Credits, 10<sup>6</sup> \$/yr</i>						
Propane (\$12.50/B)	23.46	24.83	25.72	22.56	20.12	22.24
Butane (\$14.50/B)	16.03	16.23	17.18	14.92	13.45	15.08
Sulfur (\$52.00/Ton)	0.59	0.61	0.65	0.66	0.64	0.55
Ammonia (\$120.00/Ton)	4.66	4.30	3.99	3.04	3.28	3.37
Total	44.74	45.97	47.54	41.18	37.49	41.24
Net Product cost, 10 <sup>6</sup> \$/year	620.37	622.78	581.02	537.82	542.83	588.47
Net Product cost, \$/B	37.29	40.05	42.12	45.07	44.75	39.39
<b>Equivalent Crude Price, \$/B</b>	<b>31.20</b>	<b>34.00</b>	<b>36.16</b>	<b>39.29</b>	<b>38.95</b>	<b>33.33</b>

**Table 15. Breakdown of Equivalent Crude Oil Price**

<b>Condition</b>	<b><u>1</u></b>	<b><u>2</u></b>	<b><u>3</u></b>	<b><u>4</u></b>	<b><u>5</u></b>	<b><u>6</u></b>
<b>Total Product, B/D</b>	<b>50,641</b>	<b>47,337</b>	<b>41,987</b>	<b>36,322</b>	<b>36,924</b>	<b>45,477</b>
<i>Contribution to Price, \$/B</i>						
Coal	2.92	3.17	3.61	4.24	4.16	3.29
Natural Gas	4.68	4.56	4.08	3.01	3.34	4.49
River Water	0.01	0.01	0.02	0.02	0.09	0.07
Waste Disposal	0.04	0.05	0.06	0.07	0.09	0.07
Catalysts & Chemicals	2.71	3.654	2.97	3.03	3.00	2.78
Labor	1.16	1.26	1.43	1.68	1.65	1.30
Maintenance	1.04	1.12	1.28	1.50	1.48	1.17
Capital-related costs	20.89	22.69	25.67	28.75	27.90	22.56
By-product credits	-2.25	-2.51	-2.96	-3.01	-2.69	-2.34
<b>Equivalent Crude Price, \$/B</b>	<b>31.20</b>	<b>34.00</b>	<b>36.1</b>	<b>39.29</b>	<b>38.95</b>	<b>33.33</b>

