Production and Optimization of Direct Coal Liquefaction derived Low Carbon-Footprint Transportation Fuels

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DOE Contract No. DE-FC26-05NT42448

FINAL SCIENTIFIC/TECHNICAL REPORT

(Reporting Period: 07/01/2005 to 06/30/2010)

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Disclaimer

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ABSTRACT

This report summarizes works conducted under **DOE Contract No. DE-FC26-05NT42448.** The work scope was divided into two categories – a) experimental program to pretreat and refine a coal derived syncrude sample to meet transportation fuels requirements; b) system analysis of a commercial scale direct coal liquefaction facility. The coal syncrude was derived from a bituminous coal by Headwaters CTL, while the refining study was carried out under a subcontract to Axens North America. The system analysis included H_2 production cost via six different options, conceptual process design, utilities requirements, CO_2 emission and overall plant economy. As part of the system analysis, impact of various H_2 production options was evaluated. For consistence the comparison was carried out using the DOE H2A model. However, assumptions in the model were updated using Headwaters' database. Results of Tier 2 jet fuel specifications evaluation by the Fuels & Energy Branch, US Air Force Research Laboratory (AFRL/RZPF) located at Wright Patterson Air Force Base (Ohio) are also discussed in this report.

Production and Optimization of Direct Coal Liquefaction (DCL) derived Low Carbon-Footprint Transportation Fuels

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Production and Optimization of Direct Coal Liquefaction derived Low Carbon-Footprint Transportation Fuels

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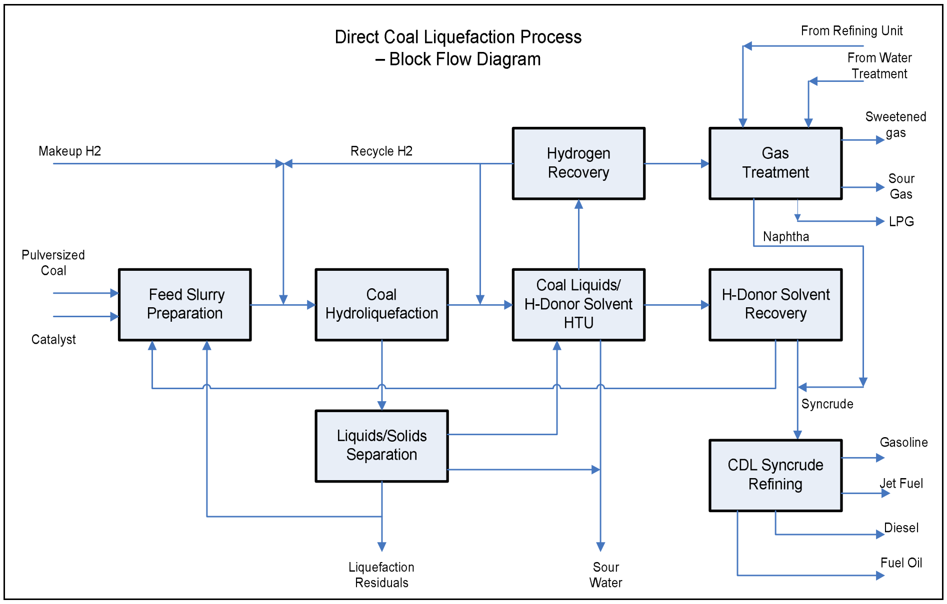
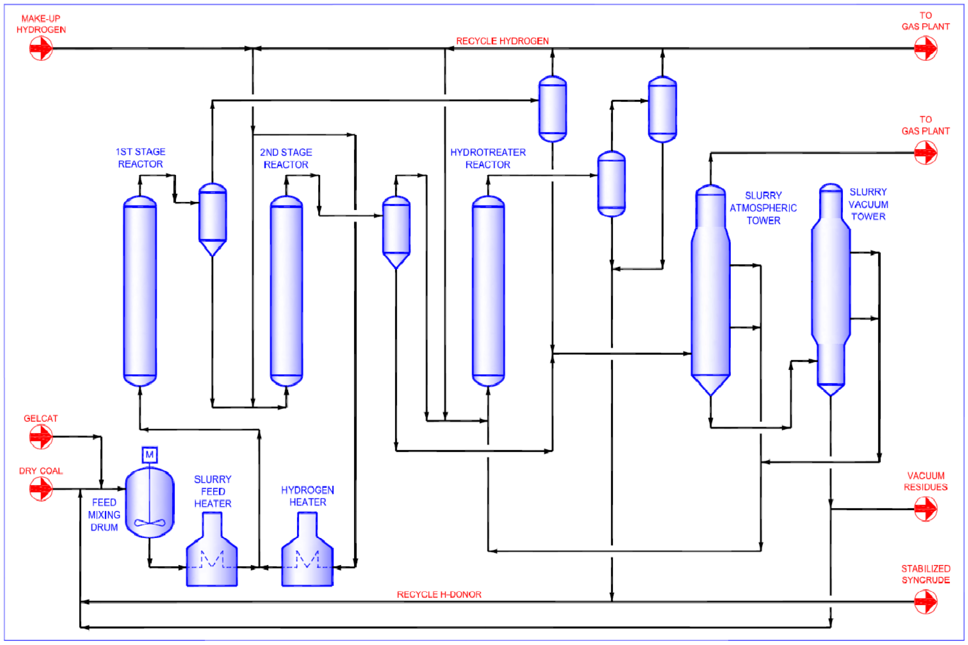
EXECUTIVE SUMMARY

This study entailed a techno-economic analysis of a direct coal liquefaction process (DCL) for production of low carbon-footprint transportation fuels. The selected process is Headwaters two-stage, dispersed iron catalyst hydroliquefaction process, a start-of-art DCL technology. This study included a conceptual design of the DCL complex which encompassed a coal conversion section, a coal derived product refining section and auxiliary units (power block, sulfur recovery unit and waste water treatment). The hydrogen supply to the complex was treated as an crossed-the-fence facility. Several production methods: steam methane reforming (SMR), coal partial oxidation (POX) with and without biomass addition, biomass POX and electrolysis.



The design basis for the DCL plant was generated from a previous bench run on Illinois No. 6 coal (Condition 1 of Run POC-5) under the 1996 DOE Proof-of-Concept Program (DOE Contract # AC22-92PC92148). This condition resulted in coal conversion of 95.5 w%, 524°C minus distillate yield of 70.8 w% and chemical hydrogen consumption of 5.5 w% (all values are in maf coal basis).

Headwaters DCL process is a two-stage hydroliquefaction process using an iron based synthetic water based dispersed catalyst. The process employed two fully backmixed reactor for effective conversion and initial cracking of the primary coal fragments. All distillate products and spent recycle solvent are hydrogenated in a direct coupled fixed bed or ebullated bed reactor. A simplified diagram is given below:



The refining data was adapted from a refining study on DCL coal liquids generated from a foreign bituminous coal with similar properties. The refining study was co-ordinated by Axens North Amercia and conducted by IFP of France. The syncrude from the DCL plant was treated through a fixed bed hydroprocessing unit which is packed with hydrotreating and hydrocraking catalysts. The treated naphtha has sufficient low nitrogen that it can be further processed in a Pt-catalytic reforming unit to produce on spec gasoline, while kerosene and diesel fractions will meet the corresponding US specifications for jet and diesel fuels. The remaining fuel oils (fraction has a boiling point higher than diesel fuel) have very low sulfur content and its amount can be adjusted based on market needs.

A 4-liter sample of 100% DCL kerosene was submitted to the Fuels & Energy Branch, US Air Force Research Laboratory (RZPF), Wright Patterson Air Force Base. The DCL kerosene was determined to pass all specifications for JP-8, with the exception of the conductivity specification which can be met with the help of additive (which is also needed for petroleum derived kerosene). The DCL liquid was noted for good low temperature properties (freeze point of -77°C) and lubricity similar to that of petroleum derived jet fuel.

Properties	**JP-Specification**	**DCL Kerosene**	**Typical JP-8**
Density, kg/L @ 15°C	775-840	0.837	0.804
Hydrogen, w% Sulfur, ppm	>13.4 <3000	13.7 <3	13.8 383
Aromatics, w%	<25	1.6	18.8
Freeze Point, °C	<-47	-77	-51

Smoke Point, mm	>19	23	22
Heat of Combustion - MJ/kg – calc. - MJ/L – calc.	>42.8	43.1 36.1	43.2 34.7
Lubricity (BOCLE) Wear scar mm	≤0.85	0.57	0.53

The DCL diesel met or exceeded current US specifications (ASTM D975), as shown below.

Properties	**U.S. Spec.**	**DCL Diesel**	**EU Spec.**
Density, kg/L @ 15°C	Not specified	0.855-0.885	>0.820 <0.845
Sulfur, ppm	<15	<5	<10
Aromatics, w%	<35	2 - 10	
Di-Aromatics, w%		0 -2	<11
Pour Point, °C		< -48	CFPP <-15
Cetane Number	>40	45-54	>51

In general because of high proportion of ring structure in the DCL diesel, its density is relatively high. There is no specification for diesel in the United State. However, it is not the case for Europe, DCL diesel will need to be blended with petroleum derived distillate to meet the density specification. It is also note that the petroleum derived cetane index tends to underestimate the cetane number significantly.

As for DCL naphtha, the catalytic reforming test confirmed that it is a good feedstock for gasoline production. The reforming severity for processing DCL naphtha is less severe than that for straight run petroleum derived naphtha of similar boiling range. The yield of C5+ reformate is relatively high than that of the straight run petroleum naphtha.

However, the DCL 360°C+ vacuum gas oils (VGO) were found to be more difficult to be cracked under fluid catalytic cracking conditions. Standardized microcat FCC test reviewed that the 360°C+ conversion for petroleum VGO typically varied between 81.8 to 85.2 w%, while that of DCL VGO was only 60.3 to 69.0 w%.

Conceptual design of a 45,850 BPSD DCL plant using Illinois No. 6 coal as feed was developed. The DCL plant requires 11,250 metric tons of run-of-mine coal which contains 7 w% moisture and 9.52 w% ash (as received basis). The product breakdown is 17,013 BPSD of gasoline, 13, 341 BPSD of kerosene, 9,040 of diesel, and 6,450 BPSD of VGO. Also, the plant produces 4.794 BPSD of LPG, 2,030 TPD of heavy VGO and 537 TPD of vacuum bottom residuals. The plant consumed 125 MW of power and 16.8 million Kcal/h of fuel gas from battery limits. CO_2 emission for the DCL plant is estimated to be 42.9 kg/bbl of distillate products. Again, this CO_2 emission value does not include emission from the H_2 plant.

The total installed cost of the DCL plant, including products refining and auxiliary units but not the H2 Plant, was estimated to be US$2,713 million. This estimate included 20% contingency on EPC cost, 13.8 w% of non-EPC cost plus financing cost. Assuming an interest rate of 7% for the 4 year construction period and 2 months of working capital, the total project cost is estimated to be $3,025 million.

It was assumed that hydrogen will be purchased across the fence from a neighboring facility or pipeline. Several manufacturing options were evaluated. The selling prices of hydrogen for the different options evaluated are listed below:

Hydrogen Production Option	CO_2 Emission[1] ton CO_2/ton H_2 produced	H_2 RSP[2] (Required Selling Price)	
		$/metric Ton H_2	$/bbl Distillate
Steam Methane Reforming (SMR)			
Low NG Cost ($5.0/MMBtu)	0.93	1,471.40	23.52
High NG Cost ($7.5/MMBtu)	0.93	1,881.40	30.08
Coal-Resid Gasification (Coal-POX)	1.53	1,837.00	29.37
Biomass Gasification (Biomass-POX)			
Low Cost ($35/ short ton)	0	3,345.97	53.49
High Cost ($75/ short ton)	0	3,885.97	62.13
Coal-Resid-Biomass Gasification			
Low Biomass Cost($35/ short ton)	0.83	2,424.82	38.77
High Biomass Cost ($75/ short ton)	0.83	2,664.82	42.60
Electrolysis			
Nuclear Power	0	3,254.20	52.03
Grid Power	0	6,118.30	97.62

Note:

1) With 90% CO_2 capture
2) An internal rate of return of 18% for the investment is assumed for all the options.

SMR is the lowest capital option. At a natural gas price of $5.00 to $7.5, the required selling price (RSP) of H_2 is estimated to be $1,471 and $1,881per metric ton, respectively. The coal partial oxidation option has a higher investment cost. At a coal price of $22.51 per metric ton, the RSP is $1,387/metric ton. The cross over point for switching from SMR to Coal-POX is estimated to be $7.23/MMBtu for the natural gas. Biomass-POX increases both capital investment and operating cost. However, CO_2 mission from biomass is considered to be neutral and can offer advantage to lower in the overall carbon footprint of the coal-to-liquids project. Due to limitation of biomass collection 100% biomass feed to the POZ unit is not practical. A case of feeding 4,000 short ton/day of biomass too the Coal-POX results 46% reduction in CO_2 emission but a higher RSP of $2,665/ton, an 45% increases in RSP. Although electrolysis also offers no Co2 emission, the RSP is 1.77 to 3.35 times that of the Coal-POX option.

Rate of return on investment was calculated for the different purchase price of H_2 as outlined above. The liquid products were priced relative to the WTI price: LPG, 1.047; gasoline, 1.034; kerosene, 1.059; diesel, 1.061; and fuel oil (VGO), 1.026. When WTI is selling at $79.58/bbl, the internal rate of returns for the different H_2 supply options are given in the table below:

(Based on Hydrogen Plant IRR = 18%)

	Steam Methane Reforming		Coal-Resid Gasification	Biomass Gasification		Coal-Resid-Biomass Gasification		Nuclear-Electrolysis	Grid Electrolysis
Feedstock Price Case	**High**	**Low**		**High**	**Low**	**High**	**Low**		
H_2 Cost (\$/kg H_2)	1.88	1.47	1.84	3.89	3.35	2.66	2.42	3.25	6.12
DCL Plant IRR (%)	22.7%	25.3%	23.0%	3.1%	10.8%	17.0%	18.9%	11.7%	n/a

Note: Equity to debt ratio = 50/50.

Using an equity to debt ratio of 50/50, only the SMR, Coal-POX and Coal-Biomass-POX cases gives an internal rate of return (IRR) above 15%. The 100% biomass and electrolysis cases yield very poor return on investment (<15%). Again the cross over point for SMR and Coal-POX is around a natural price of $7.2/MMBtu.

1. INTRODCUTION

This document summarizes all the work conducted as part of the Production and Optimization of Direct Coal Liquefaction (DCL) derived Low Carbon-Footprint Transportation Fuels, a study which was funded by the U.S. Department of Energy's (DOE's) National Energy Technology Center Laboratory under Contract No. DE-FC26-05NT42448. Headwaters CTL, LLC. was the prime contract. Part of the work, the coal liquids refining study, was subcontracted to Axens North America (Axens) of New Jersey.

The objective of this research project is to perform a techno-economic assessment of a 45,850 BPSD of coal-to-liquids facility using Headwaters' direct coal liquefaction process. This project involves not only developing a conceptual design based on Illinois No. 6 coal, but also include characterization and upgrading of raw DCL liquids to fuel grade products. In addition, this project conducts an engineering assessment on carbon emission, water usage and preliminary economics of a moderate scale DCL facility designed to produce fuel grade products.

1.1 Background

There are two major approaches to convert coal into liquids and/or chemicals: indirect and direct coal liquefaction. The ultimate goal of these approaches is to reduce the size of the coal molecules at the same time to increase its hydrogen to carbon ratio, to remove hetero-atoms (chlorine, sulfur, nitrogen and oxygen) and mineral matter from coal. Under the indirect approach all feed coal is partially oxidized with high purity oxygen (gasified) to form a synthetic gas mixture or called syngas (a mixture of carbon monoxide and hydrogen). The H_2/CO ratio of the raw syngas is adjusted through a water-gas shift reactor. The shifted raw syngas is then scrubbed by either a chemical or physical solvent to remove sulfur and nitrogen compounds (H_2S, COS and NH_3) as well as carbon dioxide. The clean and conditioned syngas reacts to form liquid hydrocarbon products. For example, in a Fischer-Tropsch (FT) synthesis reactor, the clean syngas reacts over an iron- or cobalt-based catalyst to form paraffinic hydrocarbons of various chain lengths. The large paraffin molecules (wax) produced from the FT synthesis reactor is cracked into smaller component molecules to produce naphtha and diesel fuel.

Direct coal liquefaction (DCL) is a hydrocracking process in which the coal structure is partially disintegrated into smaller molecules under high hydrogen pressure and elevated temperature. This operation is usually occurred in the presence of a hydrogen donor-solvent and catalyst(s). This approach is very similar to the existing commercial hydrocracking of petroleum residues. The partially dissociated smaller molecules retains most of the original aromatic structures and therefore require further upgrading (heteroatoms removal and hydrogen addition) to yield final products (gasoline, jet fuel and diesel) that meet the transportation fuels specifications..

An end use refining study was carried out by Bechtel under a US DOE contract (Contract No. DE-AC22-93PC91029) evaluating the properties and upgradability of DCL liquids as blending stocks in a petroleum based PADD II Refinery. Two DCL coal liquids were evaluated – a bituminous ((Illinois No. 6) coal derived liquid, DL-1and a sub-bituminous coal derived liquid (Wyoming Black Thunder), DL-2. Both liquids were generated from a two-stage coal liquefaction process configuration using ebullated bed technology (CTSL). DL-1 was a raw DCL liquid collected right after the last CTSL reactor, while DL-2 had gone through an additional fixed-bed hydrogenation stage which was directly coupled with the CTSL reactor. The study concluded that "either coal liquid can replace a significant portion of the imported crude oil when refinery is operating in an expansion mode. Gasoline, jet fuel and diesel, meeting present day specifications, can be produced and their emission characteristics are not significantly affected by the addition of coal liquid."

1.2 Objective and Scope of Work

Objective of the current contract is to further evaluate the upgradability of DCL liquids generated from Headwaters two-stage slurry catalyst technology and to provide an updated engineering assessment of the DCL process. The refining study focused in the processing pure DCL liquids without blending with petroleum derived liquids.

This study can be broken down into the following work structure. Task 1 is for project management. The remaining scope of work consists of 4 technical tasks designed to characterize and upgrade the DCL liquids, and to evaluate the impact of H2 production options on the overall economic of the slurry catalyst DCL process. Specifically, the technical tasks are:

Task 2 Characterization and Stabilization of Raw DCL Liquid
Task 3 Characterization of Stabilized DCL Liquid Fractions
Task 4 Upgrading of Stabilized DCL Liquids
Task 5 Engineering Analysis

The raw coal liquid used in this study was derived from an Indian bituminous coal (Assam coal) using a 30 kg/day pilot plant located at Headwaters R&D Center Lawrenceville, New Jersey. The pilot plant test was conducted during November-December of 2007.

The raw coal liquid was first stabilized at HCTL (Task 2) prior to shipping to the Subcontractor (Axens) for performing the characterization and refining study (Tasks 3 and 4). The actual refining experimental program was carried at IFP-Lyon (France), a sister company to Axens. The refining study aimed at producing finished products that meet transportation fuels specifications. The engineering analysis (Task 5) on the DCL plant including refining operation was developed by HCTL.

Conceptual design of a 45,850 BPSD DCL plant based on Headwaters dispersed catalyst DCL Technology was developed. Process and performance data used in the conceptual design was from two different sources: DCL Section - from a 1996 DOE funded contract (Contract No. AC22-92PC92148); Refining Section – from work carried out under this contract. Specifically, the yield structure and process performance data of the DCL process was from Condition 1 (Period #4) of the pilot plant run designated as POC Bench Run No. 5 (HTI Run 227-97) which utilized Illinois No. 6 coal as the feedstock. Synthetic crude produced from the DCL section of the plant is then subjected to refining operations according to results obtained from the refining study under Task 4.

The base case DCL plant does not has a hydrogen production facility within its battery limits. Hydrogen is assumed to be purchased cross the fence or through a pipeline.

Capital and operation costs of the mine-mouth DCL plant were estimated. Impacts of hydrogen cost on the overall operating cost and rate of return on investment were then determined. Six different H_2 production schemes for the cross-the-fence plant are evaluated:

- Steam methane reforming
- Partial oxidation
  - Coal and liquefaction residuals as feed
  - Biomass as feed
  - Coal/liq. Residuals plus biomass
- Electrolysis
  - Nuclear power
  - Purchase power from power grid

Impact of overall carbon footprint on liquid fuel production will also be discussed.

Specifically, this report described and discussed results obtained from Tasks 2 to 5.

2. HEADWATERS DCL PROCESS

Headwaters DCL Process was developed by Hydrocarbon Technologies, Inc. (HTI) in the mid-90s. The ownership of the process was transferred to Headwaters CTL, LLC. (HCTL) when the two companies merged together in August 2001. In 2002 Headwaters granted a process license to the Shenhua Group of China for constructing a single reactor train mine-mouth DCL plant in Majiata, Inner Mongolia. The Shenhua plant is rated at 20,000 BPSD based on a bituminous coal feed from Shangwan mine. This plant was commissioned in December 2008 and successfully demonstrated the concept of hydroliquefaction of coal using an iron based synthetic dispersed catalyst. Also, this plant confirmed the adaptation of a fully backmixed reactor for controlling the highly exothermic hydro-liquefaction reaction system. However, due to post-commissioning modifications has logged only 4200 hours of operation to the end of August 2010. These modifications included the addition of a feed preheated to the slurry product vacuum tower and replacing the lock hopper slurry product letdown valve. The preheater was eliminated from the original design by the EPC contractor during a cost cutting exercise. Similarly, the letdown was switched back to continuous flow type as recommended by the licenser.

A simplified block diagram for the Headwaters DCL process is shown in Figure 2.1. The key unit operations are:

- Feed Slurry Preparation
- Coal Hydroliquefaction
- Liquid/Solids Separation
- Recycle Solvent and Raw DCL Products Hydrogenation
- H-Donor Solvent Recovery
- Hydrogen Recovery
- Off-Gas Treatment

This process scheme is very similar to that of petroleum resid hydrocracking with the exception that coal, rather than petroleum resid, is the reactant.

Headwaters' DCL process is a two-stage hydroliquefaction process in which the large coal molecule is partially broken down to smaller fragments under moderate temperature of 430 to 460^{o}C and elevated pressure of 160 to 180 atmospheres. Various cracking and hydrogenation reactions are taken place under these conditions. Hydrogenation of the coal fragments and spent H-donor solvent are facilitated by maintaining a relatively high hydrogen partial pressure and the presence of a proprietary hydrocracking catalyst. After the coal conversion stage, raw coal liquids and spent H-donor solvent are processed in a close-coupled hydrogenation reactor in which heteroatoms removal, saturation of olefins and partial hydrogenation of aromatics take place.

The mildly hydrogenated coal liquid is then separated from the H-donor solvent via distillation. The rejuvenated H-donor solvent is recycled to the front end of the process for feed slurry preparation, while the net product is forwarded to the product refining section for further quality improvement.

Hydroliquefaction of coal is carried out in a series of two backmixed reactors operated under isothermal conditions at each reaction stage. Design of the backmixed reactor is adapted from commercially proven ebullated bed, a liquid phase fluidized bed, for petroleum resid hydrocracking. The backmixed action is created by recirculating a stream of reactor fluid from the top of the reactor to the bottom of the reactor using a specially designed centrifugal pump, as shown in Figure 2.2. The centrifugal pump is kept inside a high pressure housing to avoid excessive cooling and pressure drop. The flow rate of the circulating fluid is several times higher than that of the feed slurry, therefore creates vigorous mixing action between the reactor fluid and the fresh slurry feed. This high liquid velocity in the reactor prevents settling of unreacted coal and mineral matters.

Preheated coal slurry feed and hot hydrogen enters bottom of the first reactor and mixes with reactor recirculating fluid in the plenum chamber at a mixed cup temperature below that of the reactor. The blended three phase mixture (coal,/catalyst particles, H-donor solvent and hydrogen gas) passes through the bottom distributor plate and moves evenly upward toward the top of the reactor where it exits the first stage reactor.

Because of the backmixed design, the reactor temperature is very uniform with no more $5^{o}C$ difference between the top and bottom temperatures. Since the heat of reaction is absorbed by the incoming cooler slurry feed, there is no need to apply cold gas or liquid quenches along the length of the reactor. The first stage reactor effluent is send to an inter-stage vapor/liquid separator to remove light hydrocarbons and other gases /vapor (water, ammonia, hydrogen sulfide, carbon oxides, etc..). The degassed slurry stream mixes with a stream of cold high purity hydrogen prior to entering into the 2^{nd} stage reactor where additional hydrocracking and quality improvement reactions take place.

Separation of liquid products and solid residuals from the 2^{nd} reactor can be effected over a combination of atmospheric and vacuum towers or by solvent extraction. The former method is of lower cost and is usually apply when the coal is of high reactivity and low ash content, while the latter method is cost effective for low reactivity coal which also has higher ash content. Vacuum tower is being used in the conceptual design in this study.

The current design is also favor the use of an ebullated bed for hydrogenation of raw coal liquids and spent H-donor solvent. The hydrogenation reactor is a single-stage reactor and charged with Ni/Mo supported catalysts. Unlike a fixed-bed design, this liquid phase fluidized bed has a high tolerance for solids and asphaltenic matter that may present in the raw coal liquids. The supported catalyst can be replaced at a regular interval, daily or weekly, to provide constant hydrogenation activity in the reactor. Also, it can deal with occasion upset in the raw coal liquids and solid residuals separation system.

The vehicle oil for feed slurry preparation composes of H-donor solvent and vacuum tower bottoms. The blending ratio will depend on the reactivity of the feed coal and the amount of mineral matter in the feed coal.

Figure 2.1

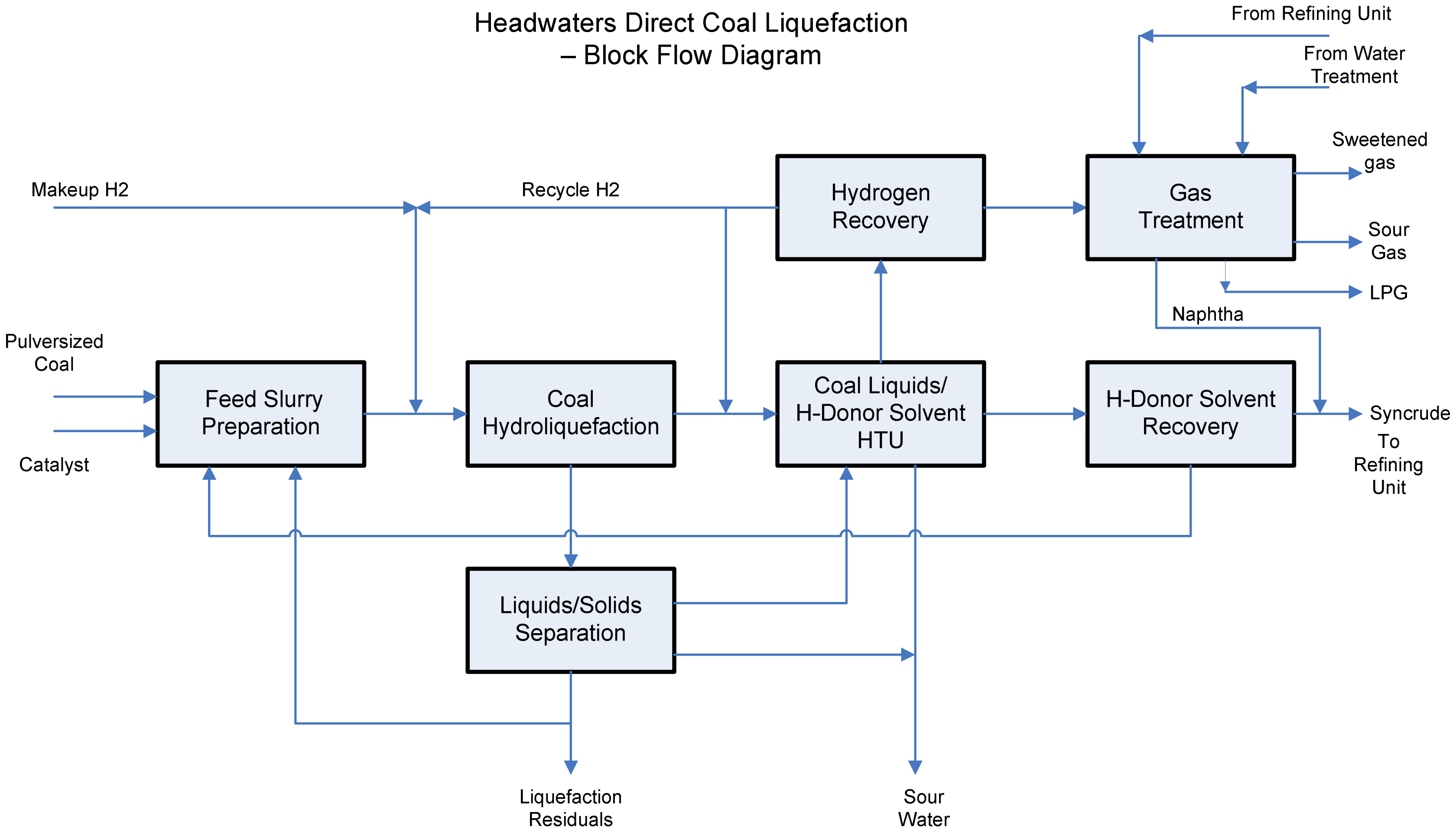
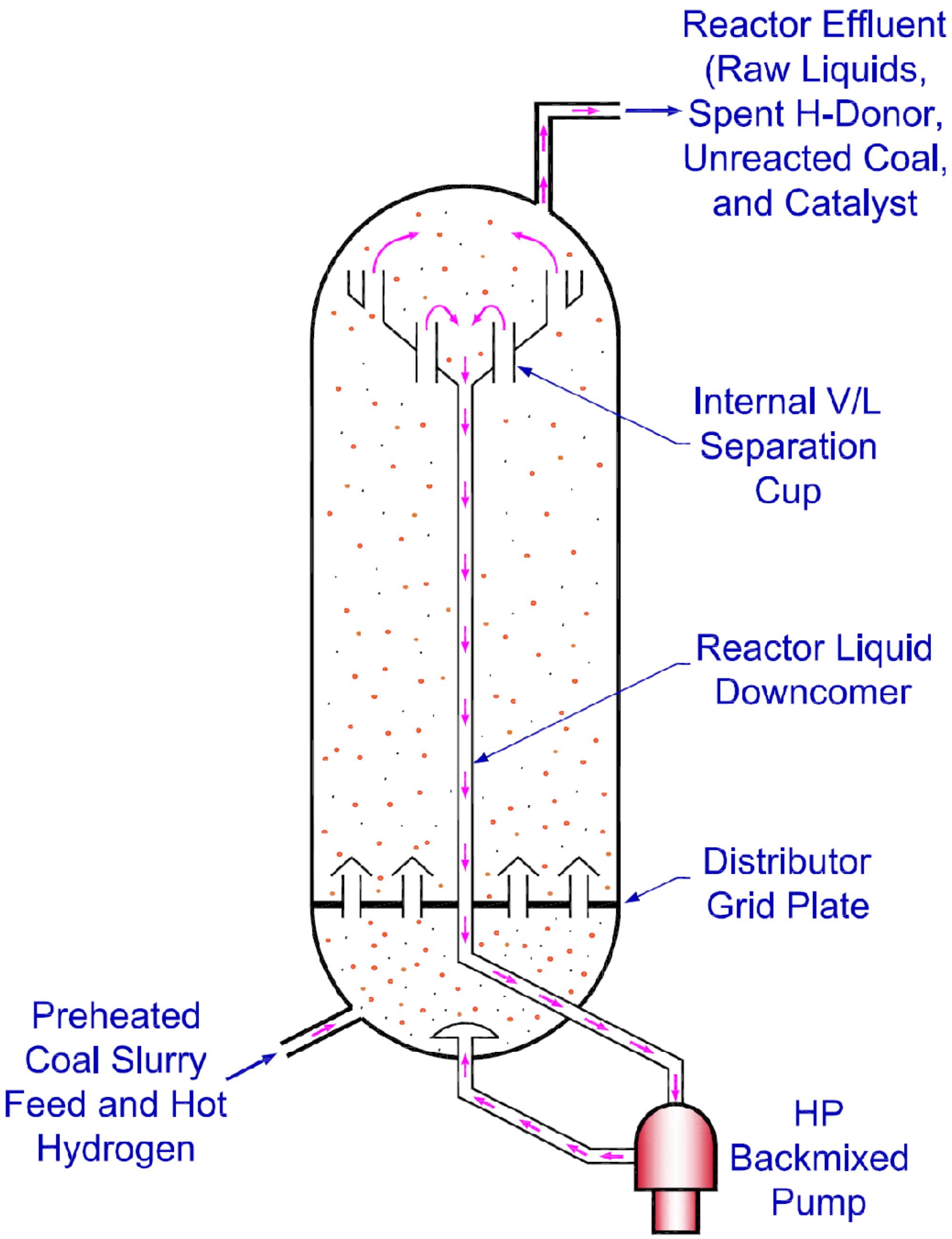

Headwaters Direct Coal Liquefaction
– Block Flow Diagram
From Refining Unit
From Water Treatment
Makeup H2
Recycle H2
Hydrogen Recovery
Gas Treatment
Sweetened gas
Sour Gas
LPG
Naphtha
Pulversized Coal
Catalyst
Feed Slurry Preparation
Coal Hydroliquefaction
Coal Liquids/ H-Donor Solvent HTU
H-Donor Solvent Recovery
Syncrude
To Refining Unit
Liquids/Solids Separation
Liquefaction Residuals
Sour Water

Figure 2.2


Reactor Effluent (Raw Liquids, Spent H-Donor, Unreacted Coal, and Catalyst
Internal V/L Separation Cup
Reactor Liquid Downcomer
Distributor Grid Plate
Preheated Coal Slurry Feed and Hot Hydrogen
HP Backmixed Pump

3. REFINING OF COAL DERIVED LIQUID

The refining characteristic of coal liquids derived from Headwaters' DCL process was evaluated under Tasks 3 and 4. The main objective of the refining study was to demonstrate DCL liquids can be refined using conventional refining processes to meet current transportation fuel specifications without relying on the blending with petroleum derived liquids.