FIGURE 1: SIMPLIFIED FLOW DIAGRAM

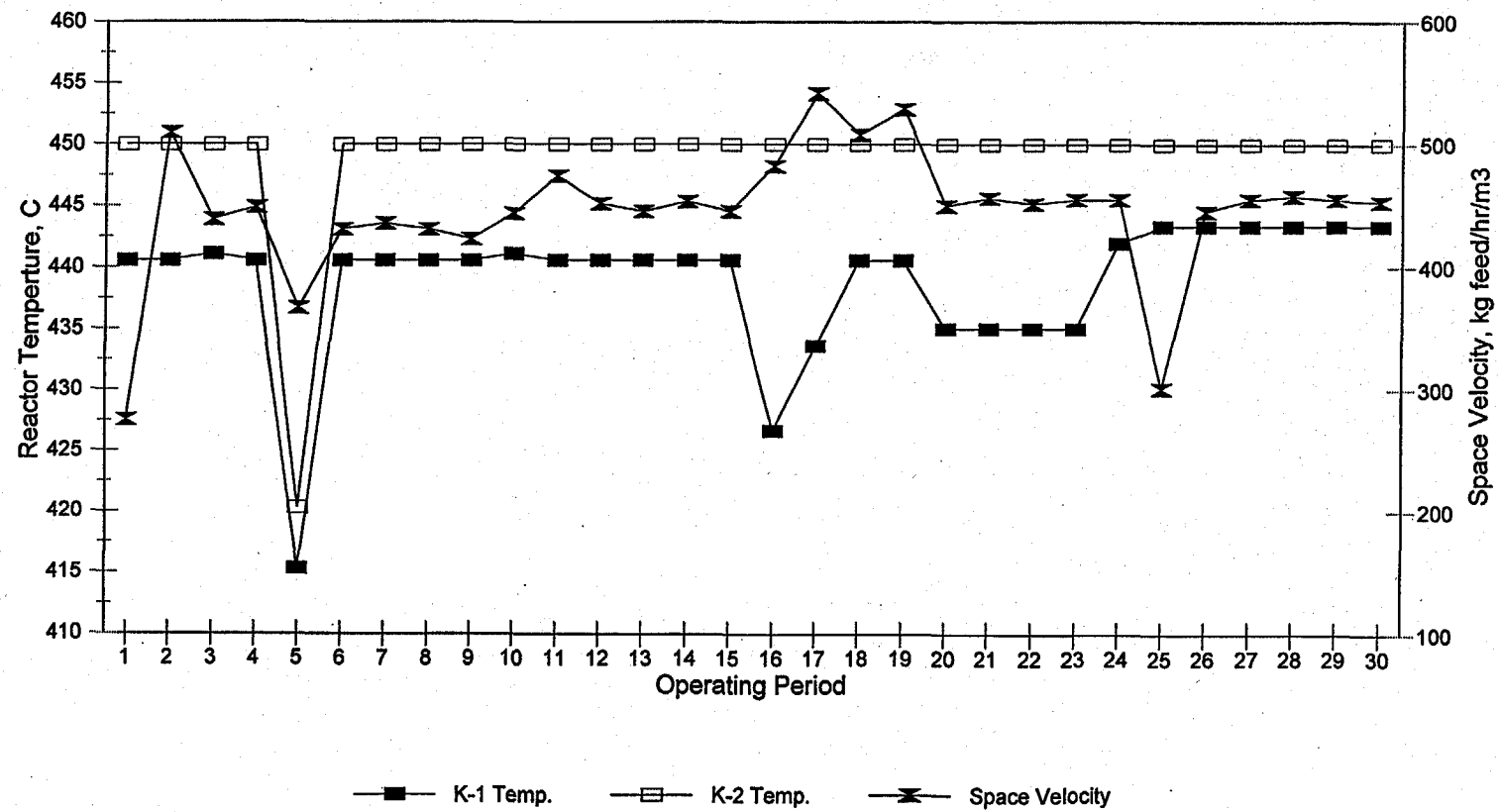


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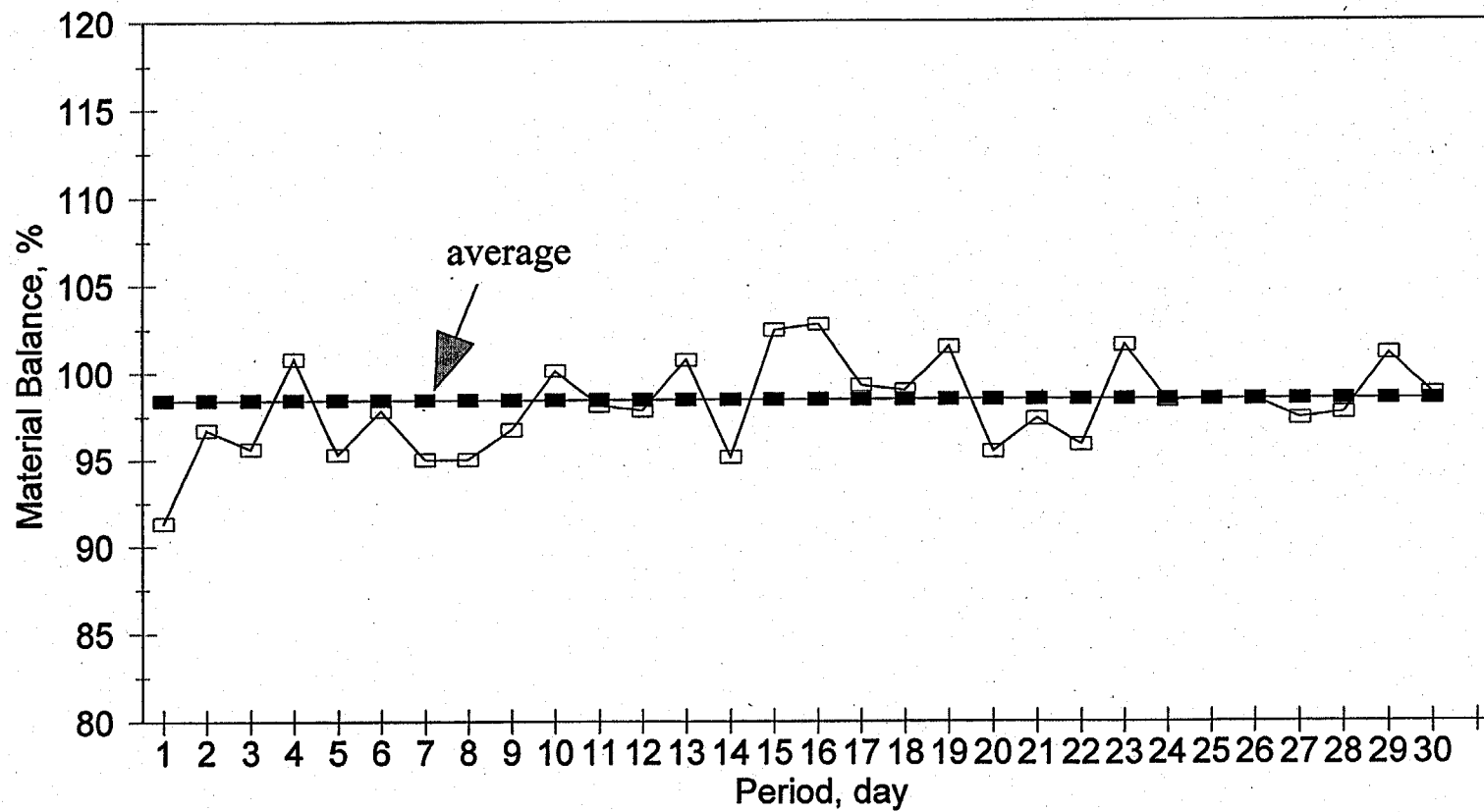
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**Figure 2**  
**Daily Operating Conditions**