A sample of raw coal liquid derived from an Indian bituminous coal was used for the entire upgrading program. The Indian coal was obtained from the Assam region and contained 3.38 w% of ash (moisture free basis). The sulfur content was 1.53 w% (moisture free basis). The H/C molar ratio was 0.855.

Raw coal was subjected to two-stage direct coal liquefaction conditions at a rate approximately 30 kg/day using a proprietary iron based catalyst. The pilot plant test was conducted in November/December 2007. The slurry product from the hot separator bottom was filtered and the filtered liquid was further distilled to recovered distillate products and a 450°C solid-free residual. Part of this heavy residual was recycled. During this test only spent H-donor solvent was hydrogenated in a fixed bed reactor. The light hydrocarbon liquids condensed from the hot separator overheads and the net hydrogenated distillate were collected as raw coal liquid products. These coal liquids were kept in several sealed containers. These coal liquids were blended together in July 2009 to produce a bulk sample labeled as L-1509. The hydrogenated distillates (left over recycle solvent from the end of the pilot plant test) were also blended to become Sample L-1510.

Sample L-1509 was mildly hydrogenated before forwarding to the Subcontractor (Axens) to perform the refining study. The objective of Axens' study was to determine optimal process conditions at which these mildly hydrogenated coal liquids can be refined to meet both the U.S. and the European specification for jet and fuels diesel. Also, in a separate series of experiment catalytic cracking of vacuum gas oil was evaluated. The refining tests were conducted using straight run coal liquids (without blending with petroleum based liquids).

3.1 Stabilization Pilot Plant Test

This task was to prepare a stabilized coal liquids for further refining to meet current transportation fuels specifications. As currently no specification is available for distillate synthetic crude oil (SCO) for refineries, in considering downstream requirements, the following criteria:

- Achieve a stable SCO considering the ASTM D2274 specification (Standard Test Method for Oxidative Stability of Distillate Fuel Oil (accelerated method). The European Stability Specification requires a value of less than 25 g/m$^{3.}$
- Achieve a stable diesel product considering a Bromine number in the diesel fraction of less than 2g/100g.
- The vacuum gas oil fraction 343°C+) should contain less than 1000 wppm nitrogen
- The SCO contains no vacuum residue (524°C+).

3.1.1 Preparation of Feed

Since this contract did not include a pilot plant for producing fresh coal derived liquids (CDL) from the direct liquefaction of Illinois coal, coal liquids generated from a recently completed pilot plant using Assam coal from India as feed were utilized. The raw Assam coal liquids have not gone through product stabilization as proposed in the DCL flow sheet considered for the current study.

A composite sample of net raw distillate products was assembled and designated as L-1509. The weight of this bulk sample was approximately 424 kg. The global properties of this sample are given Table 3.1.

A second sample composed of 25% of L-1509 and 75% of typical hydrogenated recycle solvent (L-1510) was also prepared. This sample was designated as L1509/L1510. The weight of this sample was about 473 kg. The global properties of this sample are also given in Table 3.1.

The stability of the un-hydrogenated coal liquids (L-1509) was 53 g/m^3, twice of the reference value of 25 g/m^3. However, the overall product contains fairly little heteroatoms (sulfur, 48 ppmw; nitrogen, 245 ppmw; and oxygen of 1.41 w% (by difference). The L-1509/L-1510 blended sample had a D2274 stability value of 16 g/m^3 – less than that of the reference value of 25 g/m^3.

3.1.2 Reactor Configuration and Catalyst

The stabilization test was carried out in a liquid phase fluidized bed reactor with an inner diameter of 3.0 cm. The reactor was charged with 1800 cc of Ni/Mo supported catalysts (Axens HTS-358). Expansion of the catalysts was induced by circulation of reactor liquids which were created by an internal vapor-liquid separation device and an externally driven ball check system.

A schematic diagram of the hydroprocessing pilot plant is depicted in Figure 3.1. The temperature of the raw DCL distillate was raised to 120°C through a electrically heated coil (1.27 cm diameter tubing) prior to entering the reactor. Hydrogen was introduced at two locations –

50% upstream of the feed preheater coil and 50% downstream of the preheater before entering the reactor. The latter was preheated in a separate preheated coil.

The reactor temperature was controlled at 377°C for the entire test. The reactor effluent was cooled and flashed in a series of two vapor-liquid separators. Temperature of first and second separator was controlled at 260° and 30°C, respectively.

Vent and dissolved gases (from flashing of the products) were measured and analyzed using an on-line gas chromatographic refinery gas analyzer.

3.1.3 Process Conditions and Operating Summary

The stabilization test program lasted for 12 days. A total of four process conditions were carried out. The first two conditions were on L-1509 as feed (7 days in duration), while the last two conditions used the blend feed L-1509/L-1510 (5 days in duration). Each of the feed was tested at two liquid hourly space velocities – 1.25 and 1.50 liter of feed per hour per liter of catalyst.

Material balance was performed on either 12 hours or 24 hours basis. In general, the material balance varied between 98.7 and 101.9 w% with an average of 99.5 w%.

3.1.4 Yield and Performance

Under these mild hydrogenation conditions, there was minimum hydrocracking of the light and medium boiling point materials taken place – the yield of C_1 to C_3 light hydrocarbons was below 0.1 w%. The average yield and performance are given in summary table below:

Operating Condition	**1 Average**	**2 Average**	**3 Average**
Feed	**L-1509**	**L-1509**	**L-1509 /L-1510**
Operating Parameters			
Reactor Temperature, °C	**376.8**	**376.9**	**376.8**
Space Velocity, 1/h	**1.24**	**1.45**	**1.47**
Mass Recovery, w% feed	**99.6**	**99.0**	**99.5**
Normalized Yield, w% feed			
C_1 gas	**0.02**	**0.02**	**0.01**
C_2 gases	**0.03**	**0.03**	**0.01**
C_3 gases	**0.05**	**0.05**	**0.02**
C_4 gases	**0.06**	**0.075**	**0.02**

C_5 gases	**0.36**	**0.44**	**0.23**
C_6&C_7 gases	**0.09**	**0.11**	**0.03**
Liquids	**100.08**	**99.96**	**100.0**
NH_3	**0.03**	**0.022**	**0.01**
Total	**100.70**	**100.71**	**100.33**
Process Performance, w% feed			
H_2 Consumed	**0.80**	**0.71**	**0.31**
C_1-C_3 Yield	**0.095**	**0.095**	**0.04**
C_4+ Distillates	**100.57**	**100.59**	**100.28**
HDN, w%	**84.81**	**87.06**	**88.34**
HDS, w%	**93.34**	**85.12**	**79.02**

Hydrogen consumption of Conditions 1 and 2 (with the lighter feed, L-1509) is 0.8 and 0.71, while that of Condition 3 (with the heavier feed L-1509/L-1510) is less, 0.31 w%.

3.2 Characterization of Stabilized Products

The boiling point distribution curves (simulated distillation) of the total liquid products are given in Table 3.5 and Figures 3.3 and 3.4.

The 50 w% boiling point of L-1509 was reduced slightly from 228.4°C to an average of 227.2°C, while that of the 95% point decreased from 393.7°C to an average of 321.1°C. Similarly, the 95% point of the 1509/L-1510 blend decreased from 370.0°C to an average of 350.7°C. However, there is no significant change for the 50 w% point temperature.

Although minimum hydrocracking resulted from the mild stabilization conditions, there was substantial hydrotreating taken place. Table 3.6 summarizes the hydrogen and heteroatoms content of the stabilized products.

There is a general increase in hydrogen content of the stabilized products. Hydrogen content of hydrogenated L-1509 and the blended L1509-L1510 samples was 12.73 and 12.51, respectively. As compared with hydrogen content of the respective un-hydrogenated feed, the increase is 0.61 and 0.31 w%.

The nitrogen content of un-hydrogenated L-1509 and the blended sample was 245 and 88 ppm, respectively. These values were reduced substantially an average value of 22.1 and 17.3 ppm. This is equivalent to a removal rate of 90 to 80 w%. Similar observations in sulfur removal can be seen. The removal rate was 89 w% for both samples, as shown in Figure 3.6.

The oxidative stability of the total products from the first 6 days of the stability test was subjected to ASTM D2274 analysis. With the exception of Period 3, in which the stability was 8.0 g/m^3, all values were below 3.5 g/m^3. These values are much lower than the stability criterion of 25 g/m^3.

3.3 Samples for Refining Study

Two bulk stabilized coal liquids were prepared and shipped to the subcontractor Axens/IFP (Lyon, France) for detailed characterization and conducting pilot plant testing for producing transportation fuels – namely gasoline, jet fuels, diesel and fuel oils.

The first bulk sample, totaling 327 kilograms, composed of stabilized products from Periods 1B to 7B, while the second sample, totaling of 218 kilograms, was from Period 8B to 12A. The first sample was designated as L-1514 and the second sample was labeled as L-1515.

As shown in Table 3. 7, average density (@15^{o}C) of L-1514 and L-1515 was 0.8642 g/cm^3 and 0.9102 g/cm^3, respectively. The lighter sample (L-1514) has an initial boiling point of less than 69^{o}C, 50 w% point of 222.8^{o}C and 95 w% point of 331.6^{o}C. The corresponding values for the heavier sample (L-1515) were 81.6, 267.8, and 350.8^{o}C, respectively.

Further characterization of these two samples was performed by the Subcontractor Axens/IFP, Results of detailed characterization is to be discussed in the next section.

3.4 Refining of Stabilized Coal Liquids

Objectives of the refining study are two folds: 1) to evaluate the upgrading of stabilized DCL syncrude using conventional refining technology, and 2) to generate preliminary yield and performance data for developing a rough refining cost for producing transportation fuels from the stabilized DCL syncrude.

The refining study was carried out under a subcontract to Axens North America of New Jersey. The goal was to evaluate the hydroprocessing of the stabilized syncrude in a single step so the naphtha fractions can be fed to a catalytic reformer for gasoline production, where the kerosene and diesel fractions can meet US and international specifications. The heavy distillate fractions can be used as fuel oils or feed to catalytic cracking. All refining pilot plant testing and liquid products characterizations were performed at Axens sister company, IFP located at Lyon, France.

The flow scheme for the two stabilized syncrude is given in Figure 3.7. For internal sample control purpose, upon the receipt of the two stabilized syncrude samples from Headwaters, IFP re-labelled the samples as the following:

- HCTL L-1514 equivalent to IFP S8016
- HCTL L-1515 equivalent to IFP S8020

AS shown in Figure 3.7, the two syncrude samples (L-1514/S8016 and L-1515/S8020) were used “as is” in the hydroprocessing step. Part of the heavier syncrude, L-1515/S8020, was fractionated to generate a 325°C+ VGO (S8027) for the short contact time (SCT) catalytic cracking study.

3.4.1 Hydrotreating and Hydrocracking of the Stabilized Liquids

Both stabilized syncrude samples contain very little 325°C+ VGO. According to D2287 simulated distillation analysis, the lighter sample, S8016, has about 5 w% 328°C+ VGO, while the heavier sample, S8020, has about 10 w% 328°C+ VGO. Also, S8016 contains about 70 w% 185°C+ distillates, while S8020 has about 75 w%. Both samples have an excellent oxidative stability (ASTM D2274) of less 10 g/m^3.

Detailed characterization of both samples and its TBP cuts (IBP-180°C, 180-250°C, 250-325°C, 325°C+) are summarized in Tables 3.8 to 3.11. Obviously these fractions do not meet corresponding fuel specifications and therefore require additional refining steps. The upgradability of these fractions is discussed in the section here below.

Photo of S8020 and its TBP sub-fractions are depicted in Figure 3.9. The naphtha (IBP-180°C), Kerosene cut (180-250°C) and diesel cut (250-325°C) was colorless, while the 325°C+ VGO cut was dark in color.

The hydrotreating and hydrocracking pilot plant test was carried out at IFP Lyon in December 2009 and January 2010. The U215 fixed-bed pilot plant uses a 3.6 cm internal diameter reactor. The reactor is equipped with six internal thermocouples integrated in the same thermowell and is operated in non-diluted catalyst, up-flow mode. The catalyst zones are kept at the desired temperature by six heating shells, each with skin and resistor thermocouples in order to assure a proper warming of the shell. The pilot plant is equipment with an on-line gas chromatographic refinery gas analyzer.

The reactor was charged with 750 cc of Axens HDK 776 catalyst. The unoccupied volume at the top and bottom of the catalyst bed was filled with a grading of ceramic balls. The catalyst was sulfide prior to the exposure to the coal liquids using a petroleum atmospheric gas-oil doped with DMDS.

A total of five test conditions were carried out:

Condition	Feed	Temperature	LHSV
1	S8016	Base	Base
2	S8016	Base	1.5 x Base
1B	S8016	Base	Base
3	S8020	Base	1.5 x Base
4	S8020	Base+10°C	0.75 x Base

Note: Pressure= base condition; H_2//hydrocarbon at reactor outlet = base condition

The test's initial operating condition (Condition #1) was with the S8016 feed (the lighter stabilized syncrude) and was considered unsuccessful due to significant light fraction losses that were observed on the material balances. These losses were related with the nitrogen injection and feedstock recirculation system in the feedstock tank. Condition 2 mass balance calculations were correct since they were performed after the mentioned problems were resolved. Condition #1 was repeated and reported as Condition #1B. Conditions #1B and #2 were designed to study impact of liquid space velocity. LHSV of Condition 2 was 50% higher than that of Condition #1B with all other process variables unchanged.

The heavier feed, S8020, was used in Conditions #3 and #4. Operating conditions for Condition #3 were identical to that of Condition #2. The last condition, Condition #4, has a LHSV of 25% lower than that of Condition 1B or half of that of Condition #3 and a 10^{o}C increase in reaction temperature in order to increase hydrocracking severity.

Photographs of the total liquids collected under each hydroprocessing conditions are given in Figure 3.10. Both total liquids from Condition #1B and #2 (using the lighter feed of S8016) are crystal clear but the products from Conditions #3 & #4 (using the heavier feed of S8020) are orange to yellow colored, respectively. This is result of their higher final cut point and the lower degree of conversion of aromatic hydrocarbons can be achieved heavier feed.

When increasing the space velocity (lowering in reaction severity) from Condition #1B to Condition #2, both the hydrogen consumption and aromatic carbon conversion decreases accordingly – H_2 consumption from 1.6 to 1.3 w% and HDCa from 98 to 92 w%. The overall hydrocracking performance also retarded, as the yield of the IBP-180^{o}C cut decreases. Similar observation can be observed for the heavier feedstock when reaction severity was decreased from Condition #4 to Condition #3.

The process performance and product yield structure are reported in Table 3.12, while the global analyses of the total liquid products are given in Table 3.13 and 3.14. These products have nitrogen and sulfur content below 0.4 ppm and 1.0 ppm, respectively.

The total liquid products from Condition 1B and 4, the most severe process condition for each of the feedstock, were selected for TBP fractionation and detailed characterization of the subsequent fractions (IBP-180, 180-250, 250^{o}C+). Because the amount of 325^{o}C+ fractions in both liquid products were quite low and thus not possible to separate from the 250^{o}C+ cuts.

Photo of the total liquids from Condition #1B, Condition #4 and its subfractions are shown for comparison in Figures 3.11 and 3.12, respectively. One unexpected observation is that although the total liquid product from Condition #1B was crystal clear, the 250^{o}C+ fraction derived from it has a brownish color. Given that the asphaltene and aromatic contents of the total liquid was low, and the AGO cut was less than 13 w%, the AGO fraction must experienced certain deterioration during the TBP fractionation procedure.

It should be pointed out that the mass spectrometry is given as indicative information. Because this analysis has not been adapted to the very naphtheno-aromatic nature of the DCL liquids, therefore the results presented herein can be misleading. Again, the RON and MON values that are presented in this report were obtained from GC method and the correlation that was used in predicting the individual compound has not fully been adapted for DCL liquids. These values should be treated as precise estimations.

Properties of the TBP cuts are discussed below (refers to Tables 3.15 and 3.16):

Naphtha – The octane numbers, RON and MON, are low around 60 for both samples. Therefore further treatment in a cat reformer is needed to improve its quality to meet gasoline specifications. The low octane numbers are due to the pressure of high portion of naphthenic compounds, around 70 to 75 w%. The heteroatom contents (N, S & O) are sufficiently low so it can go to the reformer directly without further hydrotreatment.

Kerosene – With the exception of its density, both kerosene cuts meet the international jet fuel specifications. The density of kerosene from Conditions #1B and #4 is 0.8525 and 0.8716 g/cm^3, respectively, as compared with a maximum specification of 0.8400 g/cm^3. Note that the jet fuel density specifications could be achieved by adjusting the boiling range of the kerosene fraction, while still meeting all other specifications. The higher density is a result of its naphthenic nature. The improvement in its smoke points from 15 and 17 in the light and heavy feeds to on-spec values of 22mm and 20 mm in the hydrotreated products, respectively. The minimum specification for smoke point is 19 mm. **Unlike coal liquids derived from the Fischer Tropsch route, these specifications are met without any blending with petroleum derived liquids**. The freeze points of both liquids are exceptionally good - below -69^{o}C.

Atmospheric Gas Oil – AGO produced from Condition #1B with the lighter feedstock (S8016) meets almost all commercial diesel fuel requirements for the US and Europe. Again these two coal derived diesel fuels have higher density (0.8886 and 0.9201 g/cm^3) than that of the European maximum specification of 0.845 g/cm^3. Depending on whether these cuts will be used as 1-D or 2-D type diesel fuel, the kinematic viscosity and/or the 90 vol% distillation temperature specifications may not be attained. The cetane number as determined by engine test confirmed that the AGO cut from Condition #1B has attained a high value of 51.6 – which is slightly higher than 51 the specification of European diesel fuel. However, the heavier AGO product from Condition #4 has a visibly lower cetane number, a higher density and viscosity than what is required for direct commercial use. Further hydrocracking of the heavier materials may be needed.

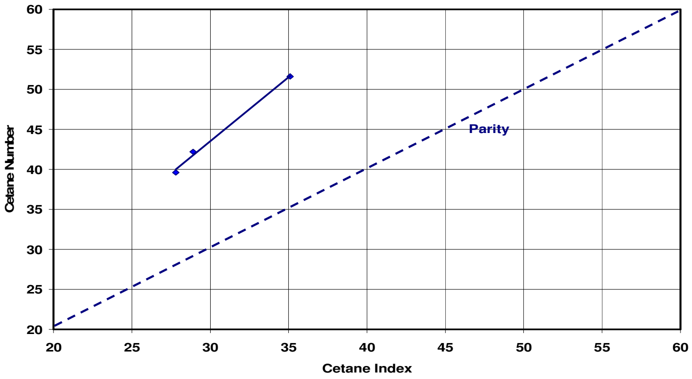
It should be pointed that cetane indexes, that were predicted using correlation derived for petroleum liquids, are significantly different from the engine cetane numbers, as shown in the following table:

TBP Cut	**Cetane Number** (CN, Engine Test)	**Cetane Index** (CI)		**Cetane Index** (CI)	
		PIR	CI/CN	**ASTM D4737**	CI/CN
Condition #1B (S8016 feed)					
180-250^{o}C	39.6	26.4†	1.50	27.8	1.46
250^{o}C+	**51.6**	35.6†	1.45	35.1	1.47
Condition #4 (S8020 feed)					
180-250^{o}C	-	14.6†	-	23.3	-
250^{o}C+	42.2	26.1†	1.62	28.9	1.46

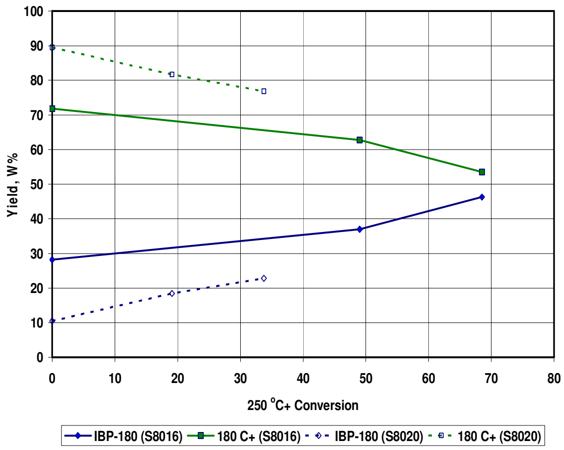
Note: † outliner

The CI/CN ratio seems to be consistent around 1.46 to 1.47, when the cetane index was determined by ASTM D4737 procedure. The same consistence does not exist between the cetane number and cetane index predicted by PIR method.

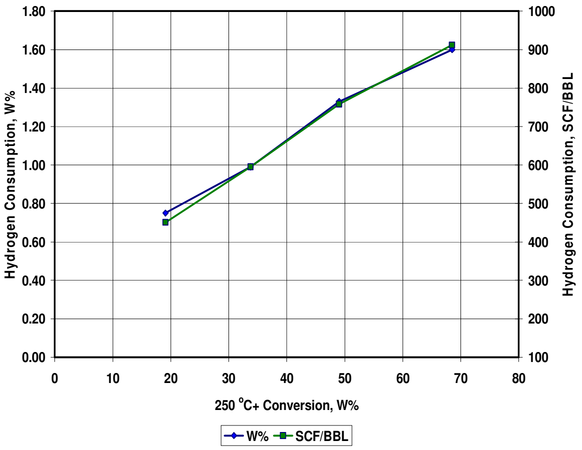
Cetane No. vs Cetane Index



Selectivity of IBP-250^{o}C vs Hydroracking Severity



H_2 Consumption vs 250^{o}C+ conversion



The selectivity of IBP-250°C tracks the 250°C+ conversion well suggesting minimum gas formation occurs during the ring-open reactions. This observation is also reflected in the H_2 consumption rate – basically there is no major different in H_2 uptake for the two feedstocks at a similar reactor severity.

3.4.2 Catalytic Reforming of Hydrotreated Naphtha

Products from Condition #1B of the Hydrotreating/Hydrocracking pilot plant test described in Section 3.5.1 above were subjected to TBP distillation. The naphtha cut (IBP-180°C) was obtained and labeled as S8062 (Sample DCL3). This naphtha cut was used a feedstock for microactivity catalytic reforming evaluation. Properties of S8062 is presented in Table 3.17.

IFP's Microcat Reforming Unit (U83) is shown in Figure 3. . This laboratory scale has four fixed bed reactors operated in parallel configuration. The effluents from each reactor are led to 6-port switching valve before a gas chromatograph (GC) for on-line characterization. Four of the ports are connected to each of the four reactor outlets. One outlet port is connected to the GC and the other outlet port is discharged into a slop pot. All connecting lines to/from the GC are heat tracked to avoid condensation.

The RON of each reactor effluent is estimated by the use of a correlation that takes into account detailed composition of the reformate. Temperature of the each reactor is automatically controlled according to the measured RON of the corresponding to a pre-set RON for each reactor effluent. For the current study only three of the four reactors were used. Under this "isoRON" mode of operation, each reactor can be operated with different feed/H_2 flow rate and temperature. All reactors were charged with the same commercial cat reforming catalyst, CR607 in this study.

The test program was designed to evaluate three different reforming severity levels (3 temperatures) to avoid excessive formation of aromatics. Results of the reforming study are given in Tabl2 3.18.

The naphtha feed contains 6.1 w% of aromatics with a corresponding octane number of 59 and density of 0.775 g/cm^3. Under the three severity conditions, the reformate attained octane number ranging from 96, 100 to 104, which is corresponding to aromatic content of 67.0, 75.0 and 81.5 w%, as plotted in Figure 3. .Over the range of severity studied, C_5+ RON shows a strong dependence against aromatics content.

The yield of H_2, C_1-C_4 and C_5+ are plotted against C_5+ RON in Figure 3.14. Linear dependency between yield of individual component and RON was observed.

According to IFP the reforming severities for processing this coal derived naphtha are less severe than that for straight run petroleum derived naphtha of similar boiling range. The C5+ reformate yield is relatively high (94.0 w% 104 RON and 96.2 w% for 96 RON.). Subsequently, the yield of H2 is relatively high (3.8 w% @ 104 RON and 2.9 w% @ 96 RON).

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3.4.3 Catalytic Cracking of Vacuum Gas Oils

The 325°C+ VGO sample (S8027), that was fractionated from the heavier coal derived stabilized syncrude (L-1515/S8020), was subjected to microcatalytic activity test using a fluidized bed, short contact time resid testing unit (SCT-RT) at IFP, as shown in Figure 3.16.

The SCT-RT unit is normally operated at low pressure (1.2 bara) and holds 15 to 30 g of catalyst. The amount of feed injected to the unit is about 1 to 3 g. This allows a flexible range of catalyst to oil ratios to be studied.

The catalyst bed is fluidized by nitrogen and is heated to 600°C. Liquid products are condensed using a refrigerated receiver cooled to -12°C. Liquids and gases products are quantified and analyzed by GC. Also, the coke formed on the catalyst surface is measured by burning off to form CO_2.

The coal derived VGO (S8027) was evaluated at three concentration levels – 100% "as is" basis, 20% and 5 w% in a straight run, hydrotreated petroleum VGO (S7923). Properties of the two VGO feeds are listed in Table 3.19. Although the final boiling point (FBP) of the coal derived VGO is lower at 539°C, as compared with the petroleum VGO which has a FBP of 598°C, it is more heavier (density of 0.9981 g/cm^3) than the petroleum VGO (density of 0.9027 g/cm^3). Again, it is due to the presence of more aromatics (71.8 w% vs 44.4 w%).

The cracking behavior of these two feedstocks is expected to be different. The addition of coal derived VGO leads to an increase of heavier liquid products and formation of more coke. The difference in cracking activity is compared by using a parameter called Standard Conversion (StdC) which is defined as (100-LCO-HCO-slurry). The shift towards a heavier product will be reflected as a decrease in StdC.

The test matrix consisted of three levels of catalyst/oil ratio, two un-blended feedstock, and two blended feedstocks (with 5 and 20 w% of S8027). Detailed yields and performance of the SCT-RT study are summarized in Table 3.20 and 3.21.

Over the three level of catalyst/oil ratios tested, the StdC for the petroleum VGO (base case) ranges from 81.8 to 85.1 w%) – the higher conversion level is corresponding to a higher catalyst/oil ratio. The coal derived VGO gives only 60.3 to 69.0 w% conversions. The conversions of the two blend feedstocks fall between that of these two unblended feedstocks, as shown in Figure 3.17.

Catalytic cracking yields at the intermediate catalyst/oil ratio are plotted in Figure 3.18. The yield of gasoline was about 53 w% with the petroleum VGO as feed, while that from the coal derived VGO feed was only 46 w% - a difference of about 8 w%.

Also, the 360°C+ conversion for each test was calculated assuming the amount of 360°C+ fraction was 95% in the petroleum VGO, while there were only 50 w% of such materials in the coal derived VGO. The conversion of 360°C+ materials for each cracking tests is listed below:

Feed Blend	**Catalyst/Oil Ratio**		
	Low Level	**Intermediate Level**	**High Level**
Petroleum VGO	92.6	91.3	89.3
5% CD VGO	90.7	90.0	89.5
20% CD VGO	88.6	87.7	86.5
100% CD VGO	67.6	66.6	65.0

The data suggested that coal derived 360°C+ materials are more difficult to be cracked.

3.5 Jet Fuel Specification Evaluation – (MIL-T-83133)

A 4 liter sample of kerosene cut sample underwent jet fuel evaluation by the Fuels & Energy Branch, US Air Force Research Laboratory (AFRL/RZPF) at Wright-Patterson Air Force Base, Ohio. The sample was labeled as 10-POSF-6875 by RZPF. Specifically, the evaluation was to determine its suitability for use as a propulsion fuel for military aviation systems according to Tier II protocol developed by AFRL/RZPF and was in comparison to the representative propulsion JP-8 (PSOF-4751).

Results of the evaluation is summarized herein Table 3.22, while details comparison are giving in the report from AFRL/RZPF attached as Appendix A.

The coal derived kerosene sample (POSF-6875) passed all current specifications with the exception of conductivity. According to AFRL/RZPF, “ the conductivity requirement would expect to be satisfied with the addition of SDA”.

The following conclusions of the jet fuel specification evaluation are extracted from the AFRL/RZPF report:

Acid Number (D3282) – The acid number of POSF-6875 (0.012 mg KOH/g) meets the JP-8 specification limit (0.015 mg KOH/g) , and is above the acid number of the JP-8 fuel (0.003 mg KOH/g).

Aromatics (D1319) – PSOF-6875 contains a lower amount of aromatics (1.6 volume %) by the JP-8 specification method D1319 than the representative JP-8 (19 volume %). This also meets the JP-8 specification limit (=maximum 25 volume %).

Distillation (D86) – The distillation temperatures of POSF-6875 are all within the specification limits. These temperatures are lower than the distillation temperatures of POSF-4751.

Freeze Point (D5972) – The freeze point of POSF-6875 (<-77°C) is well below the freeze point of POSF-4751 (-51°C), and meets the JP-8 specification maximum of -47°C.

Flash Point (D93) – The flash point of POSF-6875 (50°C) meets the JP-8 specification minimum requirement of 38°C, and is similar to the flash point of POSF-4751 (51°C).

-20°C Viscosity (D445) – The -20°C viscosity of POSF-6875 (4.8 cSt) meets the JP-8 specification of 8 cSt maximum, and is comparable to the value of the representative JP-8 (4.9 cSt).

-40°C Viscosity (D445) – The -40°C viscosity is JPTS specification, not a JP-8 specification. The -40°C viscosity of POSF-6875 (9.5 cSt) meets the JPTS specification maximum of 12 cSt, and is slightly below the representative JP-9 value (9.9 cSt).

Heat of Combustion (D4809) – The calculated heat of combustion of POSF-6875 (43.1 MJ/kg) meets the specification requirement of 42.8 MJ/kg minimum, and is nearly the same as the heat of combustion of PSOT-4751 (43.2 MJ/kg).

Thermal Stability (JFTOT-D3241) - POSF-6875 shows similar thermal stability to POST-4751 by D3241. With tube ratings if 1 and changes in pressure of 0 and 2 mm Hg, they both meet the JP-8 specification limit for thermal stability at 260°C (<3 mm tube rating and ≤25 mm Hg change in pressure).

Water Separation Index (WSIM-D3849) – The water separation index MSEP rating of 94 for POSF-6875 meets the JP-8 specification minimum rating of 90 for fuels without JP-8 additives; whereas, the MSEP rating of 78 for POSF-4751 meets the minimum rating of 70 for fuels with JP-8 additives.

Density (D4052) – The density of POSF-6875 (0.837 kg/L) is within the JP-8 specification range of 0.775 to 0,840 kg/L, and above the density of PSOF-4751 (0.803 kg/L).

Properties controlled by the mandatory addition of JP-8 Additives – (Conductivity and Lubricity) – No JP-8 additives were added to POSF-6875. Consequently, it has a low conductivity level (0 pS/m) when compared to the JP-8 specification limit range (150-600 pS/m) and the representative JP-8 value (342 pS/m). However, the lubricity value (0.57 mm wear scar) meets the JP specification limit maximum (0.85 wear scar), and is similar to the representative JP-8 value (0.53 mm wear scar).

Other non-specification analyses were also conducted. These analyses include:

a. Hydrocarbon type analysis (D6379 & D2425).

b. GC-MS/n-Paraffins analysis

c. Chromatographic analysis

d. Scanning Brookfield viscosity (low temperature)

e. Quartz crystal microbalance (QCM)

f. Metals by ICP-MS

g. Polars by HPLC and SPE

h. Volume Swell by Optical Dilatometry and Polymer-Fuel Partitioning

Detailed results of these analyses are given in AFRL/RZPF's report (Appendix A). It is interesting to note that AFRL/RXPF concluded that "based on the volume of the O-ring materials used here, PSOT-6875 should be suitable for use interchangeably with JP-8. No O-ring sealing problems would be expected assuming that all other function-critical physical properties behave in a manner comparable to the volume swell results". According to the comparison made in the AFRL/RZPF report Fischer-Tropsch derived jet fuels would have to blended with petroleum fuels in order to have comparable swelling properties.

Also, the contents of the 13 selected metals, many of which include transition metals, were below detection limits by ICP-MS analysis.

Table 3.1 Feed Analysis L-1509 & L-1510

Sample No.	**L-1509**	**25% L-1509** **75% L-1510**
	Un-Hydrogenated	Hydrogenated
API Gravity	22.5	21.5
Density @ 15^{o}C, g/cm^{3}	0.9188	0.9247
Elemental Analysis, W%		
Carbon	86.44	86.87
Hydrogen	12.12	12.20
Antek Sulfur (caustic washed)	48	24
Antek Nitrogen (caustic washed)	245	88
Oxygen Content by Difference, W%	1.41	0.93
Simulated Distillation C		
IBP	69.0	69.0
5 W%	87.8	125
10 W%	114.8	168
20 W%	158.1	208
30 W%	186.0	237
40 W%	205.9	255
50 W%	228.4	266
60 W%	241.2	278
70 W%	253.9	290
80 W%	266.2	304
90 W%	314.2	331
95W%	393.7	370
FBP	489.1	489
Oxidative Stability, g/m3 (ASTM D2274)	53	16

Table 3.2 Stabilization Test: Process Yield and Performance – Condition #1

Operating Condition	**1**	**1**	**1**	**1**	**1**	
Period	**1**	**2**	**3**	**4**	**Average**	
Operating Parameters						
Reactor Temperature, ^{o}C	**376.6**	**377.1**	**376.9**	**376.8**	**376.8**	
Space Velocity, 1/h	**1.22**	**1.25**	**1.25**	**1.26**	**1.24**	
Mass Recovery, w% feed	**101.7**	**99.0**	**98.9**	**99.0**	**99.6**	
Normalized Yield, w% feed						
C_1 gas	**0.01**	**0.02**	**0.02**	**0.02**	**0.02**	
C_2 gases	**0.02**	**0.03**	**0.03**	**0.03**	**0.03**	
C_3 gases	**0.04**	**0.05**	**0.05**	**0.05**	**0.05**	
C_4 gases	**0.05**	**0.06**	**0.06**	**0.06**	**0.06**	
C_5 gases	**0.26**	**0.40**	**0.38**	**0.38**	**0.36**	
C_6&C_7 gases	**0.08**	**0.10**	**0.09**	**0.09**	**0.09**	
Liquids	**100.08**	**100.01**	**99.88**	**100.34**	**100.08**	
NH_3	**0.03**	**0.03**	**0.03**	**0.02**	**0.03**	
Total	**100.57**	**100.69**	**100.53**	**101.00**	**100.70**	
Process Performance, w% feed						
H_2 Consumed	**0.57**	**0.69**	**0.53**	**1.00**	**0.80**	
C_1-C_3 Yield	**0.08**	**0.10**	**0.10**	**0.10**	**0.095**	
C_4+ Distillates	**100.46**	**100.56**	**100.40**	**100.87**	**100.57**	
HDN, w%	**74.84**	**88.19**	**90.08**	**86.12**	**84.81**	
HDS, w%	**97.91**	**93.64**	**91.62**	**90.17**	**93.34**	

Note: Period A - 0400 to 1600 hour; Period B – 1600 to 2400 hour

Table 3.3 Stabilization Test: Process Yield and Performance – Condition #2

Operating Condition Period	2 5A	2 5B	2 6	2 7	2 Average	
Operating Parameters						
Reactor Temperature, ^{o}C	376.9	376.9	376.9	377.0	376.9	
Space Velocity, 1/h	1.33	1.50	1.49	1.49	1.45	
Mass Recovery, w% feed	99.3	98.8	98.9	99.0	99.0	
Normalized Yield, w% feed						
C_1 gas	0.02	0.02	0.02	0.02	0.02	
C_2 gases	0.03	0.03	0.03	0.03	0.03	
C_3 gases	0.05	0.05	0.05	0.05	0.05	
C_4 gases	0.11	0.07	0.06	0.06	0.075	
C_5 gases	0.44	0.47	0.45	0.41	0.44	
C_6&C_7 gases	0.10	0.12	0.11	0.10	0.11	
Liquids	100.23	99.95	99.88	99.78	99.96	
NH_3	0.02	0.03	0.02	0.02	0.022	
Total	101.00	100.73	100.63	100.48	100.71	
Process Performance, w% feed						
H_2 Consumed	1.00	0.73	0.63	0.48	0.71	
C_1-C_3 Yield	0.09	0.10	0.09	0.10	0.095	
C_4+ Distillates	100.88	100.61	100.51	100.36	100.59	
HDN, w%	86.14	89.47	90.37	82.25	87.06	
HDS, w%	90.18	90.97	88.66	70.67	85.12	

Note: Period A - 0400 to 1600 hour; Period B – 1600 to 2400 hour

Table 3.4 Stabilization Test: Process Yield and Performance – Conditions #3 & 4

Operating Condition	**3**	**3**	**4**	**4**	**4**	**3&4**
Period	**8B**	**9A**	**10**	**11**	**12**	**Average**
Operating Parameters						
Reactor Temperature, ^{o}C	**376.8**	**376.8**	**376.9**	**376.9**	**376.7**	
Space Velocity, 1/h	**1.20**	**1.25**	**1.49**	**1.50**	**1.42**	
Mass Recovery, w% feed	**101.9**	**98.7**	**98.8**	**99.8**	**99.9**	
Normalized Yield, w% feed						
C_1 gas	**0.01**	**0.01**	**0.01**	**0.01**	**0.01**	**0.01**
C_2 gases	**0.02**	**0.01**	**0.01**	**0.01**	**0.01**	**0.01**
C_3 gases	**0.02**	**0.02**	**0.02**	**0.02**	**0.02**	**0.02**
C_4 gases	**0.03**	**0.02**	**0.02**	**0.02**	**0.02**	**0.02**
C_5 gases	**0.20**	**0.18**	**0.22**	**0.21**	**0.26**	**0.21**
C_6&C_7 gases	**0.04**	**0.03**	**0.03**	**0.03**	**0.03**	**0.03**
Liquids	**100.01**	**99.94**	**100.05**	**100.04**	**99.90**	
NH_3	**0.01**	**0.01**	**0.01**	**0.01**	**0.01**	**0.01**
Total	**100.34**	**100.23**	**100.38**	**100.35**	**100.27**	
Process Performance, w% feed						
H_2 Consumed	**0.34**	**0.23**	**0.38**	**0.35**	**0.27**	**0.32**
C_1-C_3 Yield	**0.05**	**0.04**	**0.04**	**0.04**	**0.04**	**0.04**
C_4+ Distillates	**100.28**	**100.17**	**100.33**	**100.30**	**100.22**	**100.26**
HDN, w%	**85.07**	**51.76**	**88.12**	**87.90**	**89.00**	**80.50**
HDS, w%	**85.08**	**92.73**	**81.37**	**79.13**	**76.55**	**82.97**

Note: Period A - 0400 to 1600 hour; Period B – 1600 to 2400 hour

Table 3.5 Properties of Stabilized Product – ASTM D2887 Simulated Distillation (^{o}C)

Cum. w%	1	2	3	4	5	6	Average
IBP	81.4	69.2	69.0	69.2	82.8	69.0	
5	116.6	101.9	101.9	101.8	116.4	87.4	
10	138.6	124.0	125.0	123.6	136.3	103.7	
20	182.7	157.7	160.6	155.8	176.7	142.6	
30	195.8	184.0	184.1	183.8	192.0	182.8	
40	220.4	202.3	202.9	201.2	206.8	197.6	
50	233.8	223.3	223.3	221.8	226.6	220.0	227.2
60	246.7	234.8	234.6	234.1	235.4	233.7	
70	261.3	248.4	247.4	246.6	247.6	246.1	
80	269.7	263.6	262.4	259.7	260.1	259.4	
90	303.1	283.6	276.6	272.9	270.1	273.4	
95	337.0	328.9	327.7	323.2	312.3	325.9	321.1
FBP	450.9	450.2	451.7	451.3	447.4	454.6	

Cum. w%	8	9	10	11	12	Average
IBP	74.8	80.7	81.4	81.9	82.2	
5	105.4	118.0	123.6	128.9	131.3	
10	155.1	167.2	168.9	173.9	179.2	
20	198.0	202.6	204.1	208.4	212.2	
30	231.4	233.1	233.6	233.9	234.3	
40	249.4	252.7	253.3	254.3	255.4	
50	265.2	266.0	266.2	266.4	266.7	266.3
60	270.0	270.9	272.7	273.2	273.4	
70	291.4	294.1	294.7	295.0	295.1	
80	302.1	302.9	303.3	303.7	303.8	
90	327.2	328.3	329.3	329.9	330.2	
95	350.0	350.0	350.7	351.0	351.2	350.7
FBP	453.7	452.2	453.2	454.0	454.0	

Table 3.6 Elemental Analysis and Oxidative Stability of Stabilized Products

Period	**Oxidative Stability** (ASTM D2274) g/m^3	**Elemental Analysis**			
		Carbon w%	**Hydrogen w%**	**Nitrogen ppmw**	**Sulfur ppmw**
1	1.3	85.68	12.55	5.1	12.1
2	3.3	85.80	12.69	15.6	5.7
3	8.0	86.07	12.56	20.6	4.8
4	1.7	85.77	12.89	24.1	6.7
5	3.0	86.36	12.80	22.3	5.1
6	0.4	86.09	12.66	27.9	4.7
Average of Periods 2 to 6		**86.14**	**12.73**	**22.1**	**5.4**
8	**-**	86.46	12.47	13.2	3.6
9A	**-**	86.98	12.43		-
10	**-**	86.90	12.57	16.5	2.9
11	**-**	87.14	12.58	18.6	2.9
12A	**-**	87.24	12.51	20.9	2.7
Average Period 8 to 12A		**86.94**	**12.51**	**17.3**	**3.0**
	API Gravity				
4	**31.9**				
7	**31.5**				
8	**23.5**				
9A	**23.8**				

Table 3.7 Simulated Distillation of Blended Stabilized Products

Sample	Unit	L-1514 Drum #1 (Period 1B-4A)	L-1514 Drum #2 (Period 4B-7B)	L-1515 Drum #1 (Period 8B-10A)	L-1515 Drum #2 (Period 10B-12A)
Weight	kg	151	176	105	113
Global Analysis					
Density @ 15°C	g/cm^3	0.8644	0.8639	0.9094	0.9111
Simulated Distillation					
IBP	°C	<69.0	<69.1	81.0	82.3
5 w%	°C	89.7	86.3	118.8	125.6
10 w%	°C	105.7	104.0	168.3	172.7
20 w%	°C	146.6	141.7	204.2	207.2
30 w%	°C	184.8	184.1	234.9	235.4
40 w%	°C	200.3	199.6	254.4	255.4
50 w%	°C	223.3	222.3	267.7	268.0
60 w%	°C	236.1	235.6	272.6	274.3
70 w%	°C	250.1	248.4	295.6	296.0
80 w%	°C	265.7	263.2	304.2	304.6
90 w%	°C	290.4	281.6	329.1	329.8
95 w%	°C	328.7	336.1	350.7	350.8
FBP	°C	450.8	459.1	455.0	454.1

Table 3.8 Properties of Stabilized Coal Liquids (L-1514) - 1/2

(Analyses performed by IFP, designated as S8016)

Fraction	Unit	Total Liquid	IBP-180°C	180-250°C	250°C+
TBP Distillation Yield	**w%**	100	28.22	42.26	29.52
Global Analysis					
Density @ 15°C	g/cm^3	0.8637	0.7690	0.8841	0.9413
Refractive Index @ 20°C	-	1.4719	1.4248	1.4807	1.5126
Kin. Viscosity @ T1	mm^2/s	2.259	-	2.664	10.21
Temperature, T1	°C	20	-	20	20
Kin. Viscosity @ T2	mm^2/s	1.609	-	1.863	5.523
Temperature T2	°C	40	-	40	40
Elemental Analysis					
Hydrogen	w%	12.60	14.15	12.59	11.88
Oxygen	w%	<0.20	<0.20	<0.20	<0.20
Sulfur (FX)	ppmw	17	-	-	0.0029
Sulfur (UV)	ppmw	-	1.4	0.6	-
Nitrogen	ppmw	33.6	2.4	7.5	96.9
Basic compounds	ppmw	23.0	<10	<10	52.5
Simulated Distillation					
IBP	°C	67..3	60.0	170.1	241.2
5 w%	°C	95.9	82.3	185.0	250.7
10 w%	°C	110.3	85.2	187.7	256.3
20 w%	°C	146.7	100.7	196.1	263.1
30 w%	°C	184.6	106.1	204.2	269.4
40 w%	°C	200.2	119.7	211.1	273.8
50 w%	°C	222.3	134.6	223.9	276.6
60 w%	°C	235.6	139.8	231.3	280.1
70 w%	°C	247.9	146.3	237.8	296.8
80 w%	°C	263.3	158	241.8	318.3
90 w%	°C	279.7	171.7	248.8	363.2
95 w%	°C	328.1	178.2	251.7	405.6
FBP	°C	453.0	186.4	256.9	489.9
Oxidative Stability					
Filterable		1			
Non-filterable	g/m^3	3			
Total		4			

Table 3.9 Properties of Stabilized Coal Liquids (L-1514) – 2/2

(Analyses performed by IFP, designated as S8016)

Fraction	**Unit**	**Total Liquid**	**IBP-180^{o}C**	**180-250^{o}C**	**250^{o}C+**
TBP Distillation Yield	**w%**	100	28.22	42.26	29.52
Specific Global Properties					
Bromine Index	g/100g	-	<0.8	<0.8	1.16
Maleic Anhydrid (MAV)	mg/g	-	<0.5	-	-
Molecular Weight (API2B2.1)	g/mol	158	113	155	183
Aromatic Carbon (NMR)	w%	12.4	-	-	-
CA (ndM D3238)	%	11.9	5.9	13.3	23.3
Cetane Index (PIR)	-	-	-	18.3 (outlier)	25.4 (outlier)
Centane Index (ASTMD4737)	-	-	-	20.4	32.5
Freezing Point	^{o}C	-	-	<-70	-
Pour Point	^{o}C	<-48	-	-	<-48
Smoke Point	mm	-	-	15	-
Anline Point	^{o}C	-	-	33.7	39.1
C_7Asphaltenes	w%	<0.05	-	-	-
Conradson Carbpn (MCRT)	w%	<0.1	-	-	-
Sediment (toluene Extraction)	w%	-	-	-	-
Ash	w%	-	-	-	-
Mass Spectrometry Fitzgerald					
Saturates	w%	-	-	79.8	68.4
Monoaromatics	w%	-	-	19.6	26.1
Diaromatics	w%	-	-	0.6	4.7
Triaromatics	w%	-	-	0	0.3
Sulfur Compounds	w%	-	-	0	0
GC (Carburane)					
Molecular Weight	g/mol	-	108	-	-
Hydrogen	w%	-	14.15	-	-
N-paraffins	w%	-	11.8	-	-
Isoparaffins	w%	-	17.8	-	-
Olefins	w%	-	1.0	-	-
Naphthenes	w%	-	57.6	-	-
Aromatics	w%	-	9.6	-	-
Oxygen Compounds	w%	-	2.1	-	-
Nitrogen Compounds	w%	-	0.1	-	-
Unknowns	w%	-	0.0	-	-

Table 3.10 Properties of Stabilized Coal Liquids (L-1515) – 1/2

(Analyses performed by IFP, designated as S8020)

Fraction	Unit	Total Liquid	IBP-180°C	180-250°C	250-325°C	325°C+
TBP Distillation Yield	**w%**	100	10.47	26.29	51.19	12.05
Global Analysis						
Density @ 15°C	g/cm^3	0.9109	0.7753	0.8852	0.9395	0.9981
Ref. Index @ 20°C	-	1.4926	1.4271	1.4790	1.5033	1.5309
Kin. Viscosity @ T1	mm^2/s	4.927	-	2.842	9.4	11.12
Temperature, T1	°C	20	-	20	20	70
Kin. Viscosity @ T2	mm^2/s	3.101	-	1.97	5.206	4.809
Temperature T2	°C	40	-	40	40	100
Elemental Analysis						
Hydrogen	w%	12.32	14.14	12.71	12.25	10.84
Oxygen	w%	<0.20	<0.20	<0.20	<0.20	<0.20
Sulfur (FX)	ppmw	-	-	-	-	0.0021
Sulfur (UV)	ppmw	9.7	1.3	<0.3	0.5	-
Nitrogen	ppmw	19.5	0.5	3.6	7.2	92.1
Basic compounds	ppmw	14.4	<10	<10	<10	55.5
Zinc content (Zn)	ppmw	-	-	-	-	1.0
Simulated Distill.						
IBP	°C	80.3	67.5	15.7	240.6	317.5
5 w%	°C	124.7	83.0	183.2	252.2	331.2
10 w%	°C	170.8	84.5	185.8	259.3	337.5
20 w%	°C	205.3	101.7	192.7	267.7	345.0
30 w%	°C	234.2	104.8	201.9	271.3	351.2
40 w%	°C	253.1	117.3	213.9	274.1	357.1
50 w%	°C	267.5	133.0	225.6	279.1	363.0
60 w%	°C	274.4	137.2	232.7	290.8	369.7
70 w%	°C	294.9	143.8	237.0	299.5	377.2
80 w%	°C	304.4	156.5	239.9	304.6	390.1
90 w%	°C	329.2	169.8	246.9	310.7	420.6
95 w%	°C	349.4	179.3	249.6	316.6	452.1
FBP	°C	492.6	188.0	254.7	326.0	539.0
Oxidative Stability						
Filterable	g/m^3	2				
Non-filterable		7				
Total		9				

Table 3.11 Properties of Stabilized Coal Liquids (L-1515) 2/2

(Analyses performed by IFP, designated as S8020)

Fraction	**Unit**	**Total Liquid**	**IBP-180^{o}C**	**180-250^{o}C**	**250-325^{o}C**	**325^{o}C+**
TBP Distillation Yield	**w%**	100	10.47	26.29	51.19	12.05
Specific Global Properties						
Bromine Index	g/100g	-	<0.8	<0.8	<0.8	≈2
Maleic Anhydrid (MAV)	mg/g	-	<0.5	-	-	-
Molecular Weight (API2B2.1)	g/mol	183	112	156	185	256
Aromatic Carbon (NMR)	w%	14.3	-	-	-	24.1
CA (ndM D3238)	%	11.8	5.8	9.6	10.4	28.9
Cetane Index (PIR)	-	-	-	17.4 (outlier)	25.6 (outlier)	-
Centane Index (ASTMD4737)	-	-	-	19.7	22.8	-
Freezing Point	^{o}C	-	-	<-70	-	-
Pour Point	^{o}C	<-48	-	-	<-48	0
Smoke Point	mm	-	-	17	-	-
Anline Point	^{o}C	-	-	36.8	45.6	43.7
C_7 Asphaltenes	w%	<0.05	-	-	-	0.15
Conradson Carbpn (MCRT)	w%	<0.1	-	-	-	0.24
Sediment (toluene Extraction)	w%	-	-	-	-	0.01
Ash	w%	-	-	-	-	<0.001
Mass Spectro. Fitzgerald						
Saturates	w%	-	-	83.4	76.4	-
Monoaromatics	w%	-	-	14.8	20.6	-
Diaromatics	w%	-	-	1.6	2.4	-
Triaromatics	w%	-	-	0.1	0.2	-
Sulfur Compounds	w%	-	-	0.1	0.4	-
GC (Carburane)				**MS Fischer on the SA Fraction, w%**		
Molecular Weight	g/mol	-	107			
Hydrogen	w%	-	14.14	Saturates		28.2
N-paraffins	w%	-	8.8	Aromatics		71.8
Isoparaffins	w%	-	14.6	Monoaromatics		15.3
Olefins	w%	-	0.9	Diaromatics		25.5
Naphthenes	w%	-	66.4	Triaromatics		11.4
Aromatics	w%	-	9.2	Tetraaromatics		15.3
Oxygen Compounds	w%	-	0.1	Pentaaroamtics		2.3
Nitrogen Compounds	w%	-	0.1	Hexaaromatics		2.0
Unknowns	w%	-	0.0	Sulfur compounds		0

Table 3.12 Hydrotreating/Hydrocracking Test – Operating Conditions, Performance and Yields

Ref.	**Reference**		**Condition 2**	**Condition 1B**	**Condition 3**	**Condition 4**
Operating conditions	Total pressure	(bar)	Base	Base	Base	Base
	LHSV	(L/L/h)	**1.5 * Base**	**Base**	**1.5 * Base**	**0.75 * Base**
	H2/HC ratio at reactor outlet	(NL/L)	Base	Base	Base	Base
	Temperature	(°C)	Base	Base	**Base**	**Base + 10**
Purif.	HDS	(%)	94.3	> 94.3 (1)	94.6	95.0
	HDN	(%)	> 98.9 (2)	> 98.9 (2)	> 98.3 (2)	> 98.3 (2)
	HDCa (by Ca NMR where available)	(%)	90.3	-	81.1	-
	HDCa (by ndM D3238 only) (3)	(%)	91.9	98.3	69.5	74.1
Cons.	H2 consumption by H/C	(wt%/wt)	1.34	1.60	0.76	0.99
Yields	H2S yield (H/C)	(wt%/wt)	0.00	0.00	0.00	0.00
	NH3 yield (H/C)	(wt%/wt)	0.00	0.00	0.00	0.00
	C1 yield (H/C)	(wt%/wt)	0.10	0.08	0.04	0.10
	C2 yield (H/C)	(wt%/wt)	0.18	0.12	0.07	0.16
	C3 yield (H/C)	(wt%/wt)	0.55	0.46	0.19	0.40
	C4 yield (H/C)	(wt%/wt)	0.77	1.12	0.26	0.56
	PI-180°C yield (H/C)	(wt%/wt)	36.99	46.58	18.47	22.94
	180-250°C yield (H/C)	(wt%/wt)	47.69	44.21	30.56	34.93
	250-325°C yield (H/C)	(wt%/wt)	13.88	9.30	46.35	39.28
	325°C+ yield (H/C)	(wt%/wt)	1.17	0.00	4.81	2.61
	Total yield (H/C)	(wt%/wt)	101.34	101.60	100.76	100.99

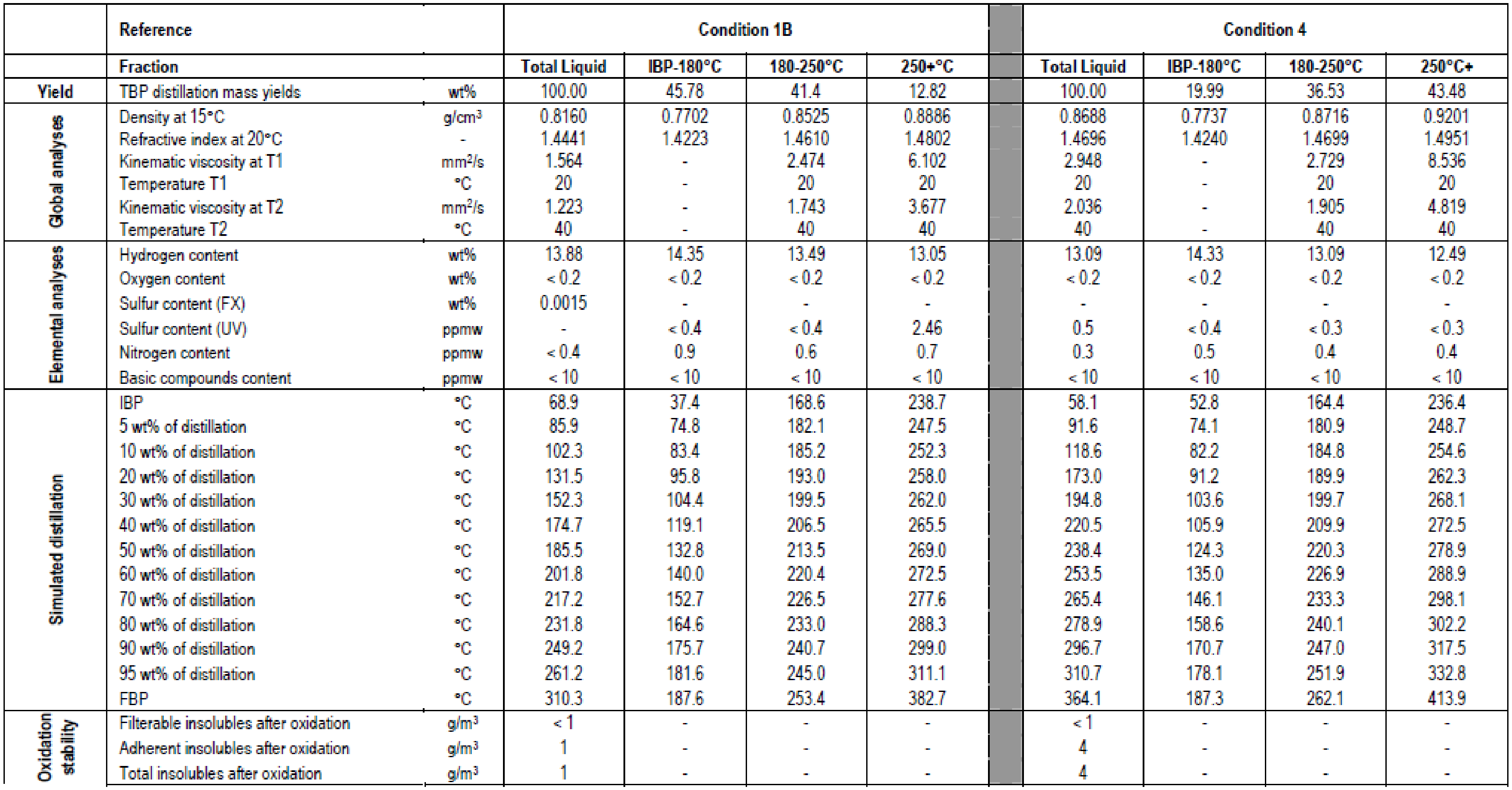
Table 3.13 Hydrotreating/Hydrocarcking Test – Product Properties 1 of 2

	Reference		Feed S8016	Condition 2	Condition 1B	Feed S8020	Condition 3	Condition 4
	Fraction		Total Liquid	Total Liquid	Total Liquid	Total Liquid	Total Liquid	Total Liquid
Global analyses	Density at 15°C	g/cm^3	0.8637	0.8323	0.8160	0.9109	0.8847	0.8688
	Refractive index at 20°C	-	1.4719	1.4518	1.4441	1.4926	1.4769	1.4696
	Kinematic viscosity at T1	mm^2/s	2.259	1.880	1.564	4.927	3.776	2.948
	Temperature T1	°C	20	20	20	20	20	20
	Kinematic viscosity at T2	mm^2/s	1.609	1.407	1.223	3.101	2.454	2.036
	Temperature T2	°C	40	40	40	40	40	40
Elemental analyses	Hydrogen content	wt %	12.59	13.64	13.88	12.32	12.92	13.09
	Oxygen content	wt %	< 0.20	< 0.2	< 0.2	< 0.20	< 0.2	< 0.2
	Sulfur content (FX)	wt %	0.0017	-	0.0015	-	-	-
	Sulfur content (UV)	ppmw	-	1.0	-	9.7	0.5	0.5
	Nitrogen content	ppmw	33.6	< 0.4	< 0.4	19.8	< 0.3	< 0.3
	Basic compounds content	ppmw	23.0	< 10	< 10	14.4	< 10	< 10
Simulated distillation	IBP	°C	67.3	73.1	68.9	80.3	75.5	58.1
	5 wt% of distillation	°C	95.9	96.4	85.9	124.7	116.3	91.6
	10 wt% of distillation	°C	110.3	104.7	102.3	170.8	155.3	118.6
	20 wt% of distillation	°C	146.7	140.0	131.5	205.3	189.0	173.0
	30 wt% of distillation	°C	184.6	171.6	152.3	234.2	219.6	194.8
	40 wt% of distillation	°C	200.2	185.0	174.7	253.1	237.4	220.5
	50 wt% of distillation	°C	222.3	198.8	185.5	267.5	253.7	238.4
	60 wt% of distillation	°C	235.6	216.4	201.8	274.4	265.3	253.5
	70 wt% of distillation	°C	247.9	229.5	217.2	294.9	273.8	265.4
	80 wt% of distillation	°C	263.3	243.3	231.8	304.4	294.5	278.9
	90 wt% of distillation	°C	279.7	259.9	249.2	329.2	305.0	296.7
	95 wt% of distillation	°C	328.1	274.7	261.2	349.4	324.8	310.7
	FBP	°C	453	341.5	310.3	492.6	402.5	364.1

Table 3.14 Hydrotreating/Hydrocarcking Test – Product Properties 2 of 2

	Reference		Feed S8016	Condition 2	Condition 1B	Feed S8020	Condition 3	Condition 4
	Fraction		Total Liquid	Total Liquid	Total Liquid	Total Liquid	Total Liquid	Total Liquid
Oxidation stability	Filterable insolubles after oxidation	g/m^3	1	< 1	< 1	2	< 1	< 1
	Adherent insolubles after oxidation	g/m^3	3	3	1	7	2	4
	Total insolubles after oxidation	g/m^3	4	3	1	9	2	4
Specific global properties	Molecular weight (API 2B2.1)	g/mol	158	146	139	183	177	168
	Aromatic carbon content (NMR)	wt%	12.4	1.2	-	14.3	2.7	-
	CA (ndM D3238)	%	11.9	1.0	0.2	11.8	3.6	3.1
	CP (ndM D3238)	%	26.2	28.7	30.2	15.0	20.5	24.0
	CN (ndM D3238)	%	61.9	70.3	69.6	73.2	75.9	72.9
	Pour point	°C	< -48	< -48	< -48	< -48	< -48	< -48
	C7 asphaltenes content	wt%	< 0.05	-	-	< 0.05	-	-
	Conradson Carbon (MCRT)	wt%	< 0.1	-	-	< 0.1	-	-

Table 3.15 Detailed Properties of Hydrotreated/Hydrocracked Coal Liquids - 1 of 2



	Reference		Condition 1B				Condition 4			
	Fraction		**Total Liquid**	**IBP-180°C**	**180-250°C**	**250+°C**	**Total Liquid**	**IBP-180°C**	**180-250°C**	**250°C+**
Yield	TBP distillation mass yields	wt%	100.00	45.78	41.4	12.82	100.00	19.99	36.53	43.48
Global analyses	Density at 15°C	g/cm³	0.8160	0.7702	0.8525	0.8886	0.8688	0.7737	0.8716	0.9201
	Refractive index at 20°C	-	1.4441	1.4223	1.4610	1.4802	1.4696	1.4240	1.4699	1.4951
	Kinematic viscosity at T1	mm²/s	1.564	-	2.474	6.102	2.948	-	2.729	8.536
	Temperature T1	°C	20	-	20	20	20	-	20	20
	Kinematic viscosity at T2	mm²/s	1.223	-	1.743	3.677	2.036	-	1.905	4.819
	Temperature T2	°C	40	-	40	40	40	-	40	40
Elemental analyses	Hydrogen content	wt%	13.88	14.35	13.49	13.05	13.09	14.33	13.09	12.49
	Oxygen content	wt%	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2
	Sulfur content (FX)	wt%	0.0015	-	-	-	-	-	-	-
	Sulfur content (UV)	ppmw	-	< 0.4	< 0.4	2.46	0.5	< 0.4	< 0.3	< 0.3
	Nitrogen content	ppmw	< 0.4	0.9	0.6	0.7	0.3	0.5	0.4	0.4
	Basic compounds content	ppmw	< 10	< 10	< 10	< 10	< 10	< 10	< 10	< 10
Simulated distillation	IBP	°C	68.9	37.4	168.6	238.7	58.1	52.8	164.4	236.4
	5 wt% of distillation	°C	85.9	74.8	182.1	247.5	91.6	74.1	180.9	248.7
	10 wt% of distillation	°C	102.3	83.4	185.2	252.3	118.6	82.2	184.8	254.6
	20 wt% of distillation	°C	131.5	95.8	193.0	258.0	173.0	91.2	189.9	262.3
	30 wt% of distillation	°C	152.3	104.4	199.5	262.0	194.8	103.6	199.7	268.1
	40 wt% of distillation	°C	174.7	119.1	206.5	265.5	220.5	105.9	209.9	272.5
	50 wt% of distillation	°C	185.5	132.8	213.5	269.0	238.4	124.3	220.3	278.9
	60 wt% of distillation	°C	201.8	140.0	220.4	272.5	253.5	135.0	226.9	288.9
	70 wt% of distillation	°C	217.2	152.7	226.5	277.6	265.4	146.1	233.3	298.1
	80 wt% of distillation	°C	231.8	164.6	233.0	288.3	278.9	158.6	240.1	302.2
	90 wt% of distillation	°C	249.2	175.7	240.7	299.0	296.7	170.7	247.0	317.5
	95 wt% of distillation	°C	261.2	181.6	245.0	311.1	310.7	178.1	251.9	332.8
	FBP	°C	310.3	187.6	253.4	382.7	364.1	187.3	262.1	413.9
Oxidation stability	Filterable insolubles after oxidation	g/m³	< 1	-	-	-	< 1	-	-	-
	Adherent insolubles after oxidation	g/m³	1	-	-	-	4	-	-	-
	Total insolubles after oxidation	g/m³	1	-	-	-	4	-	-	-

Table 3.16 Detailed Properties of Hydrotreated/Hydrocracked Coal Liquids - 2 of 2