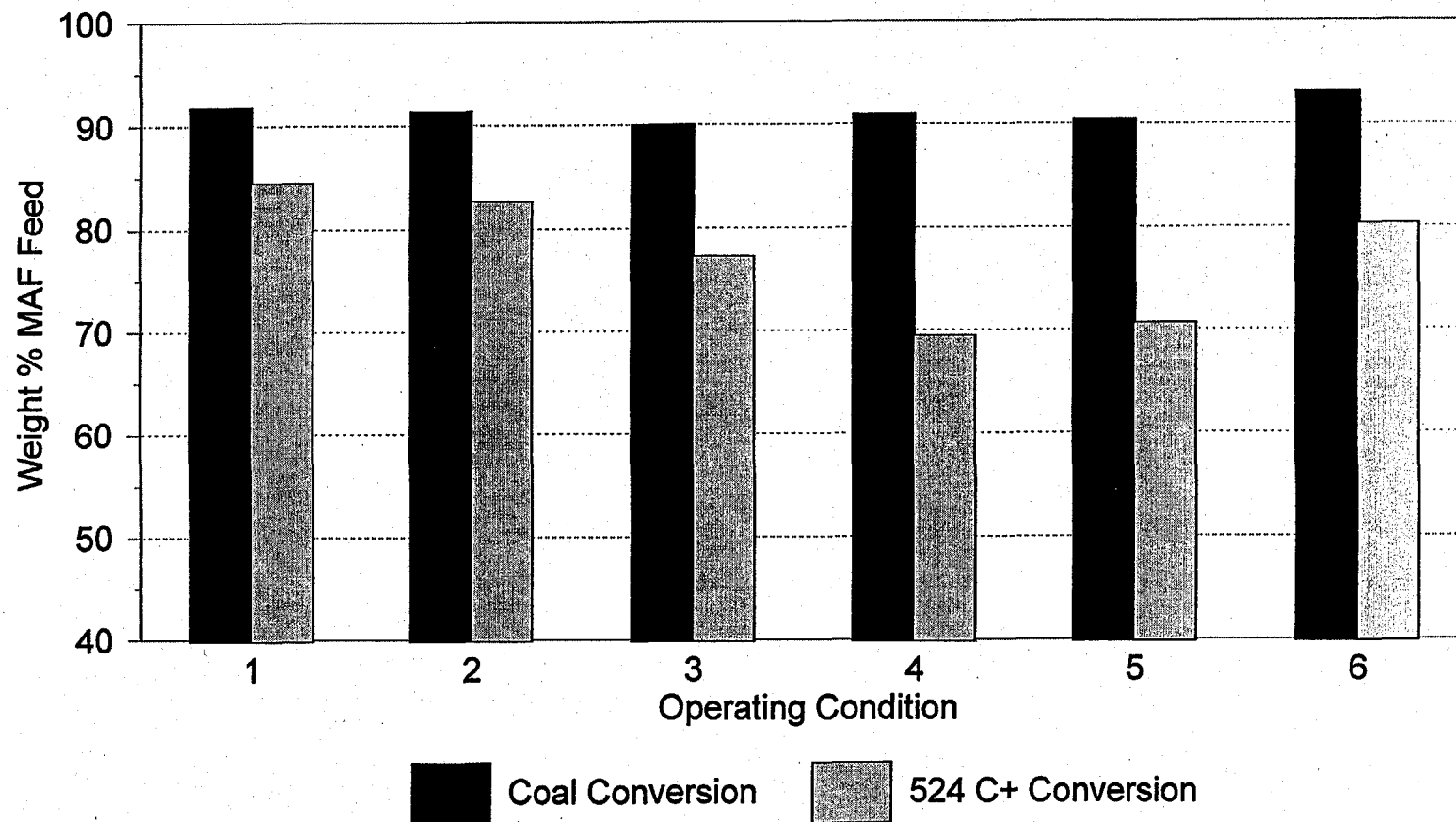




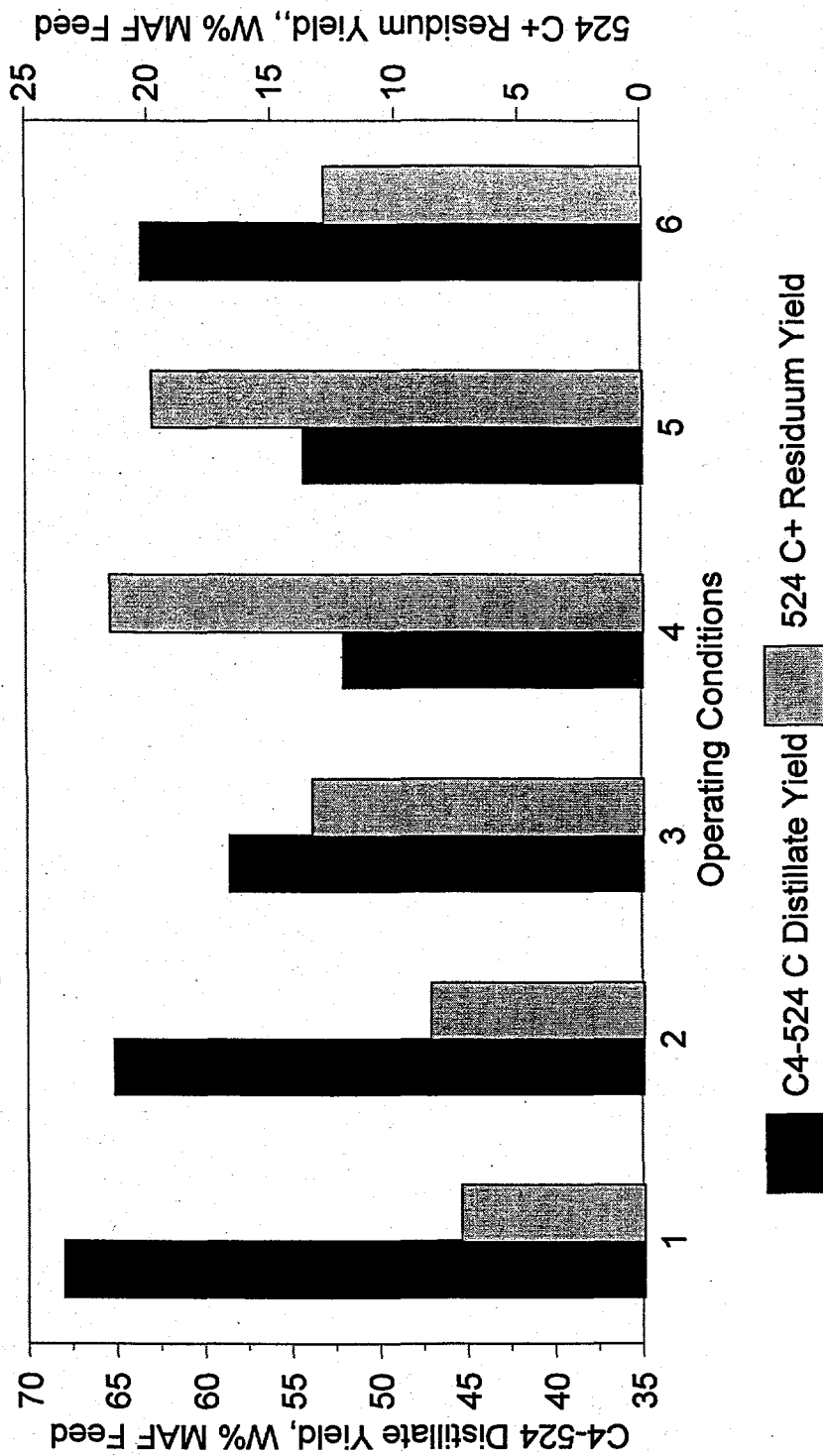
**Figure 3**  
**Daily Material Balance**