	Reference		**Condition 1B**				**Condition 4**			
	Fraction		**Total Liquid**	**IBP-180°C**	**180-250°C**	**250+°C**	**Total Liquid**	**IBP-180°C**	**180-250°C**	**250°C+**
Yield	TBP distillation mass yields	wt%	100.00	45.78	41.4	12.82	100.00	19.99	36.53	43.48
Specific global properties	Bromine index	g/100g	-	< 0.8	< 0.8	< 0.8	-	< 0.8	< 0.8	< 0.8
	Maleic Anhydrid Value (MAV)	mg/g	-	< 0.5	-	-	-	< 0.5	-	-
	Molecular weight (API 2B2.1)	g/mol	139	112	153	189	168	107	155	190
	CA (ndM D3238)	%	0.2	1.2	1.7	5.3	3.1	3.1	3.6	9.1
	Cetane Index (PIR)	-	-	-	26.4 (outlier)	35.6 (outlier)	-	-	14.6 (outlier)	26.1 (outlier)
	Cetane Index (ASTM D4737)	-	-	-	27.8	35.1	-	-	23.3	28.9
	CFR Cetane number (engine test)	-	-	-	**39.6**	**51.6**	-	-	-	**42.2**
	Freezing point	°C	-	-	< -69	-	-	-	< -69	-
	Pour point	°C	< -48	-	-	< -48	< -48	-	-	< -48
	Smoke point	mm	-	-	**22**	-	-	-	**20**	-
	Aniline point	°C	-	-	55.4	61.6	-	-	47.9	54.3
Mass spectrometry Fitzgerald	Saturates	wt%	-	-	96.8	89.2	-	-	93.9	79.8
	Monoaromatics	wt%	-	-	2.5	9.4	-	-	5.8	16.6
	Diaromatics	wt%	-	-	0.4	0.9	-	-	0.2	2.8
	Triaromatics	wt%	-	-	0	0.1	-	-	0	0.3
	Sulfur compounds	wt%	-	-	0.3	0.4	-	-	0.1	0
Gas chromatography (Carburane)	Molecular weight	g/mol	-	111	-	-	-	107	-	-
	Hydrogen	wt%	-	**14.35**	-	-	-	**14.33**	-	-
	N-paraffins	wt%	-	**7.4**	-	-	-	**6.2**	-	-
	Isoparaffins	wt%	-	**17.0**	-	-	-	**12.5**	-	-
	Olefins	wt%	-	**0.0**	-	-	-	**0.0**	-	-
	Naphthenes	wt%	-	**68.2**	-	-	-	**75.2**	-	-
	Aromatics	wt%	-	**7.4**	-	-	-	**6.1**	-	-
	Oxygen compounds	wt%	-	**0.0**	-	-	-	**0.0**	-	-
	Nitrogen compounds	wt%	-	**0.0**	-	-	-	**0.0**	-	-
	Unknowns	wt%	-	**0.0**	-	-	-	**0.0**	-	-

Table 3.17 Properties of Hydrotreated Naphtha (80-180°C)

- S8062 (Sample DCL3)

Properties	**Analysis**
Global Properties	
Density @ 15°C g/cm^3	0.775
Sulfur content (UV), ppmw	0.4
Nitrogen content, ppmw	0.5
Hydrogen, w%	14.36
Simulated Distillation, [°C]	
IBP	73.7
5 w%	86.9
10 w%	98.4
20 w%	104.4
30 w%	119.5
40 w%	129.4
50 w%	137.1
60 w%	145.8
70 w%	155.0
80 w%	165.4
90 w%	175.8
95 w%	182.9
FBP	
PONA Analysis, w%	
N-paraffins	6.4
Iso-paraffins	16.1
Olefins	0.0
Naphthenes	71.5
Aromatics	6.1

Table 3.18 Naphtha Reforming MicroactivityTest – Yields and Properties of Coal Derived Gasoline

Yields/Properties	CDL Feed	Condition #1	Condition #2	Condition #3
Yield, w%				
H_2		2.9	3.4	3.8
C_1		0.1	0.1	0.2
C_2		0.2	0.4	0.6
C_3		0.3	0.5	0.7
C_4		0.3	0.6	0.7
C_5+ liquids	100	96.2	95.0	94.0
Research Octane No.	59	96	100	104
Density @15^{o}C	0.775	0.826	0.838	0.851
PONA Analysis, w%				
N-parafiins	6.4	5.4	4.7	3.7
Iso-paraffins	16.1	20.7	16.3	12.1
Olefins	0.0	0.4	0.2	0.2
Naphthenes	71.5	6.4	3.8	2.1
Aromatics	6.1	67.0	75.0	81.8

Table 3.19 Comparison of Coal Derived VGO and Petroleum VGO

Sample Number	Petroleum VGO (S7923)	Coal Derived VGO (S8027)
Global Properties		
Density @ 15^{o}C, g/cm^3	0.9027	0.9981
Refractive Index	1.4803	1.5309
Sulfur (FX), ppmw	294	21
Nitrogen, ppmw	583	92.1
Pour Point, ^{o}C	39	0
Aniline Point, ^{o}C	91.5	43.7
C_7 Asphaltenes, w%	0.05	0.15
Simulated Distillation, ^{o}C		
IBP	307.6	317.5
5 w%	358.2	331.2
10 w%	378.1	337.5
30 w%	420.1	351.2
50 w%	451.8	363.0
70 w%	487.1	377.2
90 w%	535.6	420.6
95 w%	556.0	452.1
FBP	597.7	539.0
Saturates, w%	55.3	28.2
Aromatics, w%	44.4	71.8

Table 3.20 Catalytic Fluid Cracking (FCC) of Coal Derived VGO – Yields and Product Properties

Feedstock													
Petroleum VGO	wt%	100	100	100	95	95	95	90	90	90	0	0	0
Coal Derived VGO	wt%	0	0	0	5	5	5	10	10	10	100	100	100
Std Conversion (1)	wt%	81.8	83.8	85.2	79.6	83.3	84.3	77.2	81	81.9	60.3	65.6	69
Product Yields													
H2	wt%	0.2	0.3	0.4	0.2	0.3	0.3	0.2	0.3	0.4	0.4	0.6	0.6
C1	wt%	0.7	1.0	1.3	0.7	0.9	1.0	0.5	0.9	1.0	0.3	0.5	0.7
C2=	wt%	0.8	1.0	1.3	0.8	1.0	1.1	0.7	1.0	1.1	0.5	0.8	0.9
C2	wt%	0.5	0.6	0.8	0.4	0.6	0.6	0.4	0.6	0.7	0.3	0.4	0.6
C3	wt%	1.3	1.7	2.5	1.3	1.7	2.0	1.1	2.0	2.1	1.0	1.5	2.0
C3=	wt%	6.5	7.3	7.8	5.6	7.0	6.8	5.6	6.5	6.5	2.9	3.4	3.6
C4	wt%	6.0	7.1	8.7	5.5	6.8	7.7	5.4	7.6	7.5	3.4	4.2	5.0
C4=	wt%	6.4	6.9	6.7	5.9	6.6	6.3	5.6	5.8	5.7	2.5	2.5	2.5
PI-160°C	(LCN)	44.9	42.7	39.7	43.8	42.8	42.5	42.1	40.8	40.1	31.6	33.2	33.7
160-220°C	(HCN)	11.8	10.5	9.2	12.2	10.4	9.8	12.1	10.1	10.0	13.5	12.9	12.1
220-280°C	(LCO)	8.3	7.6	6.7	8.5	7.5	7.1	8.7	7.6	7.6	9.4	9.3	8.9
280-360°C	(HCO)	5.8	5.0	4.6	6.6	5.2	4.9	7.8	6.1	5.7	18.0	13.9	12.1
360°C+	(slurry)	4.1	3.6	3.6	5.3	4.1	3.7	6.3	5.2	4.8	12.3	11.1	10.1
Coke	wt%	2.9	4.7	6.6	3.3	5.2	6.0	3.5	5.4	6.8	3.9	5.6	7.4
		100.2	100.0	99.9	100.1	100.1	99.8	100.0	99.9	100.0	100.0	99.9	100.2
Product Quality													
PI-160°C	(LCN)												
Density, g/cm3		0.728	0.754	0.752	0.737	0.737	0.747	0.732	0.749	0.757	0.765	0.771	0.774
N-paraffins	wt%	3.6	3.5	3.6	3.6	3.7	3.6	3.6	3.6	3.5	2.5	2.4	2.4
Isoparaffins	wt%	35.1	33.5	32.4	32.3	33.4	33.0	33.9	33.0	31.7	18.6	18.5	19.0
Olefins	wt%	8.3	7.8	5.6	9.0	9.5	7.4	11.1	9.2	8.2	30.2	25.9	23.0
Naphthenes	wt%	23.0	20.2	20.7	23.8	23.3	21.5	22.1	18.6	18.4	14.4	12.1	11.1
Aromatics	wt%	29.9	35.0	37.8	31.4	30.1	34.5	29.3	35.7	38.2	34.4	41.1	44.5
RON		91.3	92.2	95.7	91.5	91.7	93.6	90.0	93.1	94.1	88.6	92.1	94.2
MON		81.8	82.5	84.5	81.5	81.9	83.2	80.9	83.4	83.8	81	83.8	85.1

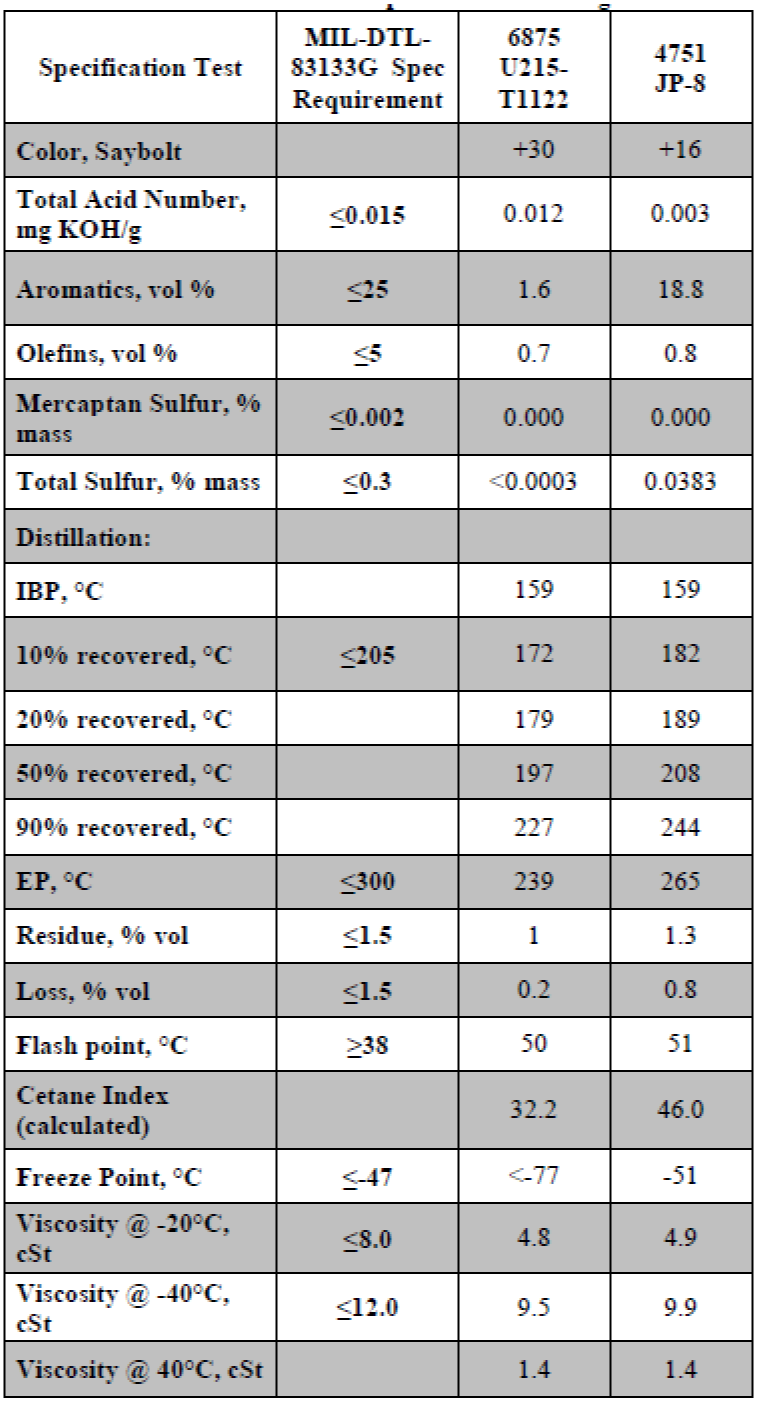
Table 3.21 Catalytic Fluid Cracking (FCC) of Coal Derived VGO – Yields and Product Properties

Feedstock													
Petroleum VGO	wt%	100	100	100	95	95	95	90	90	90	0	0	0
Coal Derived VGO	wt%	0	0	0	5	5	5	10	10	10	100	100	100
Std Conversion (1)	wt%	**81.8**	**83.8**	**85.2**	**79.6**	**83.3**	**84.3**	**77.2**	**81**	**81.9**	**60.3**	**65.6**	**69**
160-220°C	(HCN)												
Density, g/cm3		0.860	0.866	0.876	0.861	0.864	0.869	0.861	0.877	0.880	0.878	0.899	0.908
N-paraffins	wt%	2.3	2.1	1.8	2.2	2.1	2	2.2	1.8	1.7	0.9	0.7	0.6
Isoparaffins	wt%	13.5	11	7.7	11.7	11.6	9.8	13.5	9.2	8.3	8.2	5.6	4.9
Olefins	wt%	4.7	3.8	2.6	7	6.8	4	7.6	3.8	3.4	14.6	9	6.1
Naphthenes	wt%	2.1	1.8	1.3	2.4	2.5	1.9	3	2	1.8	2.9	1.9	1.5
Aromatics	wt%	77.4	81.3	86.6	76.7	77	82.3	73.8	83.1	84.8	73.4	82.7	86.9
RON		94.3	96.8	100.6	94.6	94.7	97.8	92.9	98.5	99.5	90.7	96.3	99.2
MON		83.4	85.4	88.6	84.3	84.3	86.4	83	86.9	87.7	82.1	86.2	88.2
220-280°C	(LCO)												
Density, g/cm3		0.969	0.988	0.994	0.973	0.974	0.993	0.969	0.994	0.998	0.969	0.991	1.001
N-paraffins	wt%	2.3	1.2	1.5	1.1	1.1	0.8	1.4	0.8	0.7	0.5	0.9	0.8
Isoparaffins	wt%	7.1	7.3	5.9	7.5	7.4	6.7	7.4	6.6	6.4	7	5.5	4.9
Olefins	wt%	5.9	4.2	3.9	5.7	5.6	4.2	5.9	4.4	4.1	6.2	3.2	2.7
Naphthenes	wt%	2.7	2.3	1.7	2.6	2.5	2.2	2.8	1.9	1.7	2	1.3	1
Aromatics	wt%	82	85.1	87	83.1	83.5	86.1	82.5	86.3	87.1	84.4	89	90.7
280-360°C	(HCO)												
Density, g/cm3		0.988	0.975	1.004	0.972	0.976	0.972	0.976	0.992	0.990	1.003	1.017	1.020
N-paraffins	wt%	3.6	3.5	2.7	3.2	2.8	2	4	2.2	2.1	5.1	3.5	3
Isoparaffins	wt%	12.3	12.7	7.4	17	15.5	17.4	14.2	14.2	14.7	6.8	7	7.3
Naphthenes	wt%	0.2	3	0.1	0.2	0.2	0.2	0.3	0.2	0.2	0.3	0.3	0.2
Aromatics	wt%	81	75.1	86.2	76.4	78.1	77	78.1	79.9	79.4	83.7	85.5	85.7
Saturated C15+	wt%	2.9	5.7	3.5	3.2	3.3	3.4	3.4	3.5	3.6	4	3.7	3.8

Notes

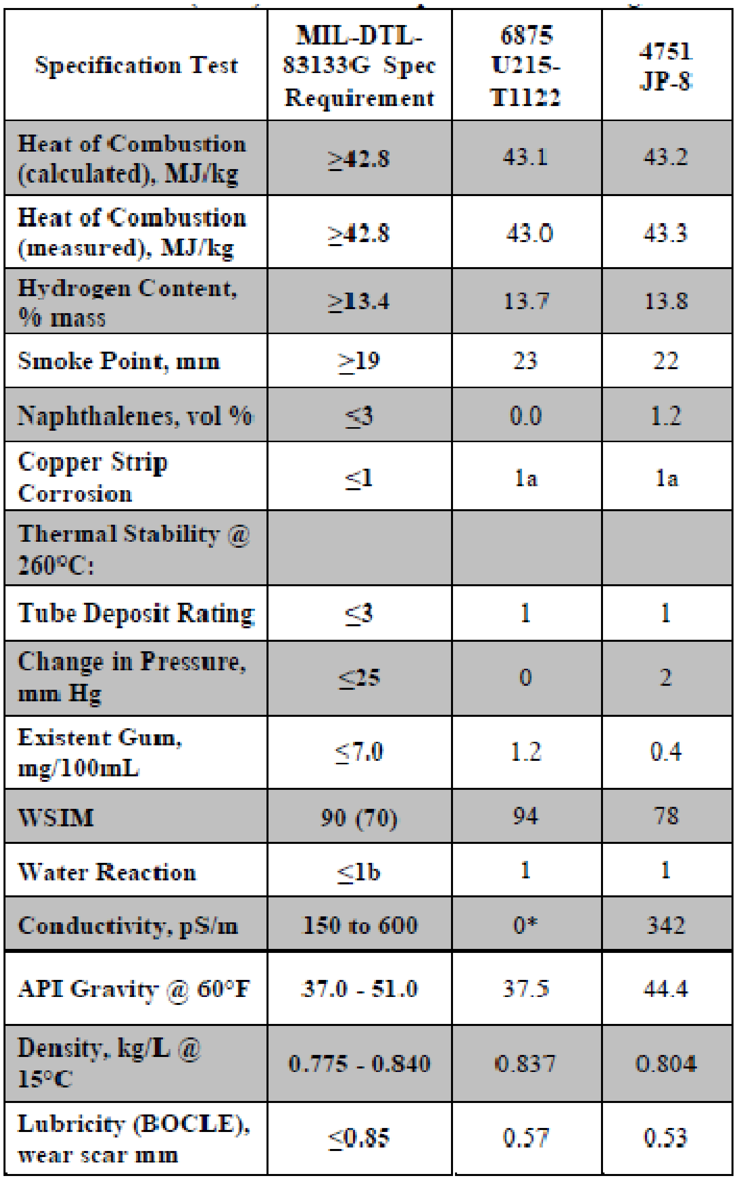
1. Conversion = 100 – LCO, wt% - HCO, wt% - slurry, wt%

Table 3.22 Jet Fuel Specification Test Results – 1/2



Specification Test	MIL-DTL-83133G Spec Requirement	6875 U215-T1122	4751 JP-8
Color, Saybolt		+30	+16
Total Acid Number, mg KOH/g	≤0.015	0.012	0.003
Aromatics, vol %	≤25	1.6	18.8
Olefins, vol %	≤5	0.7	0.8
Mercaptan Sulfur, % mass	≤0.002	0.000	0.000
Total Sulfur, % mass	≤0.3	<0.0003	0.0383
Distillation:			
IBP, °C		159	159
10% recovered, °C	≤205	172	182
20% recovered, °C		179	189
50% recovered, °C		197	208
90% recovered, °C		227	244
EP, °C	≤300	239	265
Residue, % vol	≤1.5	1	1.3
Loss, % vol	≤1.5	0.2	0.8
Flash point, °C	≥38	50	51
Cetane Index (calculated)		32.2	46.0
Freeze Point, °C	≤-47	<-77	-51
Viscosity @ -20°C, cSt	≤8.0	4.8	4.9
Viscosity @ -40°C, cSt	≤12.0	9.5	9.9
Viscosity @ 40°C, cSt		1.4	1.4

Tabl2 3.22 (continue) - 2/2



Specification Test	MIL-DTL-83133G Spec Requirement	6875 U215-T1122	4751 JP-8
Heat of Combustion (calculated), MJ/kg	≥42.8	43.1	43.2
Heat of Combustion (measured), MJ/kg	≥42.8	43.0	43.3
Hydrogen Content, % mass	≥13.4	13.7	13.8
Smoke Point, mm	≥19	23	22
Naphthalenes, vol %	≤3	0.0	1.2
Copper Strip Corrosion	≤1	1a	1a
Thermal Stability @ 260°C:			
Tube Deposit Rating	≤3	1	1
Change in Pressure, mm Hg	≤25	0	2
Existent Gum, mg/100mL	≤7.0	1.2	0.4
WSIM	90 (70)	94	78
Water Reaction	≤1b	1	1
Conductivity, pS/m	150 to 600	0*	342
API Gravity @ 60°F	37.0 - 51.0	37.5	44.4
Density, kg/L @ 15°C	0.775 - 0.840	0.837	0.804
Lubricity (BOCLE), wear scar mm	≤0.85	0.57	0.53

*** Value outside specification limit**

Figure 3.1 Headwaters' Bench Unit -Simplified Process Flow Diagram

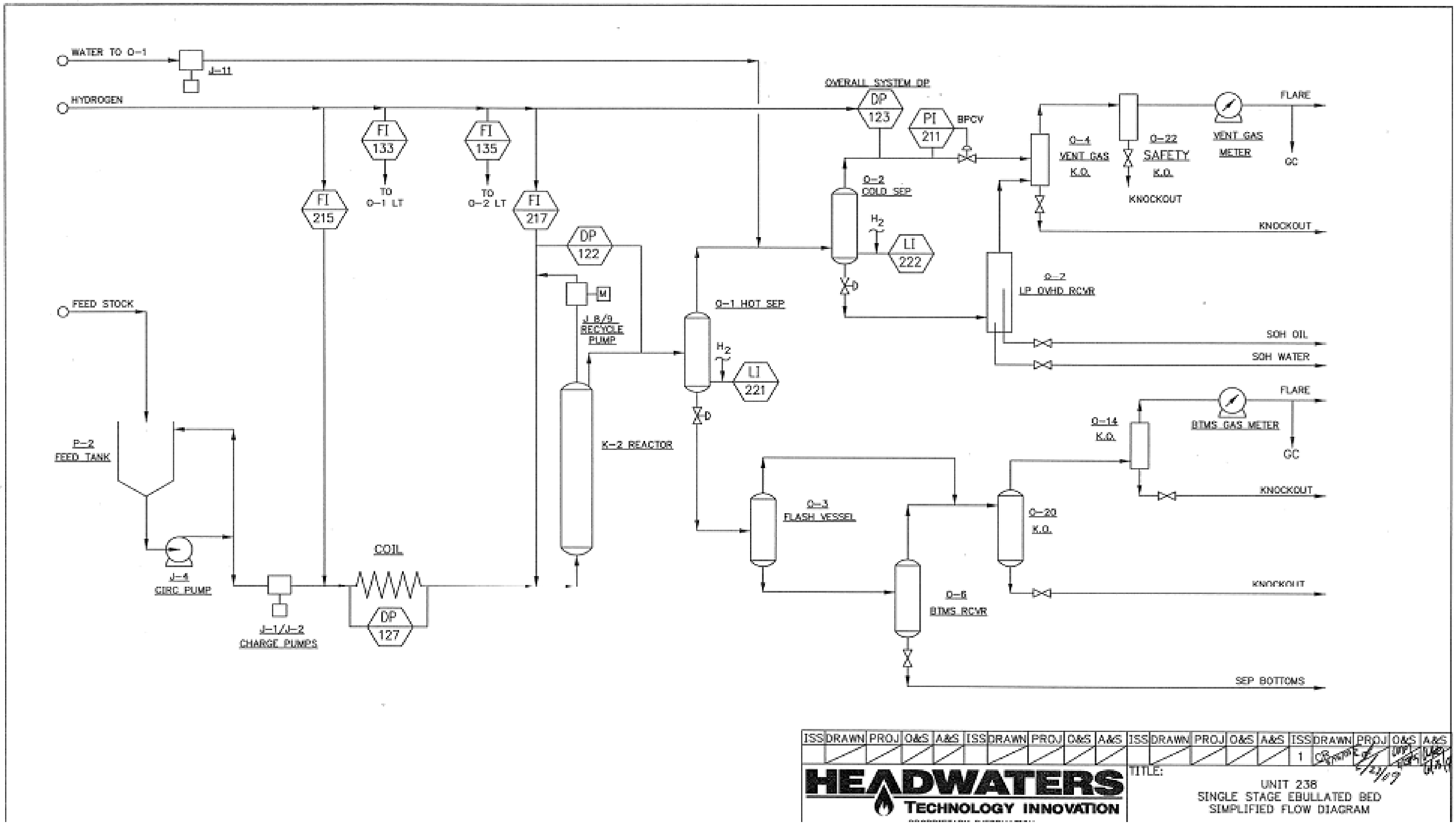


Figure 3.2 Simulated Distillation Curves for L-1509, L-1510 and 25/75 Blend.

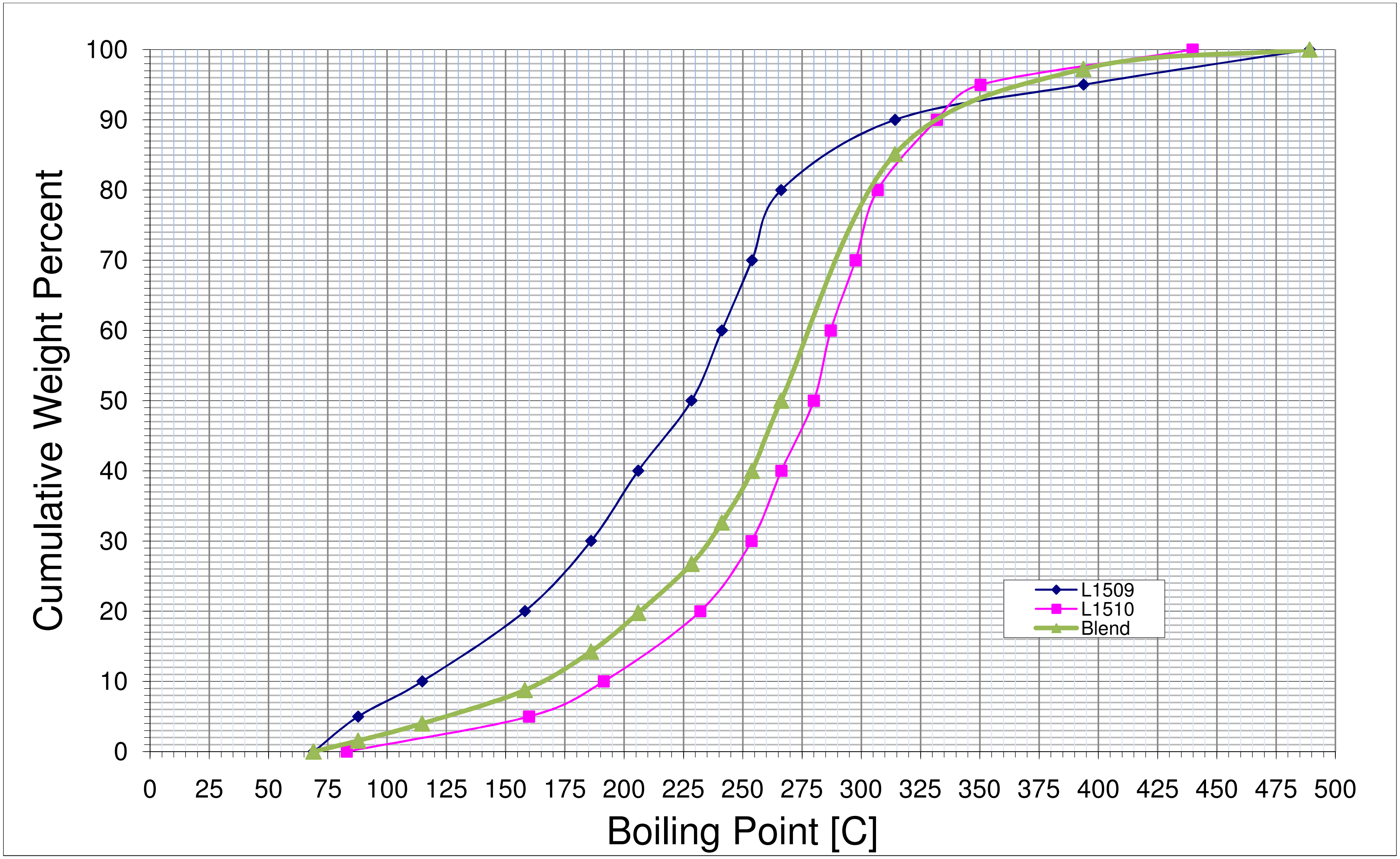


Figure 3.3 Simulated Distillation Curves for L-1509 and Stabilized Products

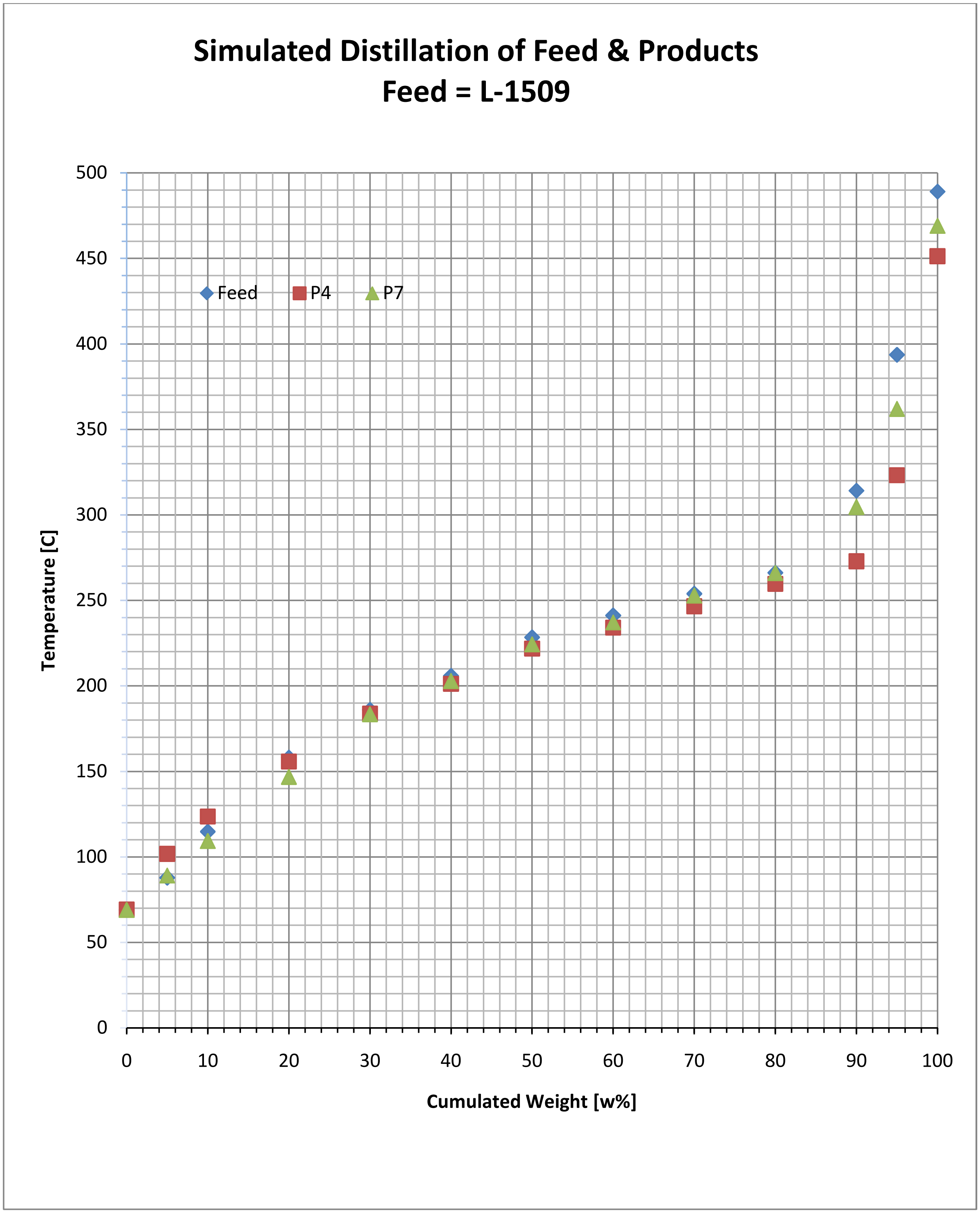


Figure 3.4 Simulated Distillation Curves L-1509/L-1510 Blend and Stabilized Products.