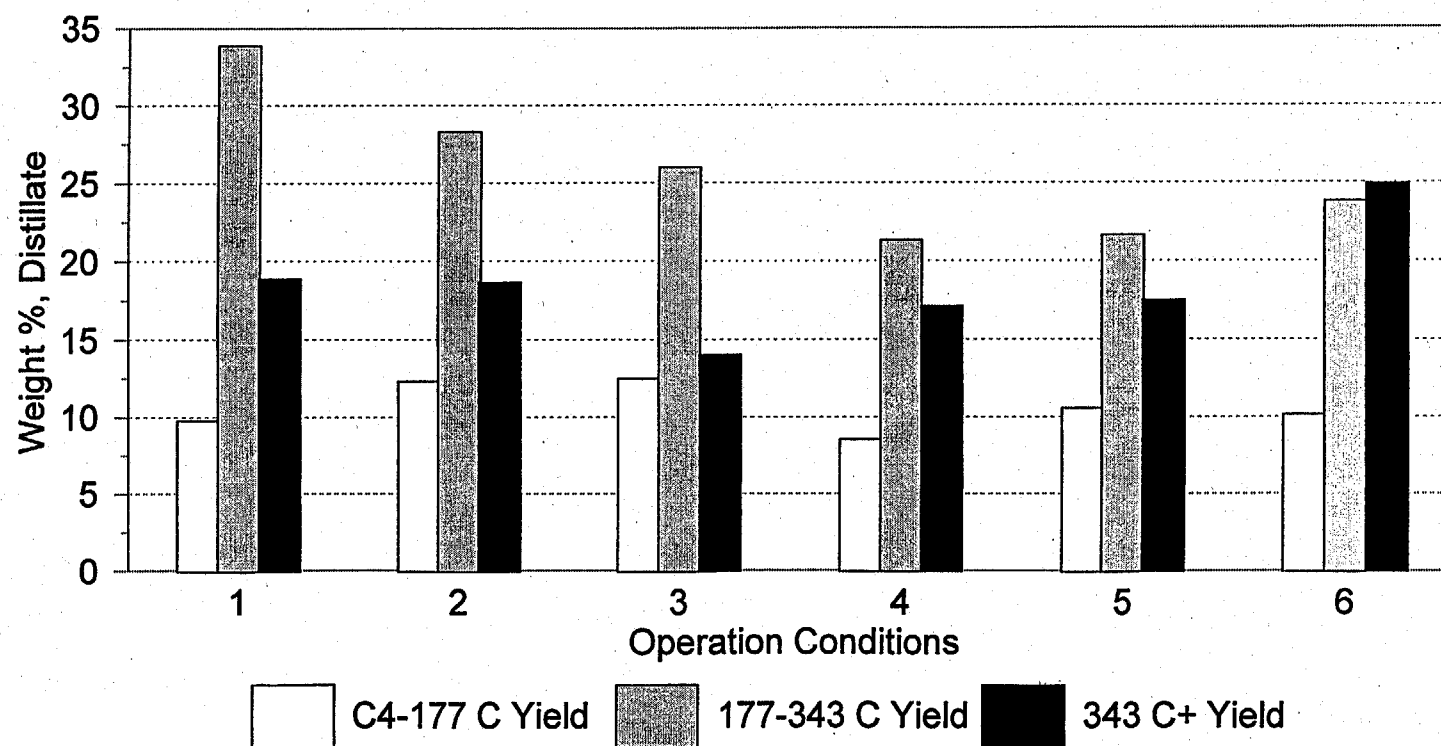
**Figure 4**  
**Coal and Residuum Conversion**



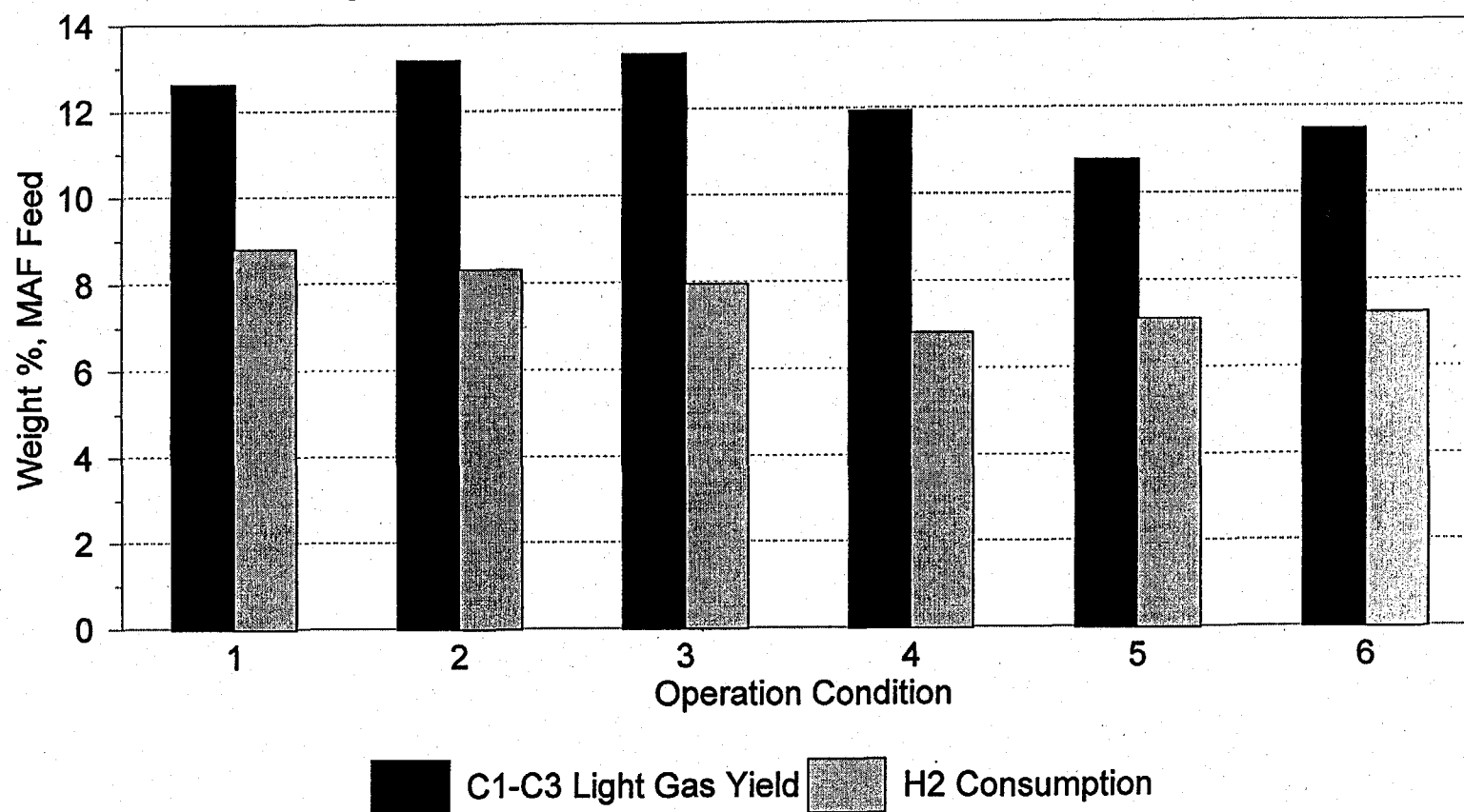
**Figure 5**  
**Distillate and Residuum Yield**