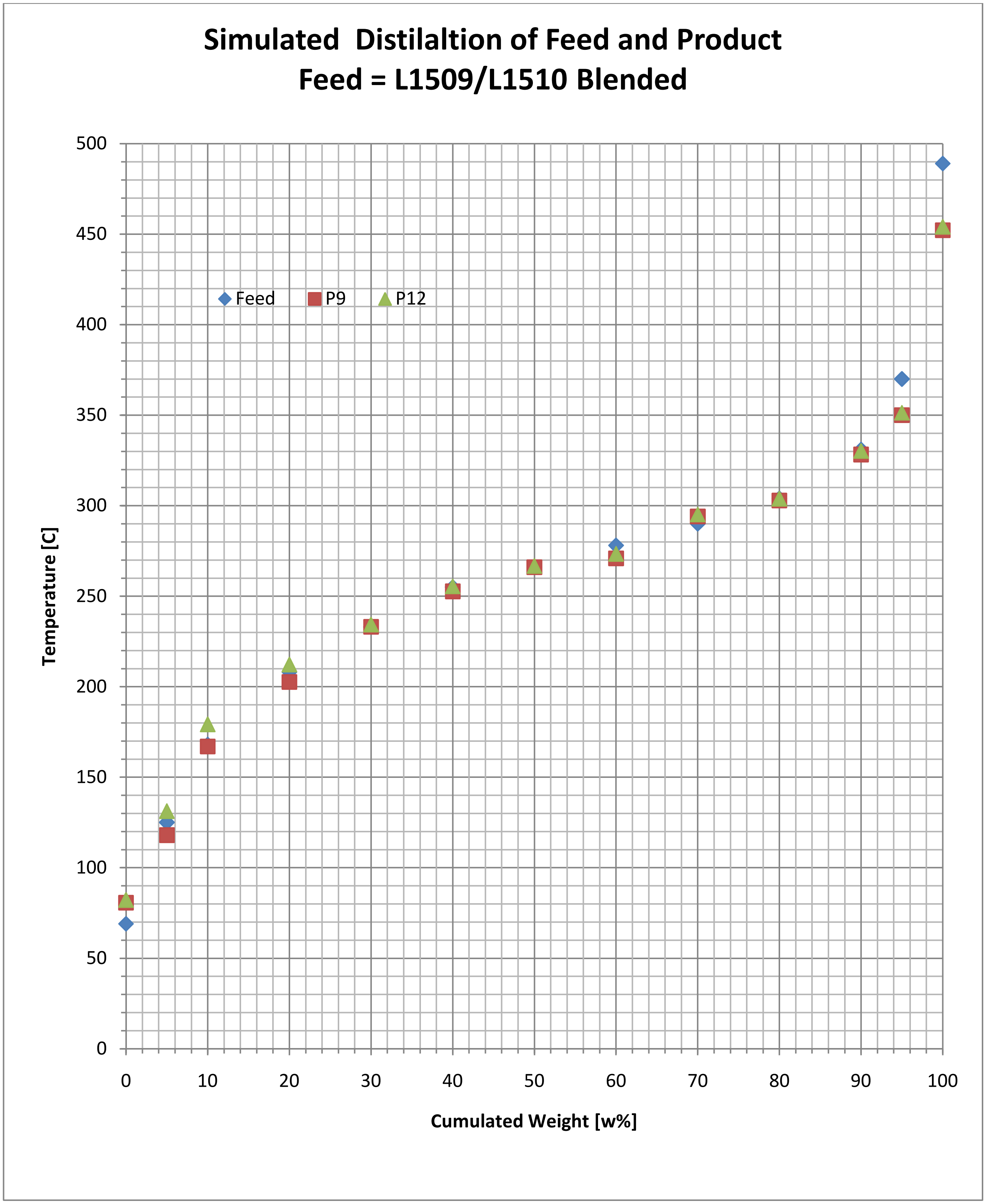


Figure 3.5 Hydrogen Content of Raw and Stabilized Products (in w%)

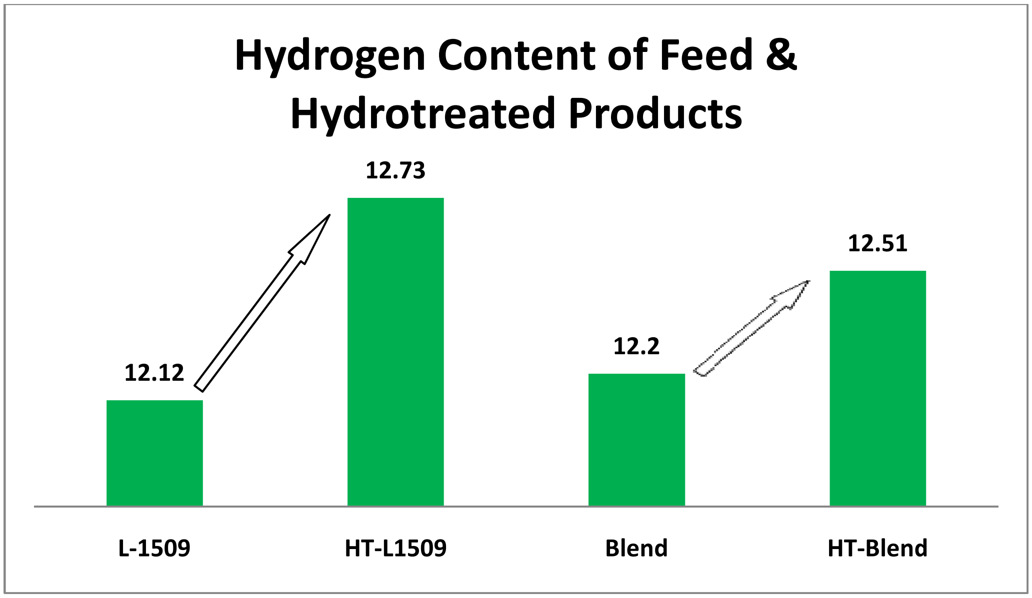


Figure 3.6 Nitrogen and Sulfur Content of Un-stabilized and Stabilized Products [in ppm]

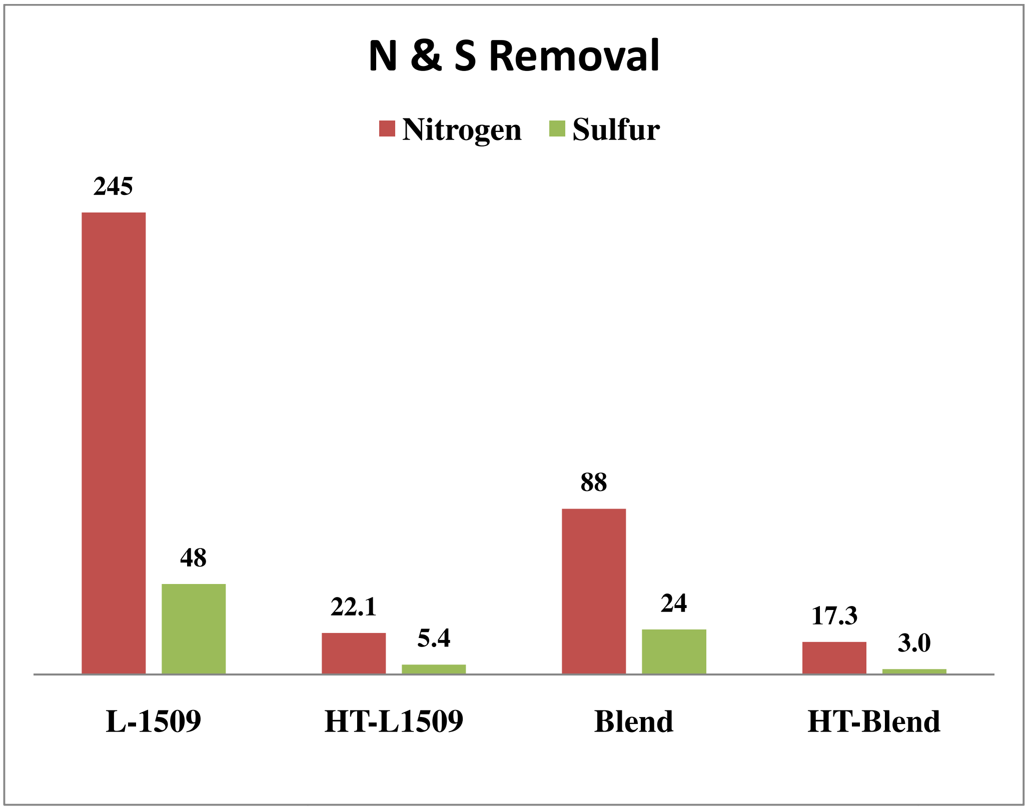
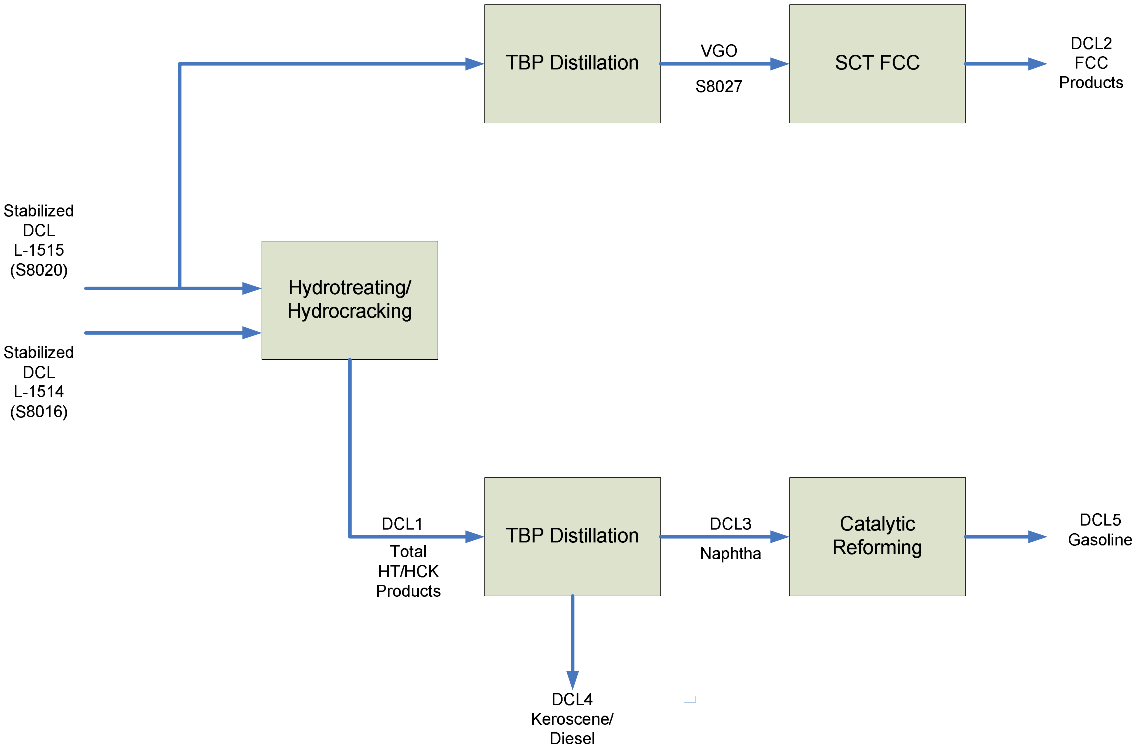


Figure 3.7 Block Flow Diagram – Axens/IFP Refining Study



Note: Detailed characterization was performed on Samples – L-1514 & L-1515, and DCL1 thru DCL5.

Figure 3.8 IFP U215 Hydrotreating/Hydrocracking Pilot Unit – Simplified PFD

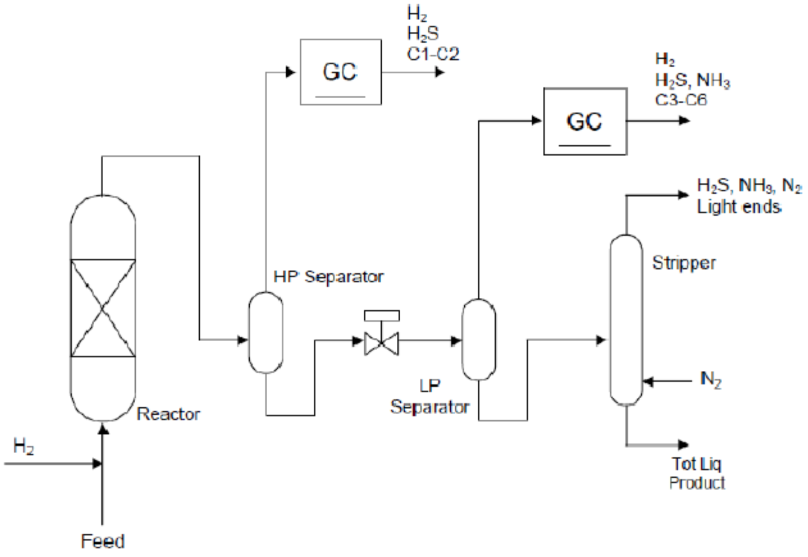


Figure 3.9 Photos of Stabilized Coal Liquids L-1515 (IFP designation – S8020)

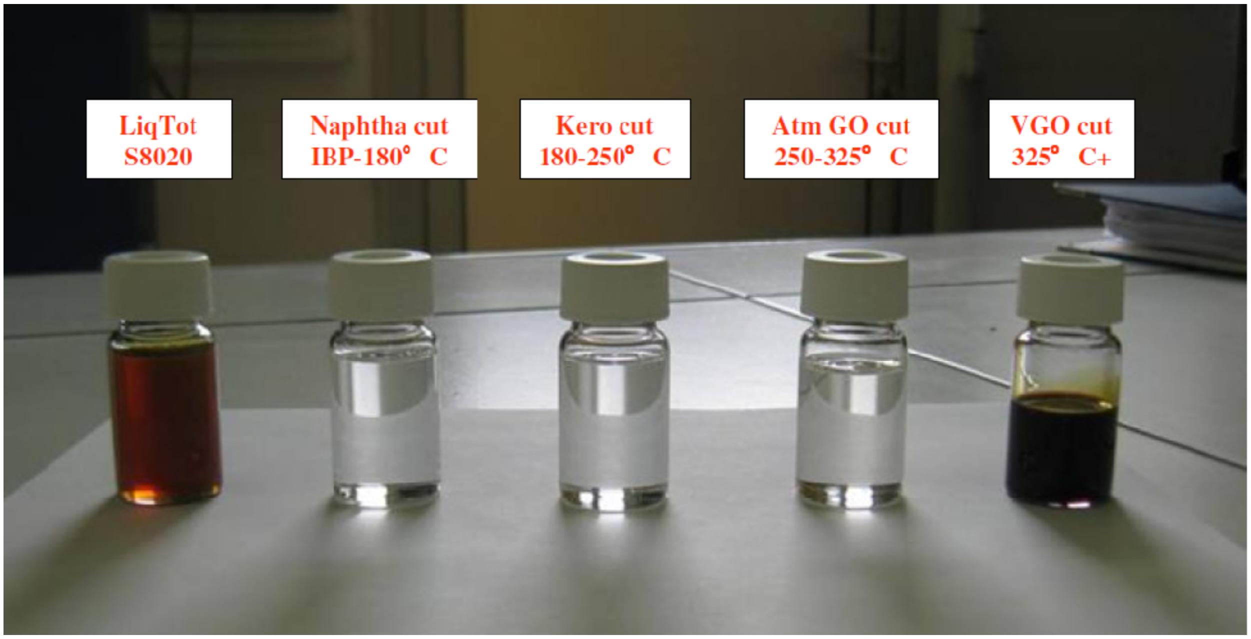


Figure 3.10 Photos of Hydrocracked Coal Liquids Derived from L-1514 (Conditions 1B & 2) & L-1515 (Conditions 3 & 4).

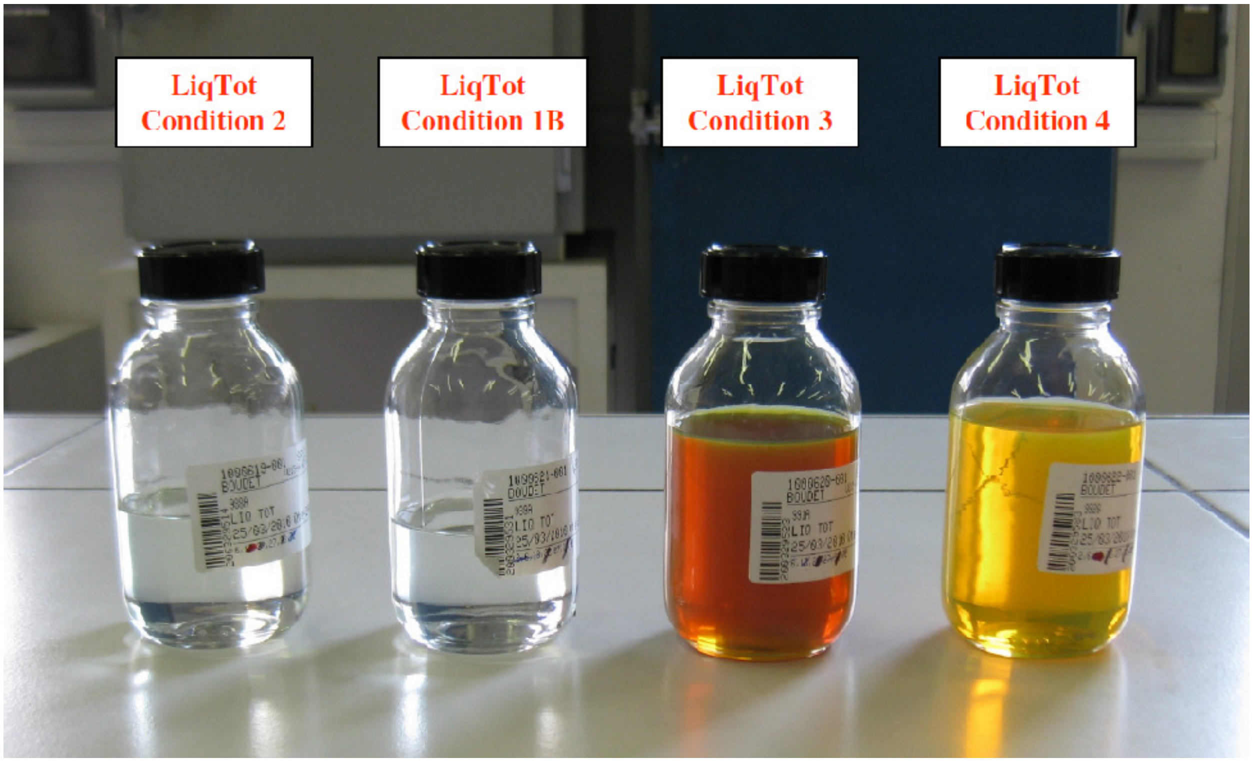


Figure 3.11 Photos of Hydrotreated/hydrocracked Product Fractions from Condition 1B

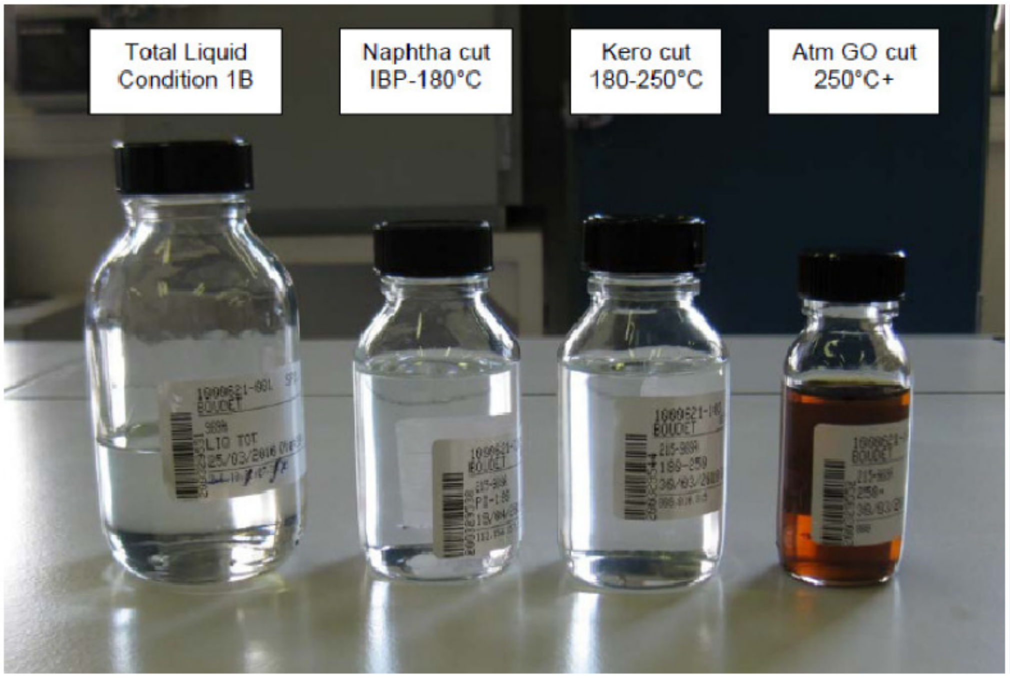


Figure 3.12 Photos of Hydrotreated/hydrocracked Product Fractions from Condition 4

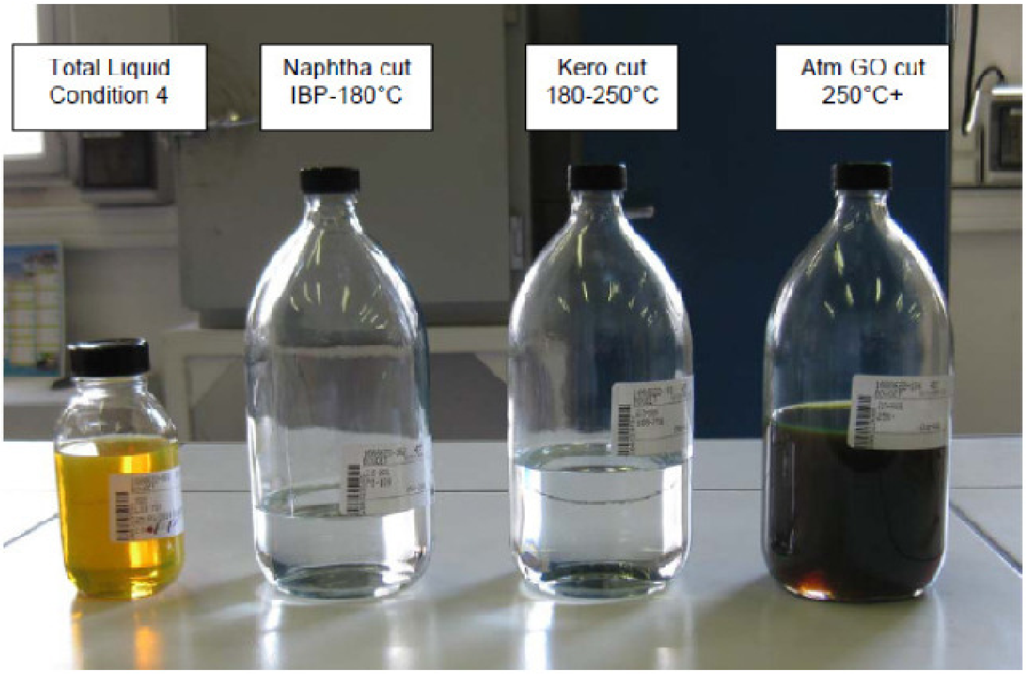


Figure 3.13 Simplified Flow Scheme of IFP Reforming Unit

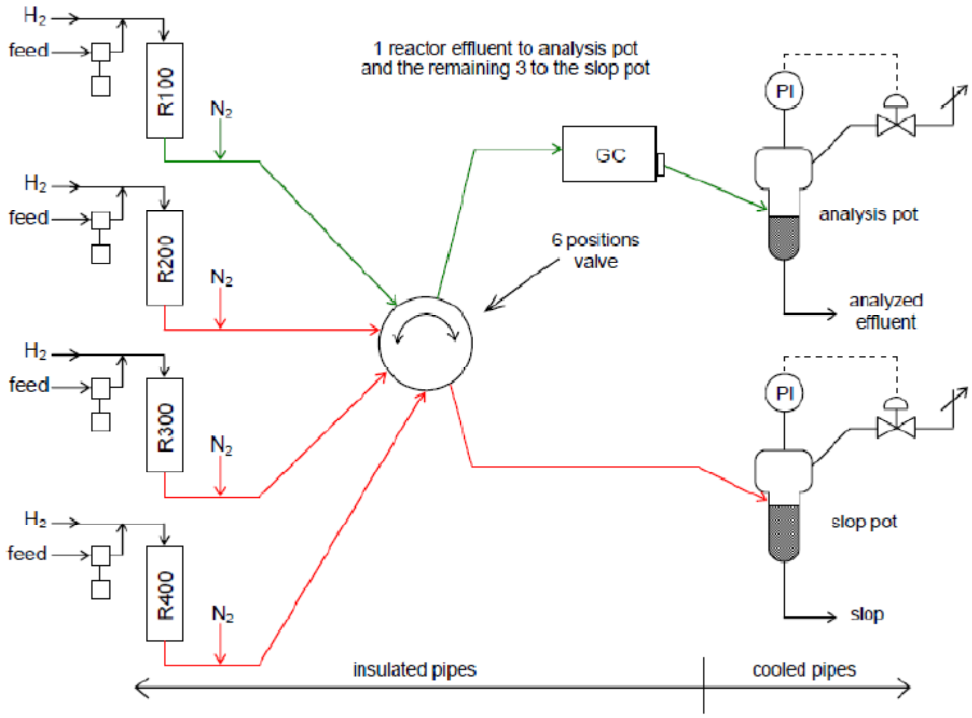


Figure 3.14 Reforming Yield from Coal Derived Naphtha

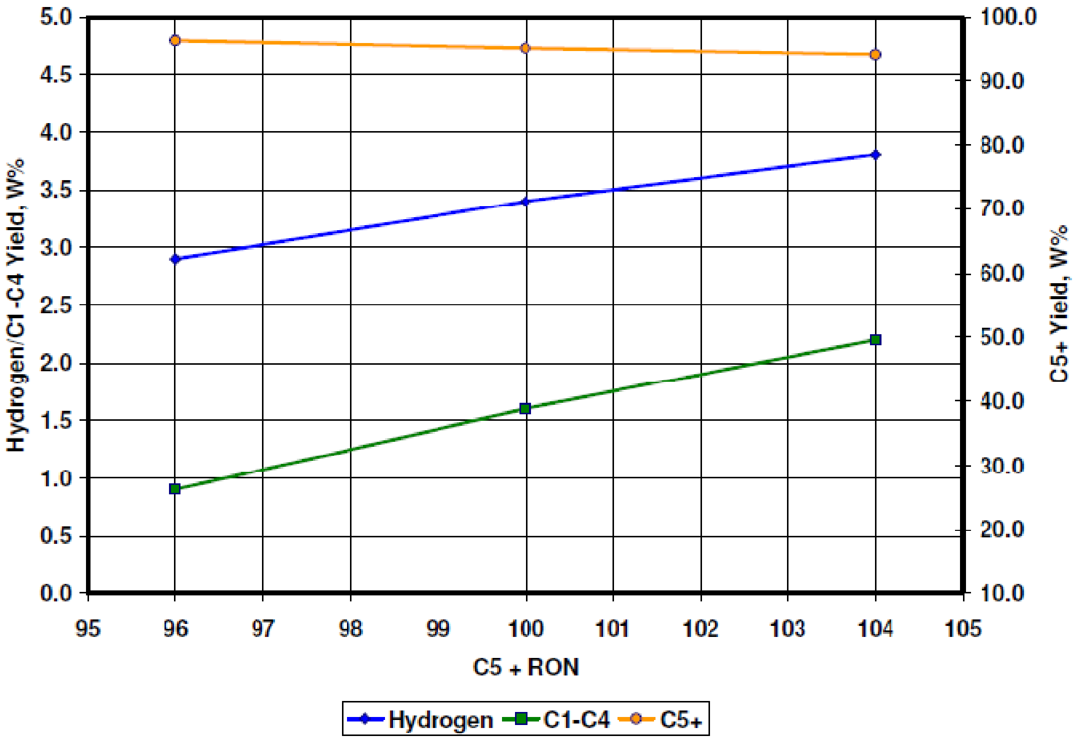


Figure 3.15 Aromatics content in Coal Derived Reformate

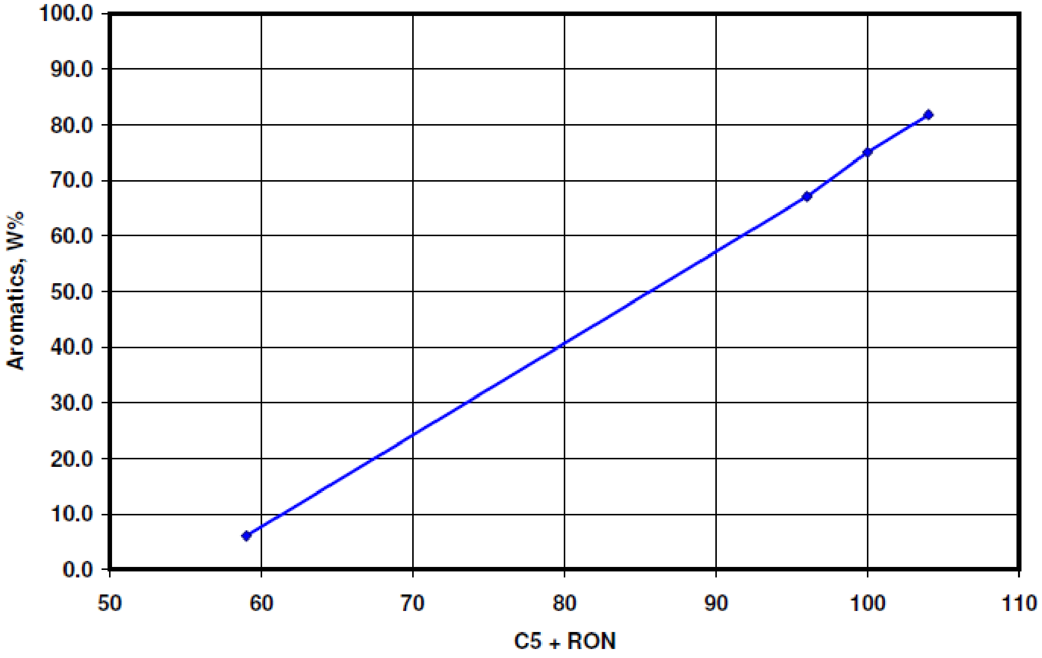


Figure 3.16 Schematic Diagram of IFP FCC Pilot Unit

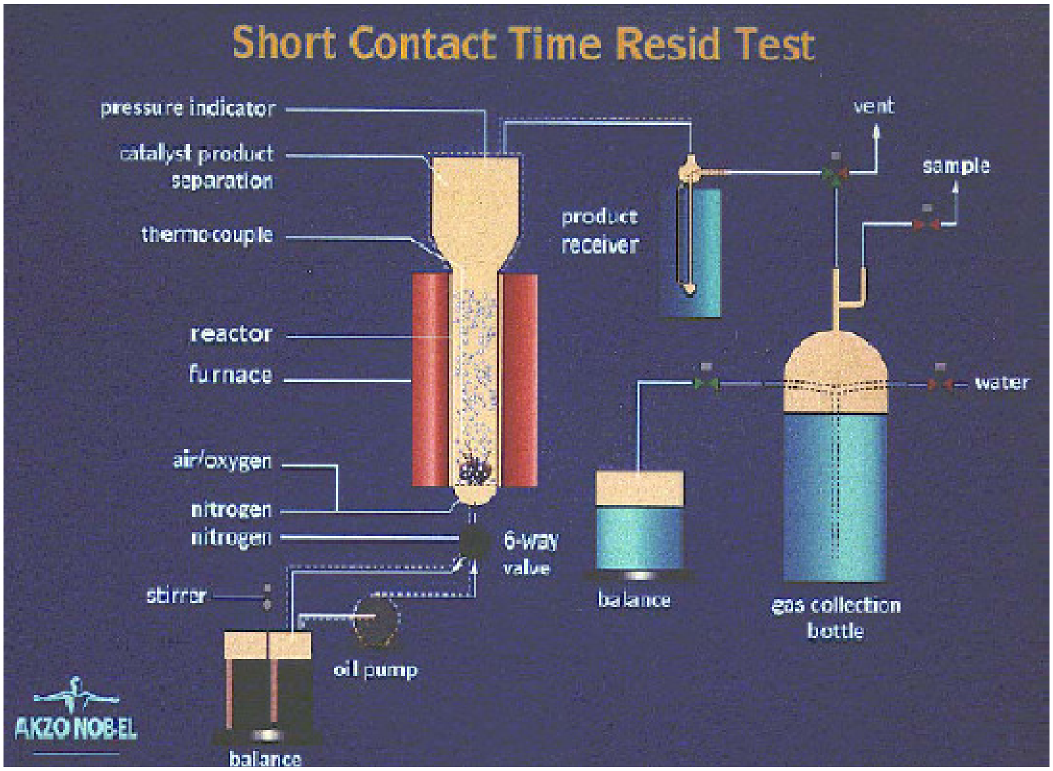


Figure 3.17 FCC Conversion as a Function of Catalyst to Oil Ratio

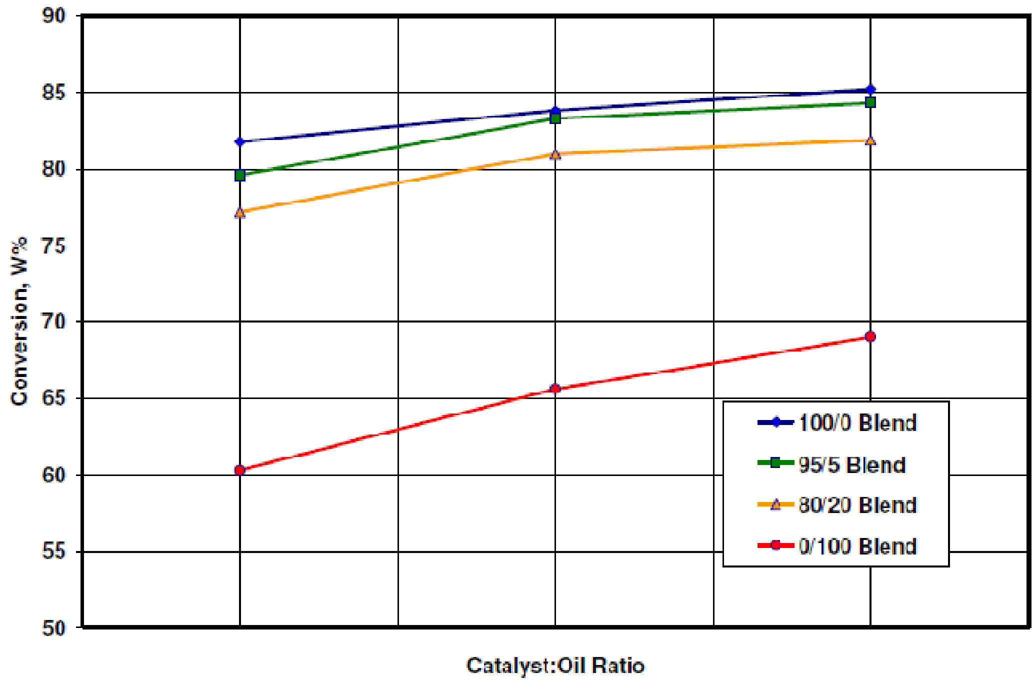
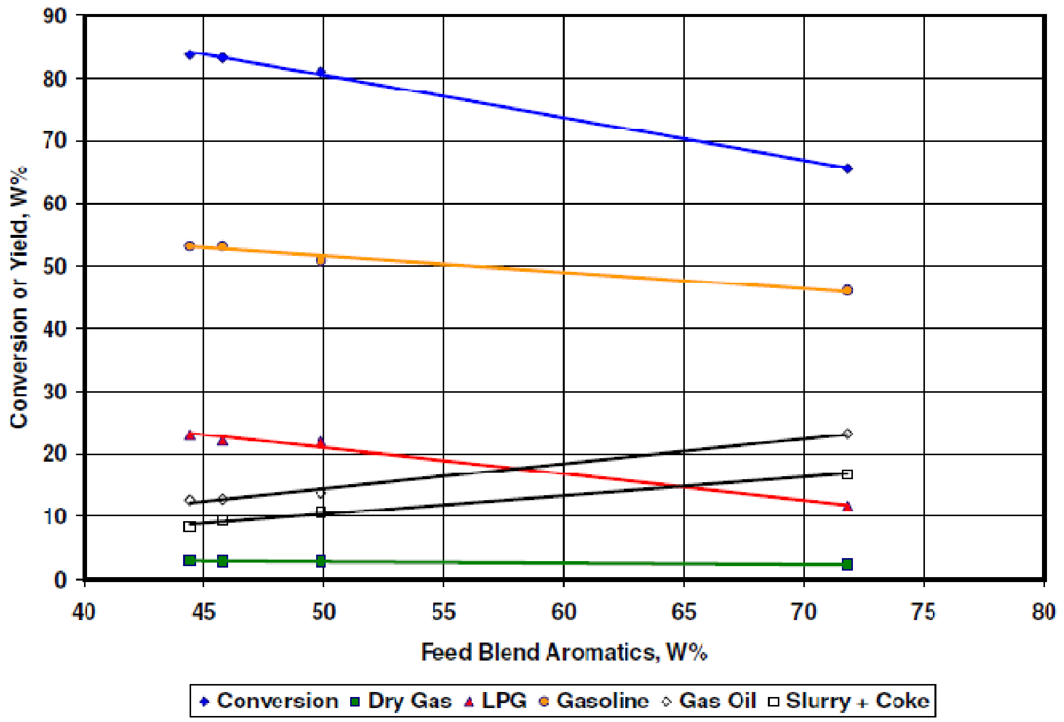


Figure 3.18 FCC Yield at a Constant Catalyst to Oil Ratio – Intermediate Catalyst/VGO ratio.



4. CONCEPTUAL PROCESS DESIGN

Conceptual design of a 45,850 BPSP DCL plant is described in this section. The conceptual plant include coal handling and preparation, coal liquefaction, coal liquids refining, auxiliary units which including sulfur recovery and waste water treatment. Since this study is focused in evaluating different option of hydrogen production, therefore the H_2 plant is not included the battery limits of the DCL complex. For this reason, the coal handling/preparation unit and the other auxiliary units are sized for the needs of the DCL and refining sections only. No doubt integrated design of the H_2 Plant and the DCL Plant will have to be considered once the method of hydrogen production has been selected.

A block flow diagram is depicted in Figure 4.1. The DCL complex is divided into four main functional blocks.

Block	. Description .
1000	Coal Preparation Unit
2000	Direct Coal Liquefaction (DCL) Unit
3000	Coal Derived Liquid (CDL) Refining Unit
4000	Other Units

The Coal Preparation Unit (Section 1000) is responsible for receiving, crushing, pulverizing and feeding of powdered coal into the feed slurry preparation section of the DCL Unit (Section 2000). Dried and pulverized coal from Section 1000 is blended proprietary iron based catalyst, process derived hydrogen donor solvent, sulfiding agent (molten sulfur), recycled heavy oils and solids residues to form the feed slurry prior to being pressurized to the system pressure. The liquefaction catalyst is a water based iron precursor that can be sprayed on to coal particles or blended with part of the donor solvent/recycle residues. The feed slurry is joined with small quantity of fresh hydrogen upstream of the gas fired the preheater in which the catalyst sulfiding reactions commenced. The preheated feed slurry is mixed with the remaining make-up and recycled hydrogen, preheated in a separate gas fired furnace, prior to entering the hydroliquefaction reaction system.

The hydroliquefaction reaction system consists two backmixed reactors, an interstage vapor-liquid separator, a direct-coupled all distillates-donor solvent hydrogenation reactor, products distillation towers, hydrogen recovery and recycle loop, and a gas plant. Under the hydrocracking conditions the large coal molecules break down into small fragments which are stabilized by reacting with hydrogen. Distillate products and recycle solvent are recovered and separated from the reactor coal, mineral matters and dispersed catalyst using a pair of atmospheric and vacuum distillation towers. The recovered intermediate products and spent H-donor solvent are hydrogenated in a direct coupled ebullated bed reactor (a liquid phase fluidized bed). The high boiling fraction and solid residues are sent to battery limits. The intermediate coal liquids are sent to the refining unit for quality improvements. After the recovery of unused hydrogen for recycling, sour off gas streams from the coal liquefaction-direct coupled hydrogenation unit as well as from the refining unit are combined and sent to a common gas plant for further treatment. The gas plant recovers condensable hydrocarbons (light naphtha and LPG), and hydrogen sulfide from the off-gas. The sweetened off-gas, which contains hydrogen, methane and ethane, combines with additional natural gas from battery limits and uses as fuel gas from all the gas fired furnaces.

Sour water from the DCL and the Refining Units are treated in a common waste water treatment unit (WWT). Sour gas recovered from the off-gas is forwarded to a sulfur recovery unit (SRU).

Products from the DCL Complex include:

Stream No.	Stream Name	Remarks
Liquid Hydrocarbons		
14	Gasoline	From Unit 3000, finished products
15	Kerosene/jet fuel	From Unit 3000, finished products
16	Diesel fuel	From Unit 3000, finished products
17	Fuel oil	From Unit 3000, finished products
18	LPG	From Unit 3000, finished products
30	Ammonia	From Unit 4200, finished products
Slurry or Solids		
9	Vacuum residuals	From Unit 2400, to OSBL (gasifier or power plant)
26	Molten sulfur	From Unit 4100, finished products
Gases		
25	CO_2/N_2	From Unit 4100, captured high purityCO_2
10 + makeup NG	Fuel gas	From Unit 2500, in plant use (gas furnaces)
Water		
33	Clarified water	From Unit 4200, recycled

Hydrogen will be purchased from battery limits either from a crossed the fence H_2 plant with a purity of 99.5 % (v/v). The hydrogen plant may produced through steam reforming of natural gas, partial oxidation of hydrocarbons (biomass, liquefaction residuals from the DCL plant), or electrolysis of water using electricity from a crossed the fence nuclear power plant or just off-grid. Details of hydrogen production options and its impact on the economy of the coal derived fuels will be discussed in Section 5 of this report.

Coal Preparation (Section 1000), sulfur recovery (Section 4100), and waste water treatment are well established technologies and therefore will be not discussed herein this report. Also, because of the lack of detailed information of the amount of phenolic compounds to be generated from Illinois coal, recovery of phenols from the waste water is not being considered in this study.

Details of the DCL Unit (Section 2000) and CDL Refining Unit (Section 3000) are discussed in the following section.

4.1 Section 2000 – Direct Coal Liquefaction unit (DCL Unit)

The DCL Unit consists of the following key units:

2100	Catalyst Manufacturing
2200	Slurry Preparation
2300	DCL Unit (DCL) & All Distillate Hydrogenation Unit (ADHU)
2400	Slurry Fractionation
2500	Gas Plant

Catalyst Manufacturing Unit (Section 2100):

This unit involves the synthesis of a Headwaters' GelCat catalyst. Due to the proprietary nature of the process, details of this unit will not be discussed in the reported.

Slurry Preparation Unit (Unit 2200):

The function of this unit is to prepare a pumpable slurry feed for the DCL unit.

Run-of-mine Illinois coal has a moisture content of about 7 w%. It is assumed that the moisture content if run-of –mine coal will be reduced to 2 w% in the pulverized step. Dried pulverized coals are then mixed with Gelcat catalyst, recycle vacuum tower bottoms from Slurry Fractionation Unit, and H-donor solvent from the All Distillate Hydrogenation Unit (ADHU).

Mixing of these streams are performed in three stages – 1) catalyst pre-mixing with H-donor solvent, 2) powdered coal pre-mixing with H-donor solvent and recycle slurry, and 3) blending of catalyst-solvent mix with coal-solvent/recycle slurry. Temperatures of the catalyst and that of the coal pre-mixing tanks are sufficient high that moisture in the Gelcat catalyst and coal can be evaporated from the slurry mixtures. Final mixing of these two streams takes place in the Slurry Feed Preparation Tank which is equipment with specially designed agitator. Part of the donor solvent is used to wash vapor from the mixing tanks to knock down any entrained coal particles. Moisture and light distillates are condensed and separated from the hot vapor stream.

DCL Unit (Unit 2300)

Slurry Feed from the high pressure slurry feed pumps enters a gas fired preheater. A portion of the make-up hydrogen is added to the slurry feed prior to entering the preheater. Temperature of the slurry feed is raised to a temperature below significant cracking reactions take place. The preheated feed slurry is joined by a hot H_2 recycle stream before entering the bottom of the first stage reactor. Gases and water generated in the first reactor are separated in a vapor-liquid separator, interstage separator, before entering the second stage reactor. Cold recycled hydrogen is used to quench the first stage liquid effluent then enters the second stage reaction stage.

The vapor from the inter-Stage Separator, after being cooled, is routed to a vapor-liquid separator without any reduction in pressure. Majority of this vapor from the top of separator is recycled and mixed with makeup hydrogen. The rest of the vapor is routed to a membrane unit for hydrogen recovery prior to discharge it to the Gas Plant (Unit 2500) for further processing. Condensed hydrocarbon liquids are directed to an intermediate products atmospheric tower in Unit 2400.

Effluents from Second Stage Reactor flow to a high pressure hot vapor-liquid separator. The hot vapor from the separator is sent directly to the All Distillate Hydrogenation Unit (ADHU), while the solids bottom stream from the separator is depressurized into a medium pressure flash drum. The bottom slurry products are further discharged into a low pressure flash drum. The depressurized slurry and recovered light distillates are fed the intermediate products atmospheric tower.

Vapor collected from the intermediate pressure drum is routed to a pressure swing system (PSA) for hydrogen recovery. The rich hydrogen stream is recycled, while the hydrogen lean sour gas is passed onto the Gas Plant for further processing

Raw coal liquids, spent H-donor solvent and liquefaction residuals are fractionated in an atmospheric tower. The concentrated slurry from the bottom of the atmospheric tower is fed into preheater before entering into a vacuum tower. More gas oils are recovered from the vacuum tower. All distillates recovered from these two towers are pressurized and fed into the ADHU for hydrotreatment. Part of the Slurry bottoms from the vacuum tower is recycled to the feed slurry preparation system, while the remaining is cooled and flicked. The bottom flicks are sent to battery limited as a by-product. These flicks can either be burnt for power generation or sent to the gasifier (for those cases in which hydrogen is being generated by coal).

All intermediate distillates and spent H-donor solvent are processed in a single ebullated bed reactor filled with a sulfide Ni/Mo supported catalyst. This reactor can handle a wide range of distillate including high boiling materials and can tolerated a small of carried over solids. The reactor is essentially operated under isothermal conditions with a small different temperature between top and bottom. The activity of the ADHU reactor is maintained by regular withdrawal of spent catalyst and addition of fresh supported catalysts. Liquid effluent from ADHU is fractionation through a series of flash. The heavy fraction is recycled as H-donor solvent while the remaining distillates are discharged as stabilized synthetic crude (syncrude) to the CDL Refining Unit (Unit 3000). The entire vapor stream from ADHU, after cooling and recovering of condensable liquids, is recycled to the DCL reactors.

Gas Plant (Unit 2500)

The Gas Plant processes low pressure and medium pressure vapor and off gas streams from the DCL and CDL Refining Units.

Low Pressure Streams:

- Atmospheric Tower overhead vapor
- ADHU low pressure vapor
- CDL Refining off gas

Medium Pressure Streams:

- PSA off gas
- Membrane off gas

Products recovered from the Gas Plant include LPG, light naphtha, sour gases (hydrogen sulfide and carbon dioxide) and sweetened fuel gas.

Because of the presence of sour gases (H_2S and CO_2) recovery of LPG is not straight forward. In order to affect the recovery of LPG and light naphtha from these vapor streams involve four key steps, as shown in Figure 4.3:

Step I To pressurize the low pressure vapor stream to about 8 to 9 kg (g)/cm^2 to knock out some Light naphtha; the compressed vapor is combined with the two other medium pressure streams.

Step II To remove the sour gases by scrubbing the combined vapor stream with an amine solution and then regenerate the rich amine solution to release the sour gases, Step III To further compress the sweetened vapor to about 40 kg (g)/cm^2 and cool it to -40^{o}C; additional light naphtha and LPG are condensed and knockout from the sweetened gas stream.

Step IV To de-ethanize and de-butanize the LPG stream.

The sour gases (H2S and CO2) are routed to the Sulfur Recovery Unit, while the sweetened gas is used as fuel gas in various furnaces. The light naphtha is blended with the stabilized syncrude from ADHU as feed to the CDL Refining Unit. LPG is sent to battery limits as product.

4.2 CDL Refining Unit (Unit 3000)

The DCL Refining Unit is designed to produce transportation fuels for direct usage. The entire stabilized syncrude is firstly processed in a hydrotreating/hydrocracking unit. The objective of this single hydroprocessing step is to yield on specification jet and diesel fuels. Also, naphtha cut from the hydrotreating.hydrocracking step will of sufficient low nitrogen and sulfur contents that it can be fed directly into a catalytic reformer for gasoline production.

A schematic flow diagram of the Hydrotreating/Hydrocracking unit is shown in Figure 4.4. The hydroprocessing unit is a typical trickle bed reactor with multiple catalyst bed arrangement. The liquid effluent from this reactor is fed into a product fractionation column from which the hydroprocessed liquid products are fractionated into naphtha cut, kerosene cut (jet fuel), diesel cut and a gas oil cut. The naphtha cut is forwarded to a catalytic reformer (not shown in Figure 4.4), while the gas oil cut (tower bottoms) can be sold as fuel oil or as feed to a fluid cat cracker (FCC) for gasoline production.

The hydrogen rich offgas from the Cat Reformer is consumed in the hydrotreating /Hydrocarcking Unit to reduce make-up hydrogen requirement.

4.3 Design Basis

Conceptual process design of a DCL complex that purchases hydrogen from a nearby or cross the fence facility is developed. The complex has a capacity of 45,850 BPSD and adapts the process configuration as described in Sections 4.1 and 4.2 above. This DCL complex consists of two maximum size reactor trains operating in parallel and uses Illinois No. 6 coal as feed. The hydroliquefaction system will be operated in bottom recycle mode in which part of the vacuum bottom residuals will be recycled. GelCat catalyst, a proprietary catalyst developed by Hydrocarbon Technologies Inc., predecessor of Headwaters CTL, LLC., will be blended or sprayed on to the feed coal during the slurry feed preparation stage. Unconverted coal, mineral matter and spent catalyst will be discharged along with high boiling residues at the bottom of the vacuum tower.

It is assumed that raw coal delivered to complex has a moisture content of 7 w% and the following ultimate analysis (moisture-free):

Ultimate Analysis,	Weight % (mf basis)
Carbon	71.20
Hydrogen	5.25
Nitrogen	1.42
Sulfur	4.02
Ash	10.24
Oxygen (by difference)	7.87
Heating Value, Btu/lb	13,290

The design conditions are selected according to Condition 1 of POC Run No. 5 (HTI Run NO. 227-97) which was conducted in August/September 1996 under a USDOE funded DCL Proof of Concept program (DOE Contract # AC22-92PC92148). The design temperature of the first and second stage reactor temperature is set at 445 and 455^{o}C, respectively.

The yield structure and process performance of the coal conversion step are summarized below:

Product	**Yield, w% maf coal**	
	Coal Conversion	**Coal Conversion + Stabilization**
Product Yield		
CO_x	1.56	1.56
H_2S	3.32	3.32
NH_3	1.40	1.40
Water	4.16	4.16
C_1-C_3	7.23	7.23
C_4-C_7	2.33	2.33
IBP-177^{o}C	16.90	17.01
177-260^{o}C	16.53	16.63
260-343^{o}C	16.05	16.15
343-454^{o}C	17.00	17.11
454-524^{o}C	4.35	4.38
524^{o}C+	10.25	10.25
Unconverted Coal	4.44	4.44
Total	**105.52**	**105.97**
Process Performance		

H_2 Consumption	5.52	5.97
Coal Conversion	95.48	95.48
IBP-524^{o}C	70.87	71.32
C_4-524^{o}C	73.20	73.65

Based on this yield structure and the information obtained from the stabilization test (described in Section 3.2) the yield pattern was adjusted. The adjusted yield structure then becomes the design basis of the Coal Conversion and All Distillation Hydrogenation Unite (ADHU).

The adjusted yield structure was fed into a DCL process model developed for the hydroliquefaction and stabilization steps. The DCL model is built upon SimSCi PROII process simulation software. The model generated the flowrate and composition of a stabilized syncrude stream which then became the feed to the product refining unit. A separate PRO II model was developed for the refining operations – Step I Hydrotreating/Hydrocracking; Step II Product Fractionation; and Step III Naphtha Reforming. Off gases from the DCL Units and the Refining Unit are combined and treated in a common Gas Plant. Sweetened fuel gases from the gas plant are mixed with purchased natural gas for providing heat to the various furnaces in the complex. There was no simulation done on the Sulfur Recovery Unit and the Waste Wash Treatment Unit. Performance and utilities requirements for these two units are prorated from published information. Also, utilities requirements for the Refining Units were provided by Axens N.A.

For this DCL complex it is assumed that gasoline, kerosene, diesel and hydroprocessed VGO from the Refining Unit are the main product streams.

4.4 Material Balance and Stream Data

The name plate capacity of the DCL plant is 45,850 BPSD and is assumed to be located at the mine mouth. The DCL plant is designed so that it will be self-sufficient in steam, preparing the required process and makeup water, treating all waste water for internal reused, but will purchase natural gas (as heat source), hydrogen and power. The overall C3+ distillate yield is 69.4 w% maf coal.

The DCL plant consumed 11,250 metric TPD of run-of-mine coal, which contains 7 w% of moisture and 9.52 w% of ash (as received basis) and produces 45,850 BPD of high quality distillable products. It should be noted that this amount of coal feed is for the DCL plant only and does not include coal may be required for hydrogen production, if partial oxidation is being used. Overall material balance for the complex is summarized in Table 4.1, while the material balance for the Refining Unit is given in Table 4.2.

The hydrocarbon products available at battery limits include:

Product	Flowrate (BPSD)
LPG	4,794
Distillates	
Gasoline	17,013
Kerosene	13,341
Diesel	9,049
Gas Oil	6,450
Subtotal	45,853
	Metric TPD
HVGO	2,030
Vacuum Tower Bottoms	536.7

Other by-products include 386.3 metric TPD of sulfur and 180.2 TPD of ammonia. The Gas Plant (Unit 2500) produces 50,363 NM^3/h of sweetened fuel gases, which has a heating value equivalent to 323 million Kcal/h. However, these fuel gases will be fully utilized in the DCL complex.

4.5 Utilities

The DCL unit, including the Gas Plant, consumes 84.9 MW of power, as shown in Table 4.4. It needs 245 MM Kcal/h (amount absorbed by the process) of fuel gas to raise the temperature of the slurry feed and make-up hydrogen to reaction conditions. Heat for drying coal in the pulverization process is assumed to come from flue gas of furnace exhaust. Process water totals to 336.2 metric ton/h. This water plus water generated from the DCL unit are routed the Waste Water Treatment Unit. Cooling water required to reduce temperature of various process stream amounts to 604 metric ton/h.

The overall utilities requirements for the DCL Complex are summarized in Table 4.5. These requirements include all requirements from Units 1000, 2000, 3000 and 4000. The total power and fuel gas requirement is 125.4 MW and 16.77 MM Kcal/h, respectively. Makeup process water is 16.6 metric ton/h, while makeup BFW is 87.5 metric ton/h – total makeup water of 104.1 ton/h (or 2,498.4 TPD). Cooling water loss is estimated to be 294 ton/h. The portable water requirement is relatively small and is 10 ton/h.

The DCL complex produce excess amount of low pressure (150 psi) steam. As shown in Table 4.5, there is going to be an excess flow of HP steam (600 psi) of 32,840 kg/h and 87,370 kg/h of LP steam. On the contrary, there is a net requirement of MP steam (300 psi) of 37,410 kg/h. The MP steam requirement can be satisfied by depressurized all the excess HP steam and reconditioning 4,560 kg/h of the LP steam. The reconditioning operation involves raising the temperature and pressure. Energy required for reconditioning is:

Thermal energy for raising the temperature LP steam:

(assuming 90% efficiency in heat transfer) = 24,510 Kcal/h

Energy for compression from 150 to 300 psi = 12.90 kw or 0.31 MWh.

Therefore, the net production of LP steam is from 87,368 Kg/h to 82, 805 Kg/h and there will be no excess HP steam.

4.6 Air Emission

The emissions of NO_x, SO_x, and particulates from the DCL complex are from the following sources:

1. Process furnaces within the DCL plant (Unit 2000)
   - Coal Slurry Feed Heaters
   - Hydrogen Heaters
   - Vacuum Tower Feed Heaters
2. CDL Refining Unit (Unit 3000)
3. Sulfur Recovery Unit (Unit 4100)

Since the DCL Complex purchases hydrogen from an independent facility outside the battery limit, emission from hydrogen production is not included emission from the DCL complex. Also, air emission from drying of run-of-mine coal from 7% to 2% moisture will use hot flue gas from the coal Slurry Feed Heaters (or Hydrogen Heaters) and therefore causes no additional emissions. CO_2 emission from hydrogen production will be discussed separately in Section 5.

Total air emissions are summarized in Table 4.7 which includes emissions from combustion sources and process emission (offgas from Sulfur Recovery Unit, SRU) and particulates from the Coal Preparation Unit (unit 1000). Composition of the sweetened fuel gas from the DCL complex is given in Table 4.6.

The total SOx emission is 5.20 kg/h or 0.125 TPD. The process off-gas from the SRU contains SO_x, NO_x, and CO_2. The combustion of H2S is staged to minimized chemical NOx generation from the possible ammonia carried over from the Waste Water Treatment Unit (Unit 4200). A tailgas treatment is provided to achieve the require sulfur conversion in the SRU. Tailgas from the SRU is normally recycled back to the amine unit so that there is no SOx emission from the SRU.

The source of particulate matter (PM) emission is in the coal preparation plant step which consists of coal handling, storage, drying and pulverization. The PM emission is reduced by employing paved roads, enclosing coal converyors, and installing efficient dust collection system for separating drying gases from pulverized coal. The total PM emission is estimated to 16.27 kg/h of which 12.21 kg/h is from the Coal Preparation Unit.

The total amount of CO_2 emission is estimated to be 1,967 metric TPD (or 81,965 kg/h). CO2 mission is mostly from heaters. All these emissions are from combustion sources and therefore cannot be recovered easily. However, if high purity oxygen is available (from the nearby or crossed the fence H_2 production plant) oxygen can be used for combustion the SRU. In such case 125 TPD (6.4 w% of the total emission) of CO_2 can be recovered in high purity.

Table 4.1 Overall Material Balance – DCL + Refining Unit (excluding Coal Preparation Unit)

HEADWATERS
COAL TO LIQUIDS

Page 1 of 1

DCL (incl. Gas Plant) + REFINING UNIT, BATTERY LIMITS MATERIALS BALANCE

			Rev No.	Date	BY	Approve
Client:	DOE Study					
Location:	Illinoise, USA		0	06/07/10	WL	RC
Project:	--		1			
Unit:	DCL Unit		2			
Unit No:	--	Job No.: --	3			

---- Streams Entering ----------

Stream ID	Stream Name	KG/HR
101	Fresh Coal to DCL Unit (2% mositure)	444,832
102	Makeup H2 to DCL Unit	28,840
129	Makeup H2 to CDL Refining Unit	1,704
103	GelCat to DCL Unit	5,360
105	Sulfur Injection to Slurry	449
	Subtotal	481,186
106	Vent Scrubber Air Leakage	51
107	Vacuum Tower Air Leakage	84
108	Vacuum Tower Ejector Motive Steam	3,350
109	Vent Scrubber Ejector Motive Steam	355
110	Stripping Steam to Stablized Syncrude	3,293
123	Atmospheric Tower Stripping Steam	5,025
111	Makeup Process water	336,255
	Subtotal	348,413
	Total Entering	829,598

------ Streams Leaving ----------

Stream ID	Stream Name	KG/HR
131	Gasoline from CDL Refining Unit	85,566
132	Kerosene/Jet Fuel from CDL Refining Unit	75,998
133	Diesel from CDL Refining Unit	53,198
134	Fuel Oil from CDL Refining Unit	39,263
113	Vacuum Tower Bottoms to BL	84,584
114	Vacuum Tower HVGO Draw to BL	22,319
	Subtotal	360,928
104	Sour Gas from Gas Plant to Sulfur Recovery	7,553
128	LPG from Gas Plant	17,577
126	Fuel Gas from Gas Plant	31,031
119	Vent Scrubber Ejector Seal Drum Vapor	160
124	Vacuum Tower Ejector Seal Drum Vapor	689
120	Sour Water Drum Vapor to BL	327
121	Vent Scrubber Separator Water to BL	12,714
122	Sour Water Drum Water to BL	398,551
	Subtotal	468,602
	Total Leaving	829,531
	IN - Out = ----->	68
		0.01%

Table 4.2 Overall Material Balance – CDL Refining Unit

HEADWATERS
COAL TO LIQUIDS

Page 1 of 1

CDL Refining Unit, BATTERY LIMITS MATERIALS BALANCE

				Rev No.	Date	BY	Approve
Client:	DOE Study						
Location:	Illinoise, USA			0	06/07/10	WL	RC
Project:	--			1			
Unit:	DCL Unit			2			
Unit No:	--	Job No.:	--	3			

---- Streams Entering ----------

Stream ID	Stream Name	KG/HR	BPSD
112	Stablized Syncrude	259,035	45,454
127	Light Naphtha from Gas Plant	6,107	1,316
129	Makeup H2 to CDL Refining Unit	1,704	-46,770
	Subtotal	266,846	46,770
	Total Entering	266,846	

------ Streams Leaving ----------

Stream ID	Stream Name	KG/HR	BPSD
130	Offgas from CDL Refining Unit	12,761	---
131	Gasoline from CDL Refining Unit	85,566	17,013
132	Kerosene/Jet Fuel from CDL Refining Unit	75,998	13,341
133	Diesel from CDL Refining Unit	53,198	9,049
134	Fuel Oil from CDL Refining Unit	39,263	6,450
	Subtotal	266,785	45,853
	Total Leaving	266,785	
	IN - Out = ----->	61	
		0.02%	

Table 4.3a DCL + Refining Units Stream Data

HEADWATERS COAL TO LIQUIDS

Headwaters DCL Technology - Direct Liquefaction of Illinois No. 6 Coal

45,850 BBL/Day Tranportation Fuels OVERALL MATERIAL BALANCE

STREAM	1	2	3	4	5	6	7	8	9	10	11
STREAM DESCRIPTION	TOTAL COAL FEED	DRIED COAL TO DCL	WATER LOSS (PULVERIZER)	MAKEUP H2 TO DCL & CDL REFINING UNITS	MAKEUP H2 TO DCL UNIT	STABILIZED SYNCRUDE	VTB TO B/L (or GASIFIER)	HVGO FROM DCL FRAC. UNIT	VTB & HVGO to B/L (or to GASIFIER)	FUEL GAS FROM DCL UNIT & GAS PLANT	SOUR GAS (FROM GAS PLANT)
COMPONENTS RATE	SOLID	SOLID	LIQUID	VAPOR	VAPOR	LIQUID	SLURRY	LIQUID	SLURRY	VAPOR	VAPOR
	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR
H2	0	0	0	28,551	26,958	36	0	0	0	2,055	1
H2O	32,812	8,897	23,915	0	0	172	0	0	0	27	416
H2S	0	0	0	0	0	312	0	0	0	206	3,680
NH3	0	0	0	0	0	54	0	0	0	8	522
CO	0	0	0	0	0	7	0	0	0	2,529	1
CO2	0	0	0	0	0	144	0	0	0	10	2,928
C1	0	0	0	0	0	139	0	0	0	10,335	2
C2	0	0	0	0	0	401	0	0	0	9,000	2
C3	0	0	0	0	0	1,365	0	0	0	5,020	2
C4	0	0	0	0	0	1,949	0	0	0	299	0
C5	0	0	0	0	0	1,180	0	0	0	15	0
C6-177C	0	0	0	0	0	57,625	0	0	0	98	0
177C-260C	0	0	0	0	0	60,543	2	0	2	13	0
260C-371C	0	0	0	0	0	76,293	40	0	40	0	0
371C-490C	0	0	0	0	0	54,486	1,148	0	1,148	0	0
490C-524C	0	0	0	0	0	4,274	888	332	1,220	0	0
524+	0	0	0	0	0	31	18,557	21,987	40,544	0	0
Coal IOM	391,295	391,295	0	0	0	0	17,374	0	17,374	0	0
CAT. SOLID	0	0	0	0	0	0	1,935	0	1,935	0	0
ASH	44,640	44,640	0	0	0	0	44,640	0	44,640	0	0
ARGON	0	0	0	TRACE	TRACE	0	0	0	0	0	0
COS	0	0	0	0	0	0	0	0	0	0	0
N2	0	0	0	1,994	1,882	24	0	0	0	1,902	1
O2	0	0	0	0	0	0	0	0	0	0	0
S	0	0	0	0	0	0	0	0	0	0	0
TOTAL RATE	**468,747**	**444,832**	**23,915**	**30,544**	**28,840**	**259,035**	**84,584**	**22,319**	**106,904**	**31,518**	**7,553**
MW			18.02	2.15	2.15	API=36.65	API = -6.86	API = -2.75	API = -4.72	14.02	36.86
VOL. RATE (NM3/HR)				318,825	301,038					50,363	5,130

Table 4.3b DCL + Refining Units Stream data

Headwaters DCL Technology - Direct Liquefaction of Illinois No. 6 Coal

45,850 BBL/Day Tranportation Fuels OVERALL MATERIAL BALANCE

STREAM	12	13	14	15	16	17	18	19	24	25	26
STREAM DESCRIPTION	LIGHT NAPHTHA FROM GAS PLANT	OFF GAS FROM CDL REFINING UNIT	GASOLINE FROM CDL REFINING UNIT	KEROSENE/JET FUEL FROM CDL REFINING UNIT	DIESEL FROM CDL REFINING UNIT	FUEL OIL FROM CDL REFINING UNIT	LPG FROM GAS PLANT	Makeup H2 to CDL unit	ESTIMATED AIR TO SRU	N2 & CO2 to B/L	MOLTEN SULFUR
COMPONENTS RATE	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	VAPOR	VAPOR	VAPOR	SOLID
	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR
H2	0	523	0	0	0	0	0	1,593	0	1	0
H2O	0	172	0	0	0	0	0	0	0	0	0
H2S	0	312	0	0	0	0	0	0	0	0	0
NH3	0	54	0	0	0	0	0	0	0	5	0
CO	0	7	0	0	0	0	0	0	0	1	0
CO2	0	144	0	0	0	0	0	0	16	3,437	0
C1	0	511	0	0	0	0	0	0	0	2	0
C2	0	1,213	0	0	0	0	1	0	0	2	0
C3	0	3,125	0	0	0	0	7,014	0	0	2	0
C4	0	5,383	0	0	0	0	9,268	0	0	0	0
C5	817	1,180	817	0	0	0	1,293	0	0	0	0
C6-177C	5,173	0	77,500	0	0	0	0	0	0	0	0
177C-260C	114	0	7,246	55,731	0	0	0	0	0	0	0
260C-371C	2	0	2	20,267	53,198	0	0	0	0	0	0
371C-490C	0	0	0	0	0	39,263	0	0	0	0	0
490C-524C	0	0	0	0	0	0	0	0	0	0	0
524+	0	0	0	0	0	0	0	0	0	0	0
Coal IOM	0	0	0	0	0	0	0	0	0	0	0
CAT. SOLID	0	0	0	0	0	0	0	0	0	0	0
ASH	0	0	0	0	0	0	0	0	0	0	0
ARGON	0	0	0	0	0	0	0	TRACE	460	460	0
COS	0	0	0	0	0	0	0	0	0	0	0
N2	0	135	0	0	0	0	0	111	26,941	26,942	0
O2	0	0	0	0	0	0	0	0	8,256	0	0
S	0	0	0	0	0	0	0	0	0	0	16,096
TOTAL RATE	**6,107**	**12,761**	**85,566**	**75,998**	**53,198**	**39,263**	**17,577**	**1,704**	**35,673**	**30,852**	**16,096**
MW	API = 78.49	23.56	API = 61.07	API = 36.73	API = 31.02	API = 24.94	58.33	2.15	28.97	29.32	32.06
VOL. RATE (NM3/HR)		12,133					7,544	17,788	27,587	23,570	

Table 4.3c DCL + Refining Units Stream Data

HEADWATERS
COAL TO LIQUIDS

Headwaters DCL Technology - Direct Liquefaction of Illinois No. 6 Coal
45,850 BBL/Day Tranportation Fuels OVERALL MATERIAL BALANCE