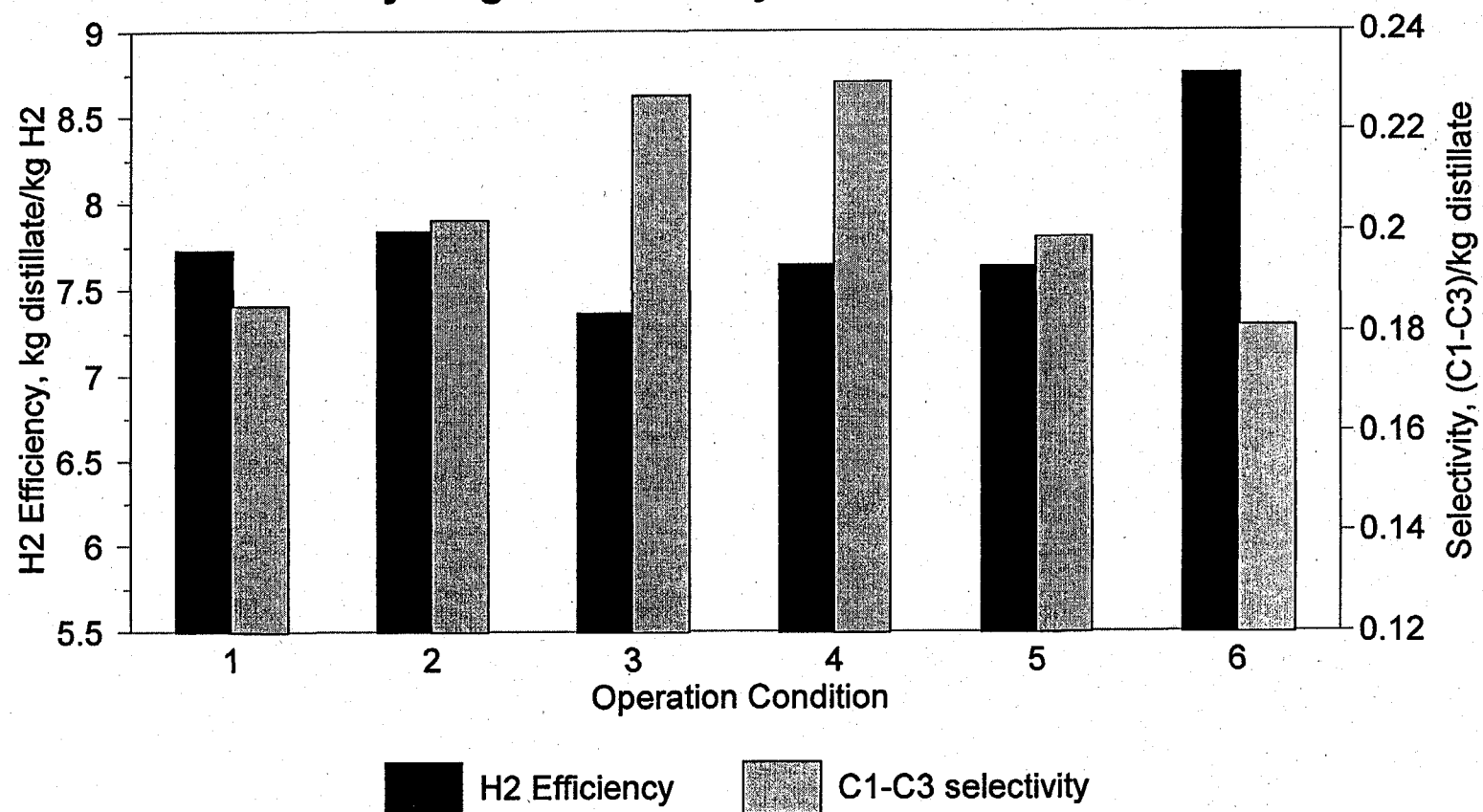
**Figure 6**  
**Distillate Fraction Yield**



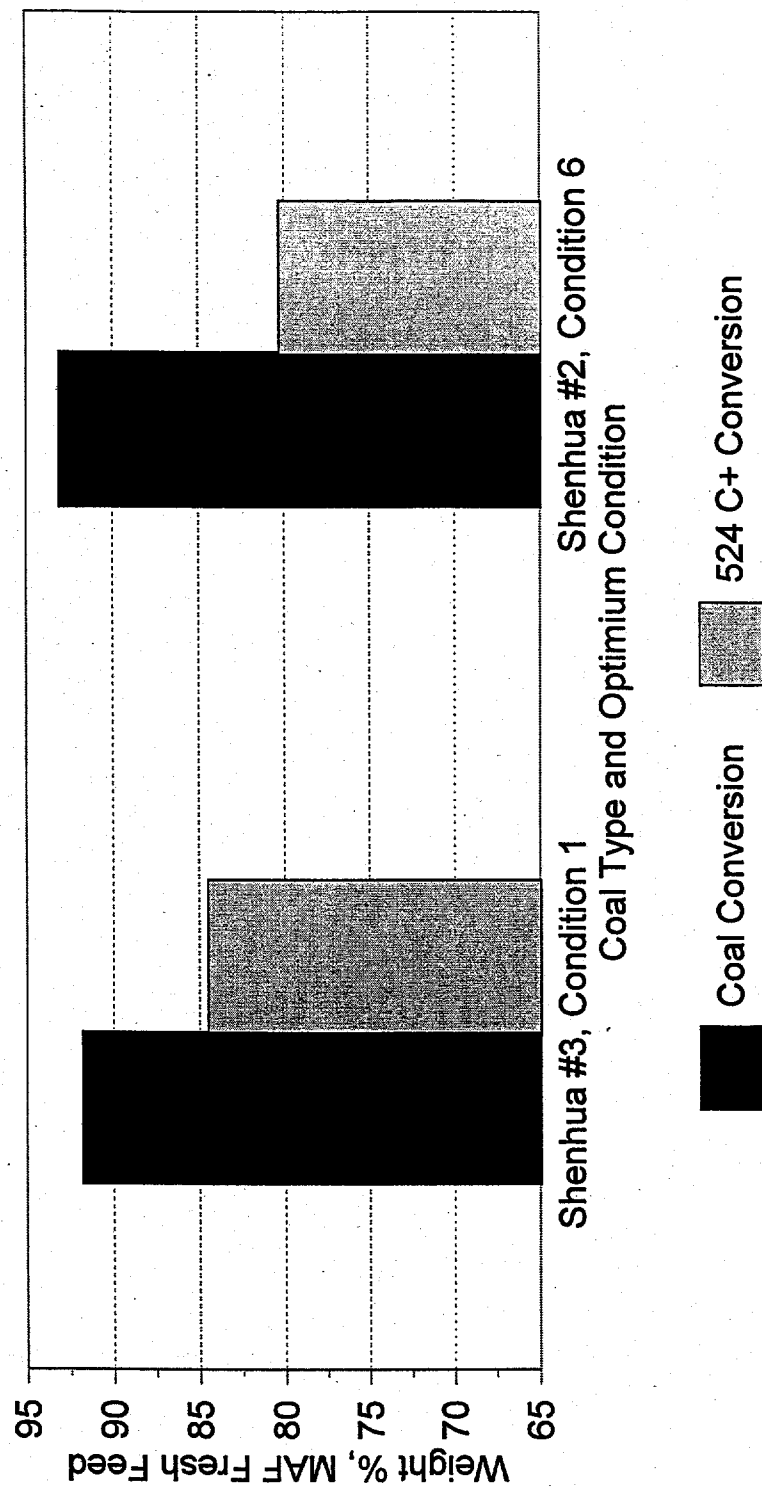
**Figure 7**  
**Hydrogen Consumption & Light Gas Yield**



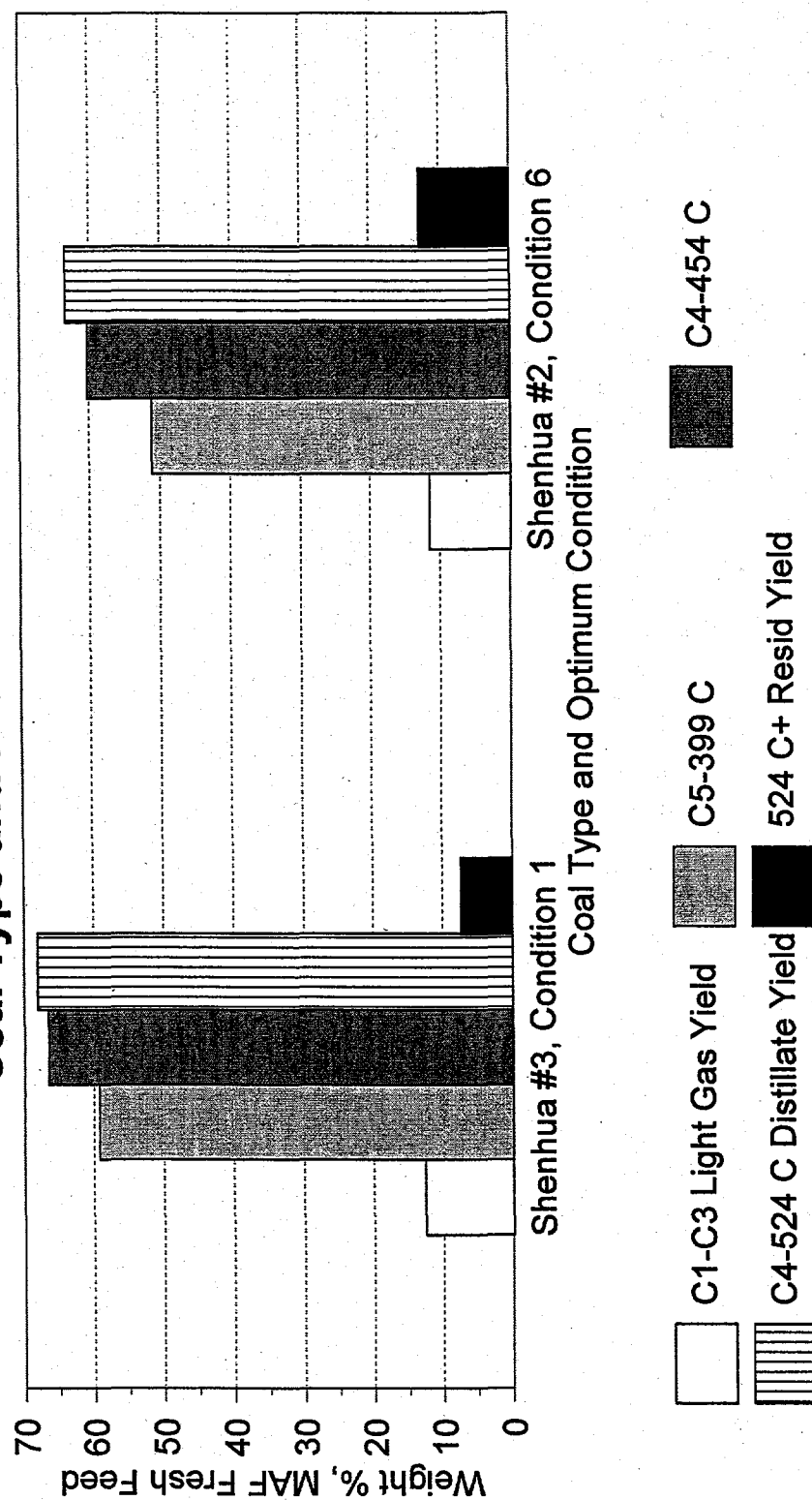
**Figure 8**  
**Hydrogen Efficiency & Gas Selectivity**