STREAM	27	28	29	30	31	32	33				
STREAM DESCRIPTION	SULFUR ADDITION TO DCL	SOUR WATER (FROM SRU)	SOUR GAS (FROM SWS)	NH3	SOUR WATER FROM DCL UNIT	WATER LOSS (EVAP.)	CLARIFIED WATER TO STORAGE TANK				
COMPONENTS RATE	SOLID	LIQUID	VAPOR	VAPOR	LIQUID	LIQUID	LIQUID				
	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR	KG/HR				
H2	0	0	0	0	1	1	0				
H2O	0	9,712	0	0	389,856	79,913	319,654				
H2S	0	1	13,906	0	13,912	6	0				
NH3	0	516	0	7,508	7,001	10	0				
CO	0	0	0	0	0	0	0				
CO2	0	0	493	0	493	0	0				
C1	0	0	0	0	2	2	0				
C2	0	0	0	0	0	0	0				
C3	0	0	0	0	0	0	0				
C4	0	0	0	0	0	0	0				
C5	0	0	0	0	0	0	0				
C6-177C	0	0	0	0	0	0	0				
177C-260C	0	0	0	0	0	0	0				
260C-371C	0	0	0	0	0	0	0				
371C-490C	0	0	0	0	0	0	0				
490C-524C	0	0	0	0	0	0	0				
524+	0	0	0	0	0	0	0				
Coal IOM	0	0	0	0	0	0	0				
CAT. SOLID	0	0	0	0	0	0	0				
ASH	0	0	0	0	0	0	0				
ARGON	0	0	0	0	0	0	0				
COS	0	0	0	0	0	0	0				
N2	0	0	0	0	0	0	0				
O2	0	0	0	0	0	0	0				
S	449	0	0	0	0	0	0				
TOTAL RATE	**449**	**10,229**	**14,399**	**7,508**	**411,265**	**79,933**	**319,654**				
MW	32.06			17.03							
VOL. RATE (NM3/HR)				9,874							

Table 4.4 DCL Unit Utilities Requirement (excluding H_2 Plant & Units 1000, 3000 & 4000)

HEADWATERS COAL TO LIQUIDS Overall Summary of Utilities Estimate

Client: DOE Unit: **DCL (with Gas Plant)**
Location: Illinois, USA
Project: DE-FC26-05NT42448 06/14/10

	Consumption	Production	Circulation
Fuel Gas, MMKcal/h	245		
Electricity, KW	84,920		
HP Steam, Kg/h	35,517		
MP Steam, Kg/h		207,108	
LP Steam, Kg/h		112.847	
BFW, Kg/h	314,710		
MP Steam Condensate, Kg/h		15,209	
LP Steam Condensate, Kg/h		3,040	
Cooling Water			603,980
Process Water	336,255		

Table 4.5 Overall Utilities Requirement Breakdown by Unit (excluding H_2 Plant)

Utility Descriptions + : comsume - : Production	Units	Unit 1000 Coal Prep.	Unit 2000 DCL Unit	3000 CDL Refining Unit	Unit 4000 Other Unit	Misc. (Cond. Polishing, Cooling Tower, and Flash Drum)	Total
Cooling Water Circ	mt/h		604	1,111	3,862	-5,577	0.0
Cooling Water Loses	mt/h					294	294.5
M/U Process Water	mt/h		336			-320	16.6
Potable Water	mt/h					10	10.0
Boiler Feed Water:							
600# HHP	kg/h				32,845	-32,845	0
300# HP	kg/h		11,783			-11,783	0
150# MP	kg/h		234,340	22,680		-257,020	0
50# LP	kg/h		68,587		9,535	-78,122	0
M/U BFW+ Cond. Blowdown	kg/h					87,532	87,532
Steam:							
600# HHP	kg/h				-32,845		-32,845
300# HP	kg/h		35,517		1,891		37,408
150# MP	kg/h		-207,108	-22,680	142,729	-309	-87,368
50# LP	kg/h	22,563	-112,847		-9,535	99,819	0
Steam Condensates							
HP	kg/h		0		-1,891	1,891	0
MP	kg/h		-15,209		-142,729	157938	0
LP	kg/h	-22,563	-3,040			25603	0
Fuel Gas	MMKcal/h		-78	87	8.31		16.77
Electric Power	MW	5.3	84.9	15	3.34	16.83	125.40

Notes:

1. BFW, Steam, & Condensate Pressure Ratings

600# HHP	42.2 , kg/cm2 (g)
300# HP	21.1 , kg/cm2 (g)
150# MP	15.0 , kg/cm2 (g)
50# LP	3.5 , kg/cm2 (g)

2. Value in minus represents production.

Table 4.6 Composition of Sweetened Fuel Gas (Stream No. 10)

Inert Gases		**Combustible Gases**	
Gases	**W%**	**Gases**	**W%**
H_2O	0.086	H_2	6.520
CO_2	0.032	H_2S	0.654
N_2	6.035	NH_3	0.025
		CO	8.024
		C_1	32.791
		C_2	28.555
		C_3	15.927
		C_4	0.949
		C_5+	0.400
Subtotal	**6.153**	**Subtotal**	**93.845**

Table 4.7 Air Emissions from the DCL Complex (excluding H_2 production)

Contaminant	**Emission (Kg/h)**				
	DCL Unit	**Refining Unit**	**SRU**	**Total**	**Total Kg/bbl**
PM	16.27	1.30	0.12	**17.69**	
CO_2	58,168	18,584	5,213	**81,965**	**42.9**
CO	44.83	14.32	1.37	**60.52**	
NO_x	60.12	23.87	0.81	**84.81**	
SO_X	3.92	1.25	0.12	**5.29**	
C_1	1.23	0.39	0.04	**1.66**	
VOC	2.93	0.94	0.09	**3.96**	
TOC	5.87	1.88	0.18	**7.92**	

Figure 4.1 Direct Coal Liquefaction Plant – Block Flow Diagram

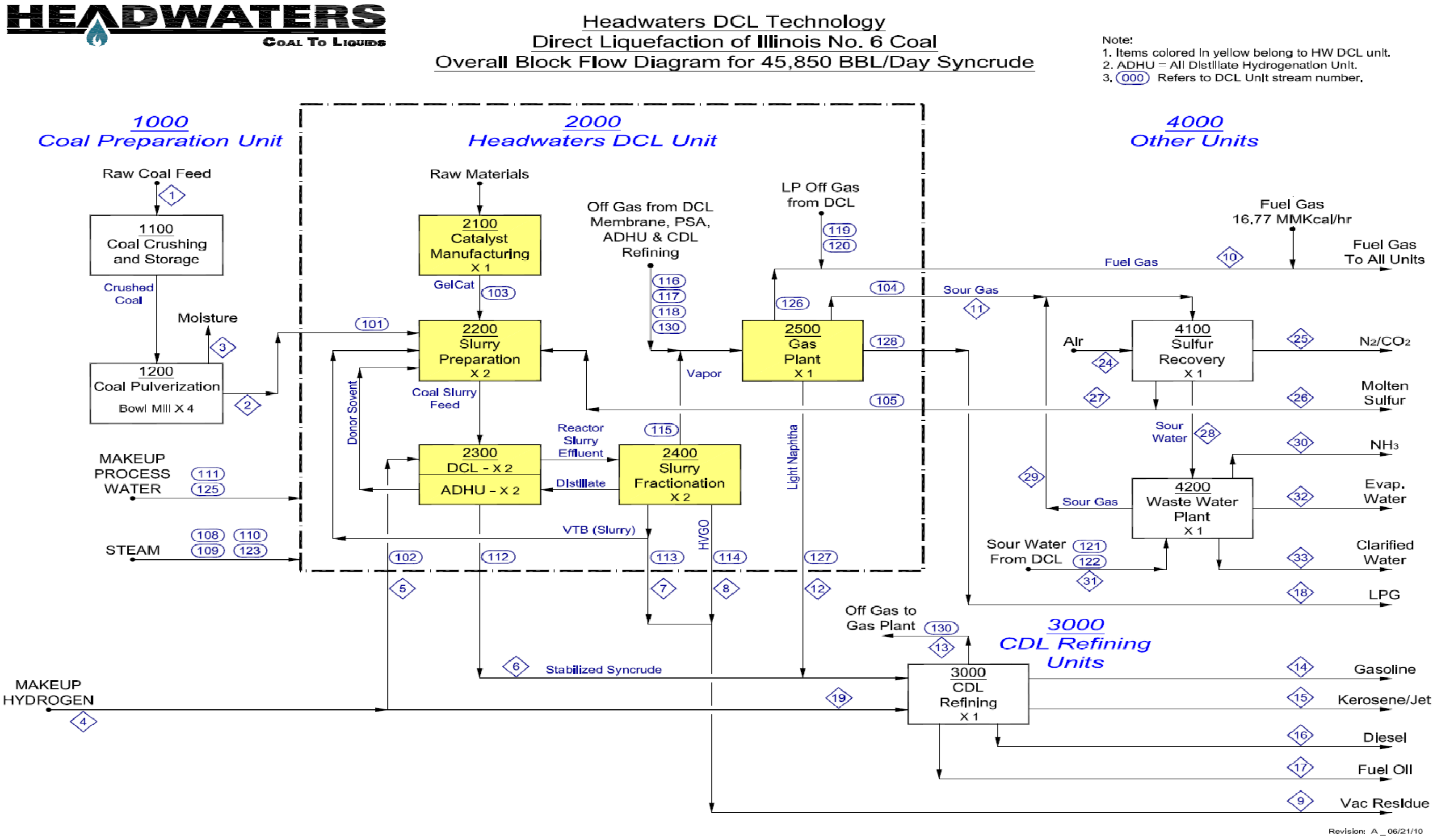


Figure 4.2 Schematic Diagram of Headwaters DCL Unit

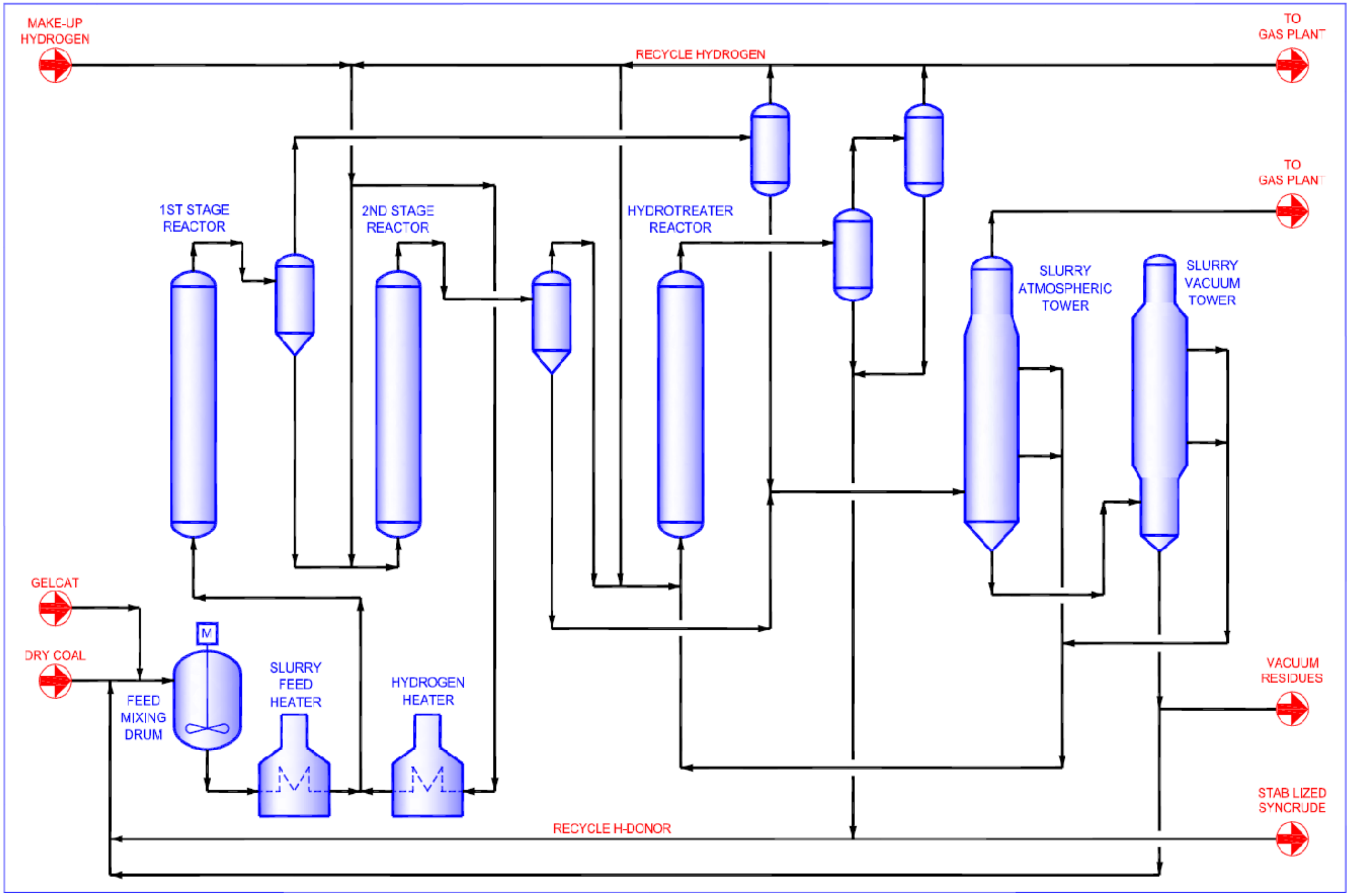


Figure 4.3 Schematic Diagram of Gas Plant

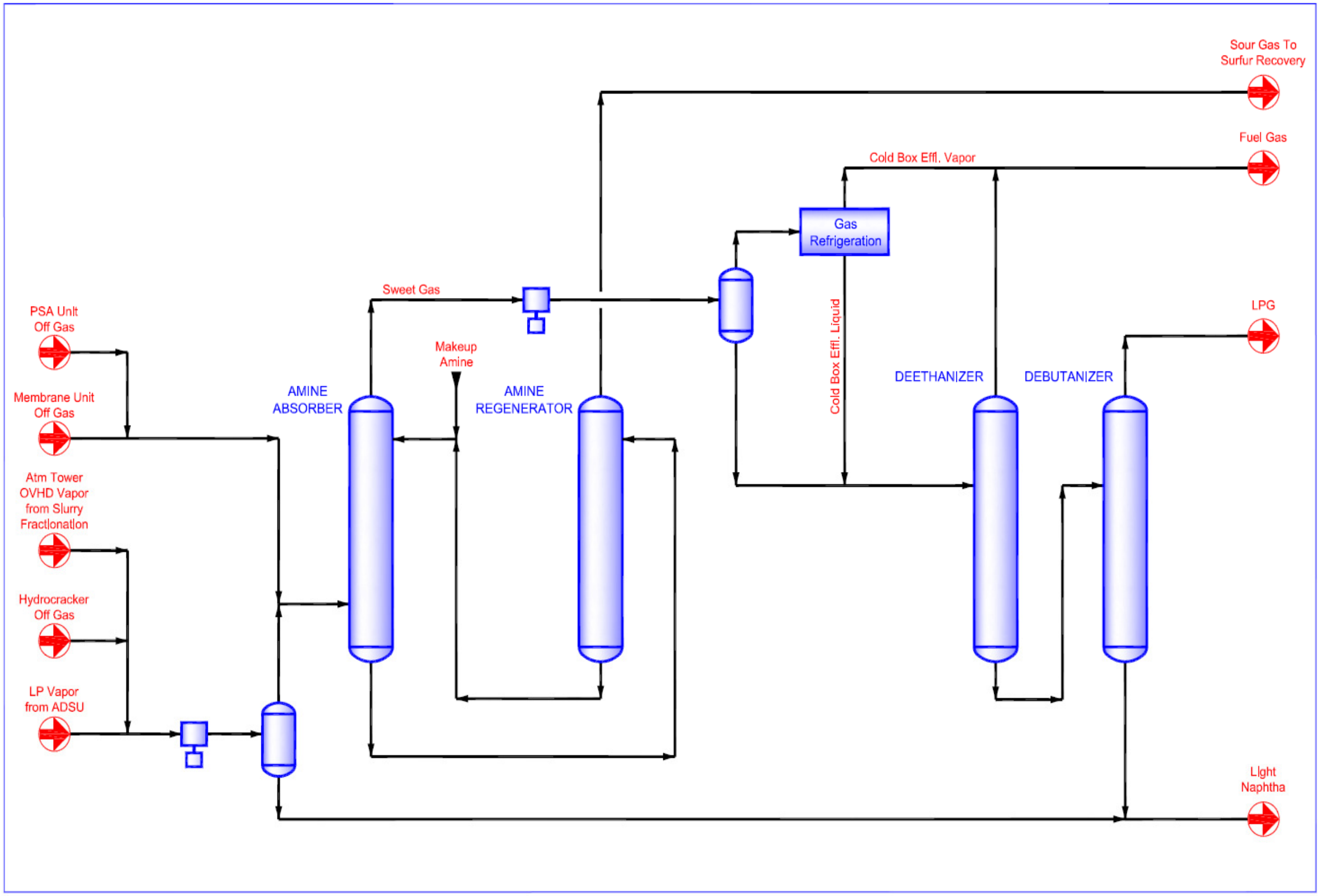
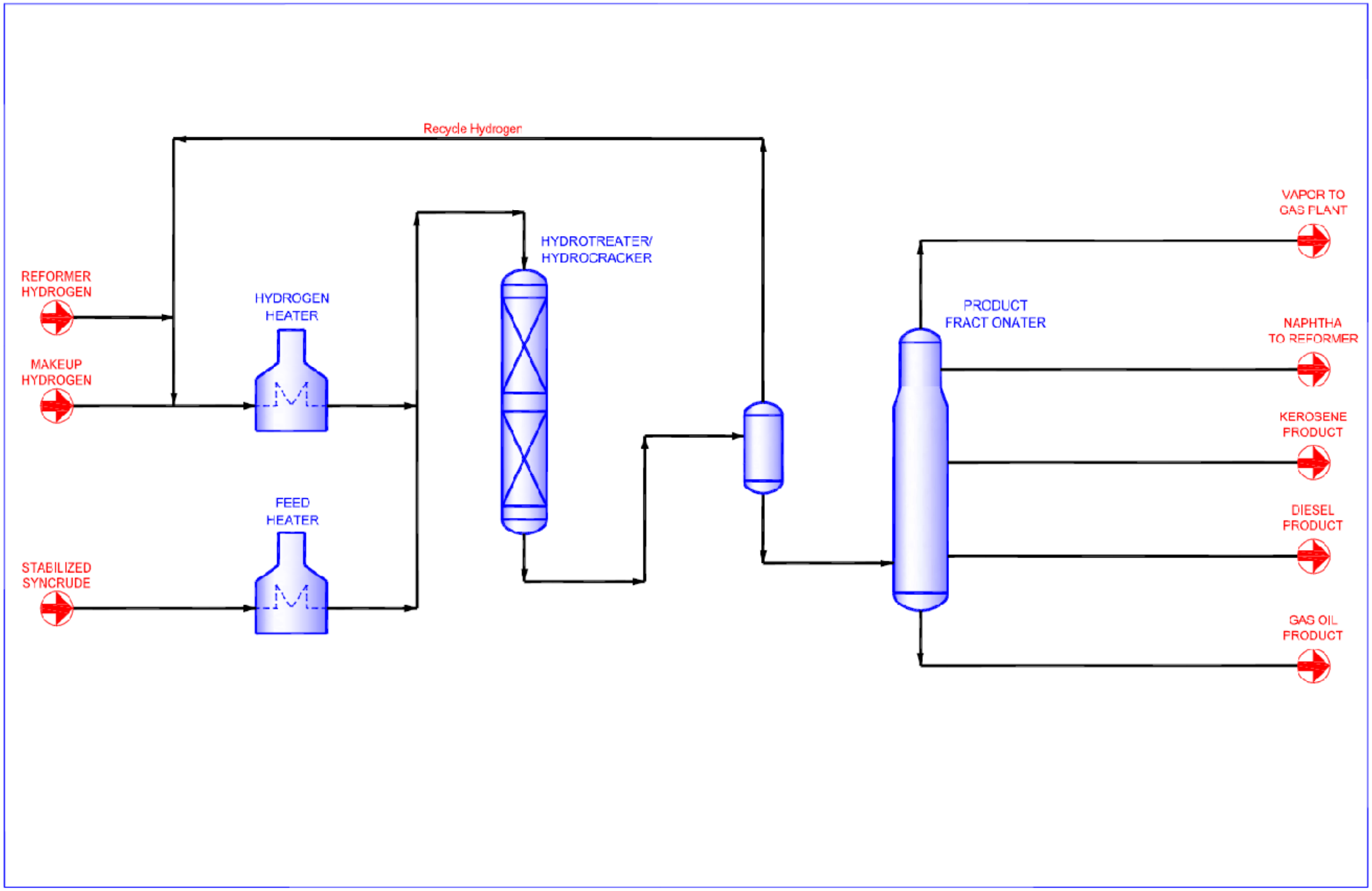


Figure 4.4 Schematic Diagram of Coal Derived Syncrude Refining Unit



5. HYDROGEN PRODUCTION OPTIONS

5.1 Introduction

In current discussions of energy supply options, considerable attention is paid to the production of hydrogen. Intrinsically, the addition of hydrogen content decreases the net carbon footprint of a hydrocarbon fuel. This means that a DCL process, which is based on the addition of hydrogen to coal, will improve the carbon footprint of a coal-based fuel. However, this improvement must be weighed against the carbon emissions that occur during the production of the hydrogen itself. To better understand this issue, a paper study was conducted of hydrogen production options.

Potentially, numerous options exist for the supply of hydrogen to a DCL plant. Traditional methods such as steam methane reforming or coal gasification may be used. Alternatively, novel approaches may be taken, including the use of energy from biomass, nuclear, wind, or solar. One can expect that each of these will have a range of benefits and shortcomings, with respect to both environmental and economic considerations. Improving the understanding of the balance of advantages and disadvantages among various hydrogen supply options was the main object of this phase of the project.

5.1.1 Case studies

A total of six cases were selected for inclusion in this study:

- Coal/Resid Gasification
- Steam Methane Reforming
- Biomass Gasification
- Coal/Resid/Biomass Gasification
- Water Electrolysis Using Nuclear Energy
- Water Electrolysis Using Grid Electricity

These cases span a considerable range of properties, in terms of commercial history, technology readiness, and reliance on fossil-based feedstocks. Coal gasification and methane reforming are well-understood, with a long history and, therefore, low technology risk. But they depend most heavily on fossil-based fuels, and will therefore present a larger carbon footprint, unless carbon sequestration measures are adopted.

Conversely, the inclusion of biomass has the opportunity to reduce the net carbon footprint, as the carbon contained in the biomass is balanced by the carbon captured from the atmosphere during the growth of energy crops. But biomass based options do not have a long operating experience. Technical and economic risks are greater, including questions surrounding the supply of biomass, as well as the technical requirements for a biomass-based process.

In theory, hydrogen production by electrolysis of water was the greatest potential for reducing carbon footprint. But this improvement can only be realized if the energy requirement can be derived from sources that are not themselves significant emitters of atmospheric carbon. To represent this option, two cases were included, one where the energy requirement for electrolysis is derived from advanced modular nuclear reactor technology, and the other where the energy is supplied as electricity from the grid. In the latter case, non-fossil sources of electricity such as wind or solar have been assumed, to create a low-carbon footprint case.

5.1.2 Parameters and assumptions

a. Production Scale

All case studies were conducted at a common production capacity, set by the net hydrogen requirements for the direct coal liquefaction and product refining sections of the facility. Based on a 48,500 BPSD DCL plant capacity, the total hydrogen requirement is 685 metric tons per day. Of this total, over 94% is required to feed the DCL block, with the remainder required for the product refining section. The value of 685 metric tons/day was taken as the net production requirement. In each of the case studies, an on-stream factor of 90% was assumed. This means that the gross design capacity of the corresponding plant (on which capital cost estimates were based) is 10% larger than the net production requirement.

The impact of the capacity requirement differs significantly among the cases studied. The requirement is well within historically proven ranges for established technologies (coal gasification, methane reforming). However, it present a more significant issue for newer technologies, especially for biomass cases, where sourcing a sufficiently large biomass feedstock could present a major hurdle.[1] These issues will be discussed in greater detail below.

b. Financial assumptions

Financial and cost parameters were selected to put the evaluation of hydrogen production on the same basis as the overall DCL/refining process design. Key financial parameters were:

-	Internal Rate of Return	18%
-	Construction Period	4 years
-	Project Life	20 years
-	Capacity Factor	330 days/year
-	Deprecitation	10 year straight line
-	Equity	50%
-	Interest Rate on Debt	7%
-	Debt Repayment Schedule	20 years
-	Income Tax Rate	34%
-	Labor Rate	$50,000/man-year

c. Feedstocks and Utilities

Because feedstocks differ between the case studies, assumptions about availability and cost for those feedstocks have a significant impact on the interpretation of the study results. Relative

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[1] "Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass", DOE/NETL report 2009/1349, January 14, 2009.

economic viability for cases can easily be skewed if more aggressive or optimistic assumptions are made for one case compared to another.

For coal and natural gas feedstocks, common assumptions were adopted for the hydrogen case studies as used for the DCL process estimate. In the case of coal, Illinois #6 was selected as the basis, with an assumed cost of $39/short ton. Natural gas was assumed at $7.50/million Btu, and a low cost case at $5/MMBtu was also included to understand sensitivity to feedstock price in this case.

The cost assumption for biomass involves more speculation. No relevant present-day commercial implementation of biomass-based hydrogen production can be used as a reference point, so a projection must be used. A wide range of assumptions are found in literature studies, ranging from optimistic target levels of about $35/dry ton,[2,3] to much higher prices, as high as $100/ton.[4] For the current study, cases were included for two biomass cost points, a low-cost case at $35/ dry ton and a high-cost case at $75/dry ton.

Grid electricity required for the corresponding electrolysis case study was assumed at $60/MWh, consistent with the assumption for utility electricity for the DCL process. It is worth noting that the electrolysis case has been assumed to be carbon-neutral, meaning that the electricity supply is based on a non-fossil source such as wind or solar. As such, the assumed price for electricity is optimistic, and the case study results for the grid electrolysis scenario must be viewed as a best-case (similar to the biomass-based case discussed above).

Water utilities were estimated at $0.31/1000 gallons for cooling water and $13.55/100 gallons for process water.

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[2] C.N. Hamelinck and A.P.C. Faaij, "Future Prospoects for Production of Methanol and Hydrogen from Biomass", NWS-E-2001-49, ISBN 90-73958-84-9, Utrecht University.

[3] P.L. Spath and D.C. Dayton, "Preliminary Screening – Technical and Economic Assessment of Synthesis Gas to Fuels and Chemicals with Emphasis on the Potential for Biomass-Derived Syngas", NREL/TP-510-34929, December 2003.

[4] "Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass", DOE/NETL report 2009/1349, January 14, 2009.

d. Carbon sequestration

A major goal of the current study is to assess the feasibility of low carbon-footprint fuels produced using DCL technology. As such, the fate of fossil carbon in hydrogen production is a key consideration. Options were considered for the treatment of fossil vs. non-fossil production methods for hydrogen. For example, each hydrogen production method could be analyzed without regard for the amount of fossil carbon present, and then the net emission of fossil carbon could be compared case-to-case. However, this creates unwanted ambiguity in the case study comparisons, making it difficult to integrate the results of economic and environmental evaluations into a unified view of the relative merits of H_2 supply methods.

The alternate approach that was adopted for the present study was to create a near carbon-neutral case for each of the technology options, so that a fair comparison could be made of the H_2 technologies on the same low carbon emission basis. This was done by assuming added costs for the fossil-based technologies to account for carbon sequestration requirements. Carbon sequestration was assumed to be 90% of all fossil-based carbon passing through the process. Biomass-based carbon was assumed to be carbon-neutral, and was therefore not subjected to the sequestration requirement. Carbon sequestration requirements were therefore set as follows:

-	Coal/resid gasification	90% sequestration
-	Steam methane reforming	90% sequestration
-	Biomass gasification	No sequestration requirement
-	Coal/resid/biomass gasification	90% sequestration of coal/resid carbon only
-	Electrolysis Using Nuclear Energy	No sequestration requirement
-	Electrolysis Using Grid Electricity	No sequestration requirement

In each of the cases where sequestration is included, it is reasonable to assume that the captured carbon dioxide will be of relatively high quality, since it originates from a water-gas shift unit. Therefore, it has been assumed that the captured carbon dioxide can be assigned a value, such that the financial evaluations of those cases which include carbon capture have a credit included for the value of the recovered carbon dioxide. The CO_2 credit was assumed to be $18/short ton.

5.1.3 Methods and resources

a. H2A model

The primary tool used for economic evaluation of the hydrogen production cases was the H2A Model. Development of this analysis tool was started in 2003 by a team from several national lab, university and industry locations. Publically available from the Department of Energy, the model is a spreadsheet program (Microsoft Excel) which allows the end user considerable flexibility to adjust the inputs to the simulation. All important factors, including financial factors, capital costs, and variable costs, can all be easily adjusted, allowing user-defined case studies to be assembled. The model provides a built-in tool for estimating carbon sequestration costs. It also includes provisions for scaling costs to different production capacity, with complete flexibility to modify scaling methods and parameters.

Along with providing the general framework of the H2A model, DOE also provides access to a series of ready-made case studies. These cover numerous options for hydrogen production, including cases which are similar to most of those selected for the present study. These ready-made cases were estimated based on varying assumptions, and at a wide range of different production capacities. As such, they required considerable modification for the purposes of the present study, as will be discussed in greater detail on a case-by-case basis below. But the ready-made cases provided a convenient starting point for the present study.

b. Other resources

A number of literature resources were utilized to obtain data needed to customize the case study evaluations for the current project.

Information related to costs and technology issues for biomass, coal, and biomass/coal hydrid technologies were obtained from “Affordable, Low-Carbon Diesel Fuel from Domestic Coal and

Biomass" (DOE/NETL-2009/1349, January 14, 2009). This study included discussions of feedstock supply issues related to biomass, and provided useful data on capital and operating structure of gasification-based syngas. Although not focused specifically on hydrogen production, the information was readily adapted.

A study from the National Renewable Energy Laboratory, "Hydrogen Supply: Cost Estimate for Hydrogen Pathways – Scoping Analysis" by D. Simbeck and E. Chang (NREL/SR-540-32525, January 2002 to June 2002) provided useful analysis of the cost factors involved in hydrogen production. The study covered multiple feedstocks for hydrogen production, including natural gas, coal, resid, biomass, and water electrolysis.

Another NREL study entitled "Preliminary Screening – Technical and Economic Assessment of Synthesis Gas to Fuels and Chemicals with Emphasis on the Potential for Biomass-Derived Syngas" by P.L. Spath and D.C. Dayton (NREL/TP-510-34929, December 2003) provided a technology review and economic discussions for biomass-based routes to hydrogen production.

A study from the National Energy Technology Laboratory, "Hydrogen Production Facilities Plant Performance and Cost Comparisons" (Final Report, March 2002) contained useful information on the effects of carbon capture on the economics of natural gas and coal-based hydrogen processes. It also included discussions of a hybrid case using a combination of coal and biomass in a gasification plant.

"Survey of the Economics of Hydrogen Technologies" from C.E.G Padro and V. Putsche of NREL (NREL/TP-570-27079, September 1999) provided helpful material, including summaries of prior literature studies of the economics of steam methane reforming, coal gasification, biomass gasification, and electrolysis

"Power Plant Water Usage and Loss Study" (August 2005, Revised May 2007) from NETL provided discussions of net water usage in IGCC plants, which was helpful in developing water usage estimates for gasification-based hydrogen plants.

Estimates of the economics for hydrogen production by electrolysis using nuclear energy were facilitated by data provided by General Atomics. Their report entitled "H2-MHR Pre-Conceptual Design Report: HTE-Based Plant" (GA-A25402, April 2006) provided details of the modular nuclear reactor concept for use of electrical and heat energy for a nuclear system to drive hydrogen production by high-temperature electrolysis. Further information on process economics were provided directly by General Atomics (personal communication).

5.2 Steam Methane Reforming

Catalytic steam reforming of natural gas (methane) is the most widely used method for commercial production of hydrogen, and generally has the lowest production cost among hydrogen production methods, at least in scenarios where supplies of natural gas are available.

5.2.1 Capital Cost

As with all of the production methods that will discussed in this section, a key requirement for this economic assessment was developing a plausible estimate for the capital cost of the required size plant. In contrast to some of the less well-developed alternative, the steam methane option has a long commercial history, and is readily employed at production scales that meet or exceed the requirement for the current estimate (685 mt hydrogen/day). Previous literature studies for large-scale SMR plants have covered capacities of 120 to 2300 mt/day.[5] These studies, from several authors, show specific total capital cost estimates of $9.00 to 14.74 per annual GJ of hydrogen (lower heating value, LHV, basis). At the higher end of the capacity range, capital cost fell in a narrower range of $9.00 to $10.82 per annual GJ. For the current study, a value of $10.50 per annual GJ was selected for the estimate of SMR plant capital cost. At the required capacity of 685 mt/day with an assumed on-stream factor of 0.9, the gross design capacity is 761 mt/day and the corresponding total capital investment for the SMR plant is $350 million. This total does not include capital cost for the carbon sequestration plant, which was estimated separately in the H2A model.

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[5] C.E.G. Padró and V. Putsche, "Survey of the Economics of Hydrogen Technologies", NREL/TP-570-27079, September 1999.

5.2.2 Feeds and Utilities

The most significant cost in steam reforming is for the natural gas feedstock. For the present study, the baseline natural gas price was fixed based on the value assumed for the evaluation of the direct coal liquefaction plant, at \$7.50/MMBtu. However, a separate low-cost natural gas case was also included in the study, at a natural gas price of \$5/MMBtu.