**Figure 9**  
**Coal Type and Feed Conversion**

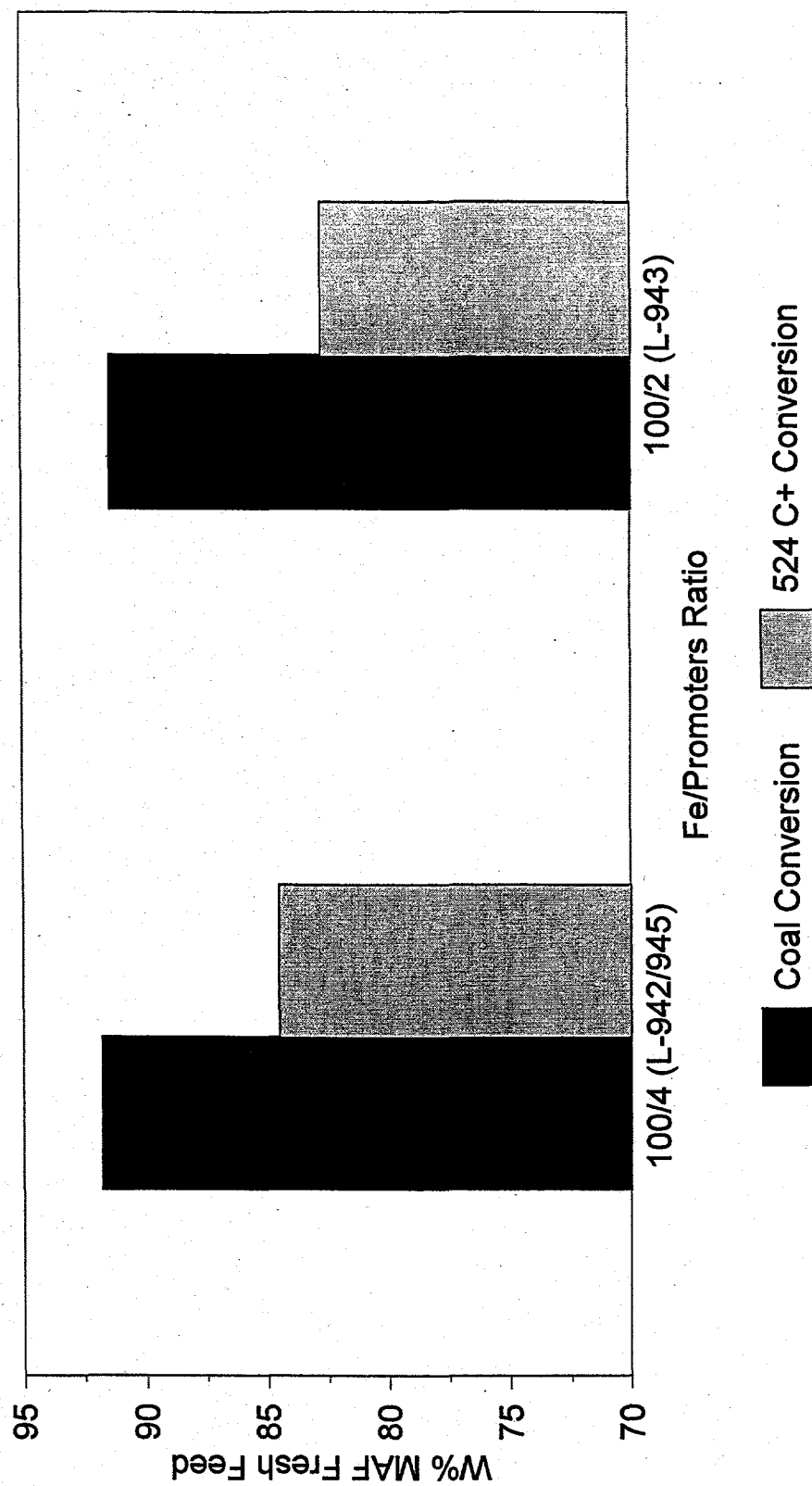


**Figure 10**  
**Coal Type and Product Yields**





**Figure 11**  
**Catalyst Type and Feed Conversion**



**Figure 12**  
**Catalyst Type and Product Yields**

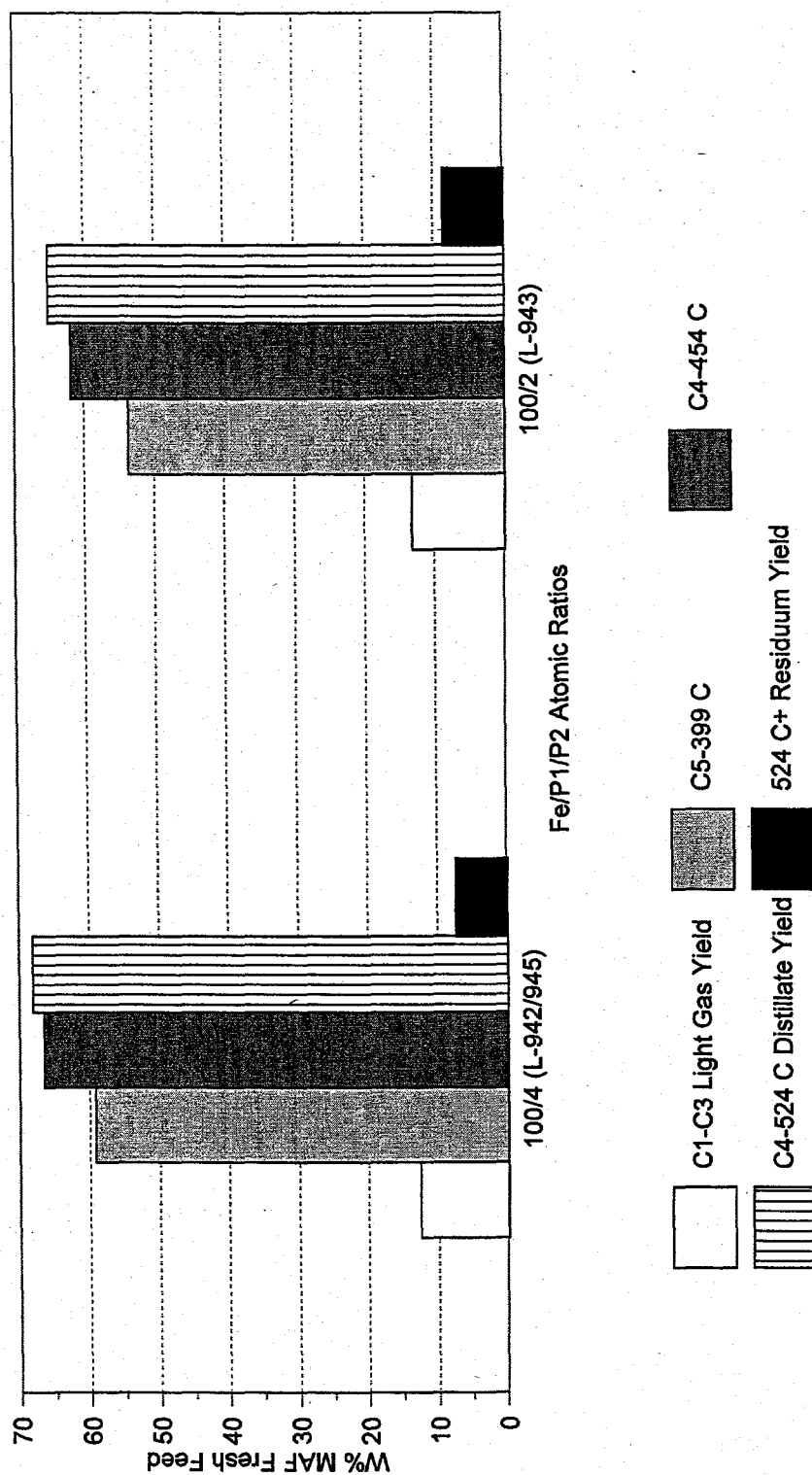


Figure 13 Coal Price Sensitivity

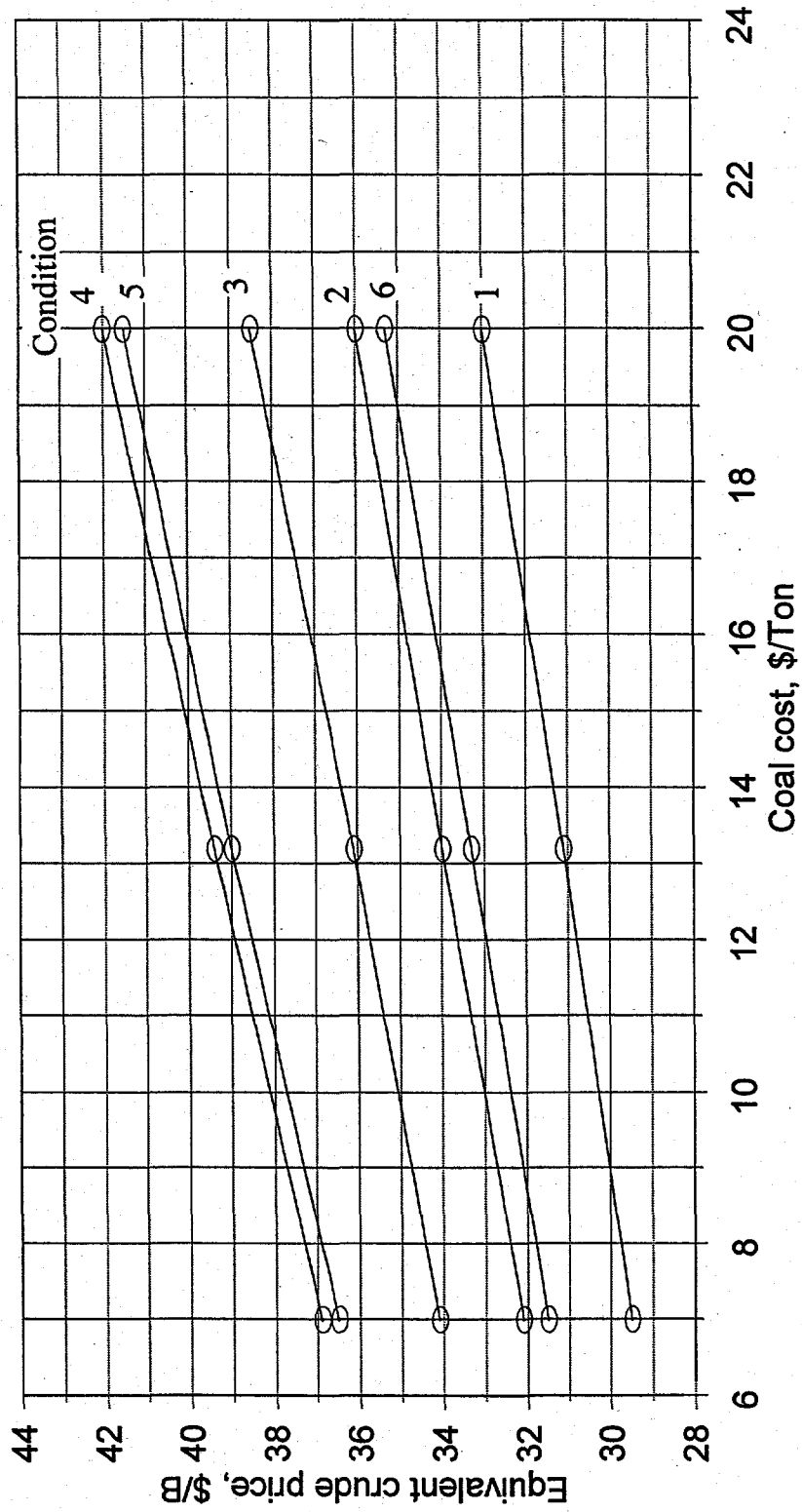


Figure 14 Gas Price Sensitivity