Other variable costs are relatively less leveraging in hydrogen production by SMR. Utility unit costs were set as follows:

Electricity	\$0.06/kWh
Process Water	\$13.60/1000 gal
Cooling Water	\$0.31/1000 gal

5.2.3 Carbon Sequestration

Carbon sequestration costs for the steam methane reforming case were calculated using the built-in utility provided with the H2A model. H2A assumes that the captured CO2 is sequestered in underground injection wells, and has built-in models for estimation of compression, injection, and pipeline costs.

Carbon capture efficiency for the SMR case was set at 90% of the total carbon dioxide produced from the feedstock, consistent with the approach selected for all cases involving fossil-based feedstocks. A specific carbon emission rate was calculated at 9.26 kg CO_2 produced/kg H_2 produced. Therefore, 90% sequestration corresponds to a rate of CO_2 capture of 8.33 kg CO_2/kg H_2. As described above, a carbon dioxide value of \$18/short ton was assumed in the evaluation of this case, which yields a carbon dioxide credit of \$0.17 per kg of H_2 produced.

5.2.4 Results

The results of the H2A model run for the steam methane reforming case (high natural gas price) are summarized as follows:

Table 5.1: Cost Estimation for SMR Case – High Cost Natural Gas

Specific Item Cost Calculation		
Cost Component	**Cost Contribution ($/kg)**	**Percentage of H2 Cost**
Capital Costs	$0.51	27.1%
Decommissioning Costs	$0.00	0.1%
Fixed O&M	$0.12	6.4%
Feedstock Costs	$1.22	64.8%
Other Raw Material Costs	$0.00	0.0%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.03	1.6%
Total	**$1.88**	

As noted above, feedstock (natural gas) cost is the dominant contributor to the overall cost of hydrogen production, accounting for 65% of the total cost. Capital cost accounts for an additional 27% of the total. The total product cost is $1.88/kg H2, which is the internal transfer price that must be borne by the DCL plant.

An alternate case was run based on a lower natural gas price of $5/MMBtu, the results of which are shown in Table V-2.

Table 5.2: Cost Estimation for SMR Case – Low Cost Natural Gas

Specific Item Cost Calculation		
Cost Component	**Cost Contribution ($/kg)**	**Percentage of H2 Cost**
Capital Costs	$0.51	34.7%
Decommissioning Costs	$0.00	0.1%
Fixed O&M	$0.12	8.2%
Feedstock Costs	$0.81	55.0%
Other Raw Material Costs	$0.00	0.0%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.03	2.0%
Total	**$1.47**	

5.3 Coal/Resid Gasification

Hydrogen production via gasification is also an industrially important technology. In addition to existing gasification installations, next generation power generation by Integrated Gasification Combined Cycle (IGCC) has garnered considerable attention over recent years. As such, a significant amount of literature is available covering various aspects of gasification.

For the case of direct coal liquefaction, the gasification has unique synergies that are not shared by other hydrogen production methods. For one, the use of coal as a major feedstock is consistent with eth DCL plant. Clearly, a DCL installation will have access to adequate supplies of coal, whereas the availability of other feedstocks such as natural gas or biomass may be more questionable, depending on the plant location. In addition, the DCL process produces a heavy residual by-product which can be consumed captively for additional hydrogen generation, thereby reducing the net coal requirement for the hydrogen plant. If other methods are selected for hydrogen generation, then an external market must be found for the residue.

5.3.1 Capital Cost

Several sources of information were compared in order to arrive at a reasonable estimate of capital cost for the coal/resid gasification case. These sources were compared based on specific capital cost, expressed as dollars per daily metric ton of feed (coal + DCL vacuum resid).

In “Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass” (DOE/NETL-2009/1349, January 14, 2009), specific capital costs for gasification-based Fischer-Tropsch liquid plants are given on a daily barrel of liquid product basis. For a 100% coal plant with carbon capture, the specific capital is estimated at $106,000 per daily barrel of F-T liquids. For a 50,000 barrel per day complex processing 21,700 ton per day of coal, the total capital cost would be estimated at $5.3 billion. However, for the current purposes, this value is too high, as it includes costs for the F-T conversion and product refining which are not relevant to the required hydrogen production for the DCL plant in the present study. Therefore, an estimate of the fraction of total capital that could be assigned to hydrogen production was required.

The above mentioned report included a chart which shows a breakdown of the capital costs for one of the cases studied. Although it was for a different case (15% biomass, 85% coal), it was assumed that the 100% coal case would have a similar breakdown of capital costs. Of the capital cost fractions, 49.3% could be directly attributed to the coal gasification section (feed handling and prep, gasification island, and carbon capture. An additional 19.1% was related to the F-T plant and other downstream sections. The final 32.9% was related to engineering and construction, contingencies, etc. To extract the fraction of the total capital related to hydrogen production, it was assumed that a fraction of the E&C/contingency costs could be assigned to the hydrogen plant in direct proportion to the fraction of direct plant capital cost related to hydrogen production (i.e. 49.3%/(49.3% + 19.1%)). As such, 72% of the E&C/contingency costs were allocated, along with the full 49.3% of cost directly attributable to syngas production, leading to the conclusion that a hydrogen-only plant would have 73% of the capital of corresponding full F-T Liquids plant, or a capital cost of $3.9 billion for a plant processing 21,700 tons per day of coal. Therefore, the specific capital cost of the hydrogen plant is estimated at about $180,000 per short ton of coal, or about $196,000 per metric ton of coal.

For comparison, a capital cost estimate was developed based on the default data contained in the H2A model for coal gasification. For the H2A default case, a plant producing 277,000 kg hydrogen per day has a capital cost of $390 million with carbon capture. At 7.85 kg coal consumed per kg H2 produced, this corresponds to a capital cost of about $180,000 per daily metric ton of coal.

A third source of coal gasification data was also available, in the form of an estimate provided by GE Energy to Headwaters as part of 2009 pre-feasibility study of a proposed direct coal liquefaction project. In the study, GE Energy provided a coal/resid co-gasification case for which the total capital cost was $1.66 billion for a plant processing a total of 8475 short tons of total feed per day (7688 metric ton per day) and producing 433 MMSCFD of hydrogen (1,096,000 kg H2/day). This corresponds to a specific capital cost of $216,000 per daily metric ton of (coal+resid) feed, or $1514 per daily kg of hydrogen produced.

Overall, the agreement is relatively good between the total capital estimates from the three sources. Because it was provided directly by a technology licensor, the capital cost derived from the GE Energy report was selected for the current case study. This had the added merit of providing a conservative estimate.

5.3.2 Feeds and Utilities

The gasification plant has two major feedstocks, coal and DCL residue. The amount of DCL residue available is fixed by the scale of the corresponding DCL plant, so the coal amount is adjusted to meet the total hydrogen production requirement for the plant. For a total production rate of 685,000 kg hydrogen per day, the coal and residue feed rates were estimated at 121,298 kg/hr and 106,903 kg/hr, respectively.

The coal feedstock was priced based on Illinois #6 coal at a cost of $39 per short ton, with a lower heating value of 0.0274 GJ/kg.

For the DCL vacuum residue, an internal transfer price was set. This was based on the assumed market value that the residue would have in the other cases where the residue is not used for hydrogen production. This approach was required in order to put the different cases on a fair and equal basis. This residue value was assumed to be $20.42 per short ton, corresponding to $0.0225 per kg of residue, at a lower heating value of 0.0121 GJ/kg.

Other variable costs used for this case were as follows:

Electricity	$0.06/kWh
Process Water	$1.66/1000 gal

5.3.3 Carbon Sequestration

As for the SMR case, carbon sequestration costs for the gasification case were calculated using the built-in utility provided with the H2A model. Consistent with other cases, the carbon capture efficiency was set at 90% of the total carbon dioxide produced from the feedstock. Since the carbon contained in the DCL vacuum residue is fossil-derived, its carbon was included in the carbon capture requirement. For coal, the specific carbon emission rate was set at 87.5 kg CO2 produced/GJ LHV. For DCL residue, the corresponding carbon content was set at 112.8 kg CO2 produced/GJ LHV.

As in other carbon sequestration cases, a carbon dioxide value of $18 per short ton was assumed, yielding a credit for carbon dioxide captured. For the coal/resid case, this yields a credit of $0.27 per kg of hydrogen produced.

5.3.4 Results

The results of the H2A model run for the coal/resid gasification case are summarized as follows:

Table 5.3: Cost Estimation for Coal/Resid Gasification Case

Specific Item Cost Calculation		
Cost Component	**Cost Contribution ($/kg)**	**Percentage of H2 Cost**
Capital Costs	$1.35	73.5%
Decommissioning Costs	$0.00	0.2%
Fixed O&M	$0.17	9.4%
Feedstock Costs	$0.28	15.2%
Other Raw Material Costs	$0.00	0.0%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.03	1.7%
Total	**$1.84**	

Capital cost is the largest contributor to the overall cost of hydrogen production, accounting for almost 74% of the total. The total product cost is \$1.84/kg H2, which is the internal transfer price that must be borne by the DCL plant.

5.4 Biomass Gasification

Among the case studies included in this report, biomass gasification is one of the more speculative, given the lack of large-scale commercial installations using biomass feedstocks to generate industrial hydrogen. Although in principle, hydrogen production by gasification of biomass should be technically feasible, there are more uncertainties due to the immature status of the technology. A major source of uncertainty is related to the scale of feedstock supply. To be a suitable method for supply of hydrogen to a DCL complex, a very large and reliable supply of biomass must be available.

To develop, an idea of the scope this issue, it is instructive to consider the magnitude of the biomass supply that would be required. As a starting point, data presented in "Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass" (DOE/NETL-2009/1349, January 14, 2009) has been used. A plant processing 100% biomass at a rate of 4000 ton/day generates about 223,000 lb/hr of clean syngas (15,200 lbmol/hr). Per mol of syngas, this is estimated to yield 0.79 mol of hydrogen, or a total of 12,000 lbmol/hr of hydrogen product, equivalent to 262,000 kg H2/day.

For the DCL complex of the present study, a hydrogen supply of 685,000 kg H2/day is required. Consequently, the biomass requirement for the DCL complex can be estimated at over 9,000 tons/day. However, according to the abovementioned DOE/NETL report, 4000 tons/day of biomass is the maximum economically feasible supply that can be obtained in all but a few ideal locations. This assumption was based on collection of biomass from a 30 to 50 miles radius, where only marginal lands are used and major changes to land use are avoided.

At more than 2 times this scale, the required hydrogen plant for the DCL complex is therefore of questionable feasibility. However, for comparison purposes, the limitation on biomass supply was suspended, and the 100% biomass case computed. This will enable some comparison of the theoretical merits of a 100% biomass case compared to the other technology case. But it will be essential to bear in mind that the 100% biomass case may be of low practical importance.

5.4.1 Capital Cost

To develop a plausible capital cost estimate for a 100% biomass gasification facility of the required size, reference was again made to the recent DOE/NETL report.[6] From this report, capital cost estimates are provided for a facility processing 4000 tons per day of biomass to produce 5000 bbl/day of Fischer-Tropsch liquids. As in the coal gasification case above, the biomass-to-FT liquid case must be modified to obtain a capital cost estimate for a hydrogen production facility, which would share much of the same equipment (gasifiers, gas clean-up), but would omit significant sections as well (F-T reactors, fuel upgrading).

While the NETL report does not provide a capital cost breakdown for the 100% biomass case, this information is provided for a 15% biomass/85% coal case. For the present analysis, it has been assumed that the same capital cost breakdown can be applied to the biomass-only case. Of the portion of the capital cost associated with direct plant costs, roughly 63% is associated with the equipment required for hydrogen production (feed prep, gasification, gas clean-up). By assuming that the same proportion (63%) of the indirect capital costs can also be assigned to hydrogen production, a modified capital cost can be developed for the analogous hydrogen plant. Using this methodology, the 4000 ton/day plant has a capital cost of $694 million.

To determine the corresponding rate of hydrogen production, it is noted that the 4000 ton/day plant produces 15,200 lbmol/hr of clean syngas. As noted above, a yield of 0.79 mol hydrogen per mol syngas has been assumed, resulting in a total hydrogen production rate of 12,000 lbmol/hr, or 262,000 kg H2/day. Therefore, the specific capital is $2,648/daily kg of hydrogen produced.

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[6] "Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass", DOE/NETL report 2009/1349, January 14, 2009.

To arrive at a capital cost estimate for the hydrogen plant required to supply the full-scale DCL facility, the capital cost must be scaled to a net production of 685,000 kg H2/day. With an assumed on-stream factor of 0.9, this corresponds to a gross design capacity of 761,000 kg H2/day, or a scale factor of 2.9 relative to the 4000 ton biomass/day plant described in the DOE/NETL report. The latter report was estimated to require six gasification trains, so the full scale plant in the current study would require roughly 18 parallel trains. It seems unlikely that a significant economy of scale can be achieved under these circumstances, so it has been assumed that the capital cost will scale in linear fashion, leading to a total capital cost estimate for the full-scale hydrogen plant of $2.02 billion.

5.4.2 Feeds and Utilities

For the biomass feedstock, two sub-cases were included in the study to reflect a range of possible feedstock pricing. A low case was included with a biomass price of $35/short ton, and a high price case at $75/short ton.

Other variable costs used for this case were as follows:

Natural Gas	$7.50/MMBtu
Electricity	$0.06/kWh
Cooling Water	$0.21/1000 gal
Process Water	$13.60/1000 gal

5.4.3 Carbon Sequestration

With 100% non-fossil feedstock in case, carbon sequestration was not included.

5.4.4 Results

The results of the H2A model run for the coal/resid/biomass gasification case are summarized as in the following tables, with the low biomass case in Table V-4 and the high biomass cost case in Table V-5.

Table 5.4: Cost Estimation for Biomass Gasification Case, Low Biomass Price

Specific Item Cost Calculation		
Cost Component	**Cost Contribution ($/kg)**	**Percentage of H2 Cost**
Capital Costs	$2.09	62.5%
Decommissioning Costs	$0.01	0.2%
Fixed O&M	$0.27	8.1%
Feedstock Costs	$0.56	16.7%
Other Raw Material Costs	$0.21	6.3%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.21	6.3%
Total	**$3.35**	

Table 5.5: Cost Estimation for Biomass Gasification Case, High Biomass Price

Specific Item Cost Calculation		
Cost Component	**Cost Contribution ($/kg)**	**Percentage of H2 Cost**
Capital Costs	$2.09	53.8%
Decommissioning Costs	$0.01	0.2%
Fixed O&M	$0.27	6.9%
Feedstock Costs	$1.10	28.3%
Other Raw Material Costs	$0.21	5.4%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.21	5.4%
Total	**$3.89**	

Capital cost is the largest factor in the overall cost of hydrogen production, accounting for more than 50% of the total production cost in both cases. Of the remainder, the largest contributor is feedstock. It must be recalled that this 100% biomass case is quite optimistic, as it assumes that very large supplies of biomass can be obtained, amounts of biomass that are over 2 times the maximum economically feasible levels cited in recent reports. This suggests that the real cost of biomass feedstock for the subject facility is likely to be markedly higher, owing to the greater geographical radius from which feedstock must be obtained.

5.5 Coal/Resid/Biomass Gasification

As noted above, a major issue related to the 100% biomass case is the projected limitations in the economically feasible supply of biomass to a hydrogen production facility. A potential alternative is a hybrid gasification case, where a combination of several feedstocks is used to optimal effect. Biomass is used at the maximum feasible level for a single-facility supply (4000 tons per day, as discussed above). DCL vacuum residue is also used, making captive use of the available low cost material, and also allowing the DCL plant operator to avoid the potential difficulty of finding a suitable market for this material. Finally, coal is used only as needed to fill out the balance of the hydrogen requirement for the DCL plant.

5.5.1 Capital Cost

To estimate the capital cost of a hybrid gasification plant, it was assumed that both the coal/resid and biomass gasification sections would require multiple trains, such that the plant could be considered as two parallel plants. As such, specific capital costs developed for the coal/resid and 100% biomass cases were used directly, in proportion of the relative amounts of the respective feedstocks being processed by the hybrid plant.

The biomass feed rate was assumed to be fixed at the maximum feasible level of 4,000 tons per day. The biomass section would then account for about 283,000 kg per day of hydrogen product. From the 100% biomass case above, the specific capital cost for the biomass plant is $2650/daily kg of hydrogen produced, yielding a total capital contribution from the biomass section of $832 million.

The hydrogen plant is assumed to consume the entire available resid from the DCL plant, a total of 2,566 mt/day, from which about 272,000 kg/day of hydrogen is produced. At a specific capital of $1,514/daily kg of H2, the resid gasification contributes $457 million to the total capital cost.

The balance of the hydrogen production, approximately 131,000 kg/day, is derived from coal gasification. At a specific capital of $1,514/daily kg of H2, coal gasification contributes $220 million to the total capital cost.

Combining these estimates yields a total capital investment of $1.51 billion for a hydrogen plant at a gross design capacity of 761,000 kg/day of hydrogen, which yields the required net capacity of 685,000 kg/day at a 0.9 on-stream factor.

5.5.2 Feeds and Utilities

As noted above, usage rates for the three feedstocks to the hybrid case were set by the following algorithm: (1) biomass usage at the projected maximum economically feasible rate of 4000 tons/day, (2) DCL vacuum residue usage at 100% of the amount produced by the DCL plant, (3) coal usage as needed to fulfill the balance of the hydrogen requirement.

Unit costs for these feeds were set at the same levels used in above cases. The usage rates and costs are summarized as follows;

Feedstock	Specific Usage Rate	Unit Cost
Coal (Illinois #6)	1.34 kg/hg total H2	$39/short ton
DCL Vacuum Residue	3.74 kg/kg total H2	$20.42/short ton
Biomass	5.30 kg/kg total H2	$35/short ton (or $75/short ton)

Prices for utilities were set as:

Electricity	$0.06/kWh
Cooling Water	$0.21/1000 gal
Process Water	$13.60/1000 gal

5.5.3 Carbon Sequestration

Carbon capture costs were calculated using the built-in utility provided with the H2A model. Carbon capture efficiency was set at 90% of the fossil-based carbon dioxide produced from the feedstock. In this case, only the carbon dioxide derived from the coal and DCL vacuum residue were included in the 90% carbon capture requirement. For coal, the specific carbon emission rate was set at 87.5 kg CO2 produced/GJ LHV. For DCL residue, the corresponding carbon content was set at 112.8 kg CO2 produced/GJ LHV.

5.5.4 Results

The results of the H2A model run for the coal/resid/biomass hybrid gasification case are summarized as follows:

Table 5.6: Cost Estimation for Coal/Resid/Biomass Hybrid Case – Low Biomass Cost

Specific Item Cost Calculation

Cost Component	Cost Contribution ($/kg)	Percentage of H2 Cost
Capital Costs	$1.67	68.9%
Decommissioning Costs	$0.00	0.2%
Fixed O&M	$0.20	8.2%
Feedstock Costs	$0.36	14.8%
Other Raw Material Costs	$0.00	0.0%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.19	7.8%
Total	**$2.42**	

Table 5.7: Cost Estimation for Coal/Resid/Biomass Hybrid Case – High Biomass Cost

Specific Item Cost Calculation		
Cost Component	**Cost Contribution ($/kg)**	**Percentage of H2 Cost**
Capital Costs	$1.67	62.7%
Decommissioning Costs	$0.00	0.2%
Fixed O&M	$0.20	7.5%
Feedstock Costs	$0.60	22.5%
Other Raw Material Costs	$0.00	0.0%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.19	7.1%
Total	**$2.66**	

Capital cost is the largest factor in the overall cost of hydrogen production, accounting for more than 60% of the total production cost in both low- and high-cost biomass scenarios. Of the remainder, the largest contributor is feedstock.

5.6 Electrolysis using Nuclear Energy

In light of the interest in finding routes to producing fuels with reduced carbon footprint, the use of nuclear energy has been proposed. As a method to generate electricity with no fossil carbon emissions, nuclear-generated electricity could be coupled to water electrolysis to generate hydrogen without associated carbon emission. Conceptual designs have been developed for systems utilizing advanced modular nuclear reactor designs integrated with electrolysis. For example, a version using high temperature electrolysis is described in “H2-MHR Pre-Conceptual Design Report: HTE-Based Plant” (GA-A25402, April 2006), a joint report of General Atomics, Idaho National Laboratory, and Texas A&M University. This integrated system uses both the electricity and waste heat generated by a modular helium reactor (MHR) to drive a high temperature electrolysis module. The combined use of electrical and heat energy has the potential to significantly increase the thermal efficiency of hydrogen production compared to only using the electrical power in conventional low-temperature electrolyzers.

5.6.1 Capital Cost

The main driver for the cost of hydrogen production using nuclear energy is capital cost. The report on the high temperature electrolysis system cited above gives a total capital cost estimate of $2.58 billion for a plant producing 828,000 kg/day of hydrogen (at 100% capacity), of which $1.42 billion is associated with the nuclear reactor module (Modular Helium Reactor), and the remaining $1.16 billion is associated with the high-temperature electrolysis hydrogen production system.

The conceptual plant design consists of multiple modules, so it was assumed that the capital investment would scale linearly with the plant capacity. For the current study, the gross design capacity requirement for the DCL and product upgrading sections is about 761,000 kg/day, so the total capital cost for the nuclear-based hydrogen plant can be estimated at about $2.4 billion. At an on-stream factor of 0.9, this plant produces the required net hydrogen supply of 685,000 kg/day.

5.6.2 Feeds and Utilities

The pre-conceptual design report provides an estimated fuel cost of $0.265/kg hydrogen produced. This was used directly for the current estimate.

The integrated MHR-HTE system was assumed to be a closed system with respect to cooling requirements, so the only other feed or utility input for the plant was demineralized water for the electrolysis system at $13.60/1000 gal.

5.6.3 Results

The results of the H2A model run for the nuclear-based electrolysis case are summarized as follows:

Table 5.8: Cost Estimation for Nuclear-Based Electrolysis Case

Specific Item Cost Calculation		
Cost Component	**Cost Contribution ($/kg)**	**Percentage of H2 Cost**
Capital Costs	$2.45	75.2%
Decommissioning Costs	$0.01	0.2%
Fixed O&M	$0.50	15.5%
Feedstock Costs	$0.26	8.1%
Other Raw Material Costs	$0.00	0.0%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.03	1.0%
Total	**$3.25**	

Capital cost is the largest factor in the overall cost of hydrogen production, accounting for 75% of the total production cost of $3.25 per kg of hydrogen. Of the remainder, the largest contributor is operations and maintenance costs, accounting for about 15% of the total. Nuclear feedstock cost is a relatively minor contributor at only 8% of the total cost.

There is no carbon sequestration cost associated with this case.

5.7 Electrolysis using Grid Electricity

The final case included in the present study is the use of grid electricity to drive a conventional low-temperature electrolysis system for hydrogen production. Theoretically, this case has the potential to be carbon-neutral, depending on the source of the electricity which drives the electrolysis. If exclusively non-fossil sources of electricity are used (nuclear, solar, wind, water, etc.), then the hydrogen production has no associated emission of fossil carbon. For the purposes of this study, this is the assumption that has been adopted.

5.7.1 Capital Cost

Built-in capital cost data in the H2A electrolysis model were used as the starting point for the capital cost estimation. The system contained in the H2A is a grid powered electrolyzer system with a total hydrogen production capacity of 52,300 kg/day. The system was based on the Hydro bi-polar alkaline electrolyzer system, and consists of 50 electrolyzer units, each capable of producing 1,046 kg of hydrogen per day.

Based on the multiple-train design for the benchmark case in the H2A model, it was assumed that the capital would scale linearly with the total production capacity. As with other cases in this study, the on-stream factor was set at 0.9. For the DCL system, the required net hydrogen production rate of 685,000 kg/day (or 761,000 kg/day gross design capacity) translates to a total installed capital cost of $1.37 billion. The system consists of approximately 728 individual electrolyzer units.

5.7.2 Feeds and Utilities

Estimation of the cost for the electricity feedstock is the key question for the overall economics of the grid electrolysis case. Electricity cost is the largest contributor to the overall production costs, and electricity cost can be expected to vary considerably depending on the generation method. This is particularly a concern for the current study, as the assumption has been made that the electricity generation method to be used is carbon neutral. In some cases (wind, solar), these carbon-neutral generation methods are likely to be more costly than conventional methods of electricity supply. However, for the current estimate, an optimistic, competitive grid electricity cost of $0.06/kWh has been assumed. This optimistic assumption must be borne in mind when evaluating the results of the evaluation.

The electrolysis modules also require process feed water and cooling water. Prices were set as:

Cooling Water	$0.21/1000 gal
Process Water	$13.60/1000 gal

5.6.3 Results

The results of the H2A model run for the grid electrolysis case are summarized as follows:

Table 5.9: Cost Estimation for Grid-Based Electrolysis Case

Specific Item Cost Calculation		
Cost Component	**Cost Contribution ($/kg)**	**Percentage of H2 Cost**
Capital Costs	$1.82	29.8%
Decommissioning Costs	$0.00	0.1%
Fixed O&M	$0.35	5.8%
Feedstock Costs	$3.21	52.4%
Other Raw Material Costs	$0.60	9.8%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.13	2.1%
Total	**$6.12**	

Feedstock (electricity) cost is the largest factor in the overall cost of hydrogen production, accounting for 52% of the total production cost of $6.12 per kg of hydrogen. Of the remainder, the largest contributor is capital cost, accounting for 30% of the total. It is important to note with the grid electrolysis case that the total production cost will be sensitive to cost of the supplied electricity. As noted above, an optimistic assumption of $0.06/kWh was made for this analysis, which may not be representative of the true costs for some non-fossil sources of electricity. In such cases, the cost of hydrogen production will be correspondingly higher.

Because of the assumption of a non-fossil source for all supplied electricity, there is no carbon sequestration cost associated with this case.

5.8 Discussion of results

5.8.1 Cost comparison

Results of the cost estimation for the cases included in this study are summarized in Table V-10.

Table 9.10: Summary of Cost Estimation for Hydrogen Production Cases

	Steam Methane Reforming		**Coal-Resid Gasification**	**Biomass Gasification**		**Coal-Resid-Biomass Gasification**		**Nuclear-Electrolysis**	**Grid Electrolysis**
Feedstock Price Case	**High** $7.50/ MMBtu NG	**Low** $5.00/ MMBtu NG		**High** $75/dry ton biomass	**Low** $35/dry ton biomass	**High** $75/dry ton biomass	**Low** $35/dry ton biomass		
CO_2 Capture	Yes (90%)		Yes (90%)	No		Yes (90% of fossil carbon only)		No	No
Capital, $billion									
H_2 Production	0.35		1.15	2.02		1.51		2.4	1.37
CO_2 Capture	0.12		0.17	0		0.12		0	0
Total	0.47		1.32	2.02		1.63		2.4	1.37
H_2 Cost ($/kg H_2)									
Capital	0.51	0.51	1.35	2.09	2.09	1.67	1.67	2.45	1.82
Feed	1.22	0.81	0.28	1.10	0.56	0.60	0.36	0.26	3.21
Balance	0.15	0.15	0.21	0.70	0.70	0.39	0.39	0.54	1.09
Total	1.88	1.47	1.84	3.89	3.35	2.66	2.42	3.25	6.12
CO_2 Captured (kg/kg H_2)	8.33		13.76	0		7.5		0	0
CO_2 Credit ($/kg H_2) (included in totals above)	0.17		0.27	0		0.15		0	0
Net Fossil CO_2 Emission (after CO_2 capture) kg CO_2/kg H_2	0.93		1.53	0		0.83		0	0
Water Usage (gal/kg H_2)	4.8		8	8		8		2.4	2.4
Notes on Water Usage	H2A default		based on NETL report on water usage in IGCC	assumed same as coal/resid case		assumed same as coal/resid case		H2A default	assumed same as nuclear case

Based on overall hydrogen production cost, steam methane reforming and coal/resid have similar cost, depending on the assumption for natural gas price. At the higher natural cost price of \$7.50/MMBtu, the two cases are very close at \$1.84-1.88 per kg hydrogen. As expected, the SMR cost is quite sensitive to natural gas price, such that the low cost natural gas case (\$5/MMBtu) has a significantly lower cost of \$1.47 per kg hydrogen.

The other gasification cases (100% biomass, Hybrid coal/resid/biomass) are markedly more expensive, driven by costs associated with the biomass gasification. This includes both capital cost and feedstock costs, both of which are significantly higher on a unit hydrogen production basis for biomass compared to coal and resid. Biomass feedstock price has a significant impact on both cases where biomass is used, with the effect most pronounced for the 100% biomass case, as would be expected.

The differences in cost among the various cases are driven by differences in both capital and feedstock cost, where feedstock is defined in the broad sense to include both material feedstocks (i.e. the chemical source of the hydrogen itself), as well as the energy feedstock which drives the process. In the case of the reforming and gasification cases, the material feedstock and energy feedstock are the same (natural gas, coal, etc), but for the electrolysis case they are separate, including both a material feedstock (water) which supplies the hydrogen atoms which accounts for only a small fraction of the cost and an energy feedstock (nuclear fuel or grid electricity) for which costs are much more significant.

For steam methane reforming, the key cost driver is natural gas cost. Natural gas has been a volatile commodity in recent years, proving to be difficult to predict, making projections of future costs for reforming-based hydrogen difficult at best. Among fossil-based resources, natural gas has the highest hydrogen-to-carbon ratio, and is therefore the most environmentally attractive. This can lead to competition for natural gas feedstocks among different end uses, which can include power generation, heating, and even direct use as transportation fuel. But in geographic areas where large reserves of natural gas are known, and particularly in remote areas where gas resources are underutilized, the SMR option is very likely to be cost competitive. Of course, the latter also depends on the presence of other requirements for direct coal liquefaction (namely, coal), which will reduce the number of viable geographical regions.

The situation is quite different for gasification cases, where lower-value feedstocks are used, and feedstock costs therefore account for a much smaller share of the overall cost of hydrogen production. In these cases, it is capital cost which is the key driver. Large multi-train gasification complexes are very costly, operating at extremely high temperature and requiring highly specialized equipment. Among the three versions of gasification processes included in this study, the capital cost is lowest for the coal-resid case, and higher for cases that include biomass gasification. It should be noted that the multi-train, multi-feed complexes assumed for these cases do not use mixed feedstocks. Different feedstocks (coal, resid, biomass) would be segregated and processed separately in parallel process trains, each designed specifically to handle the particular feedstock.

In considering the economics for the gasification cases, it should be recalled that the 100% biomass case has a built-in problem, requiring supplies of biomass feedstock that are considerably larger than published estimates for the maximum feasible supply for a single biomass-based facility. As such, the result for the 100% biomass facility should be interpreted as an optimistic “best case scenario”, for which real feedstock costs could be markedly higher.

The two electrolysis cases present a considerable contrast. On the one hand, the nuclear-based option is capital-intensive, with highest overall capital cost of all the studied cases, but the lowest feedstock cost. This creates some risk for this option, since the case study assumes the availability of commercially unproven next-generation technology for both power generation (modular helium reactors) and electrolysis (high temperature electrolysis). If technical uncertainties lead to higher capital costs, then the overall economics of the nuclear-based option, for which capital cost is very leveraging, will be significantly impacted.

Conversely, the grid electrolysis option has more moderate capital cost, but very high feedstock (electricity) cost, much higher than the next most costly feedstock (natural gas for the SMR case). Further, the unit cost for grid electricity used in this estimate ($0.06/kWh) is most representative of present-day costs for conventional supplies of grid electricity. However, the grid-based electrolysis case has been assumed to have a zero-carbon footprint, meaning than non-fossil sources of electrical power are required. While some zero-carbon power sources would be available in this cost range (nuclear, hydroelectric, geothermal), at least in certain geographical regions, other types of zero-carbon power generation (wind, solar) are likely to be more expensive. Because the cost of hydrogen produced from grid-based electrolysis is very sensitive to electricity price, the overall economics will be directly impacted by higher costs.

5.8.2 Carbon sequestration costs

Table V-10 also shows information related to carbon sequestration for the three relevant cases where fossil-based feedstocks provide all or part of the feedstock requirement. In each of these cases, a credit for the value of the captured carbon dioxide was included in the evaluation (at \$18/ton of captured CO_2). This credit is shown in the table on a unit hydrogen basis, and provides a significant benefit for the corresponding cases, especially for the coal/resid gasification case where the amount of captured CO_2 is relatively large. Overall, the CO_2 capture credit compensates for much of the cost of sequestration, such that the economics of the fossil-based cases are not significantly worsened by the CO_2 capture requirement.

5.8.3 Conclusion

Overall, this case study suggests that carbon capture costs would not be leveraging in the selection of hydrogen production technology. Even with the addition of carbon sequestration, steam methane reforming and coal/resid gasification are markedly less expensive than any of the non-fossil cases, suggesting the best approach for a low carbon footprint hydrogen supply is to employ one of the conventional technologies in combination with carbon capture.

So even with a low carbon footprint set as a pre-condition of technology selection, alternative technology options such as biomass gasification or water electrolysis based on non-fossil energy sources would only be economically competitive if carbon capture costs are significantly higher than those estimated here.

6. ECONMICAL ASSESSMENT

Capital cost, operating cost and rate of return on investment of a 45,850 BPSD DCL plant that will purchase hydrogen and power from external sources are discussed in the section. The financial analysis is conducted using an in=house financial model which takes into account of the following variables:

1. Capital cost
2. Feed stock cost (coal, hydrogen, catalyst/chemical, water and power)
3. Crude oil price.
4. Product price (in relationship with crude oil price)
5. Capacity utilization
6. Debt to equity ratio
7. Interest rate
8. Tax rate

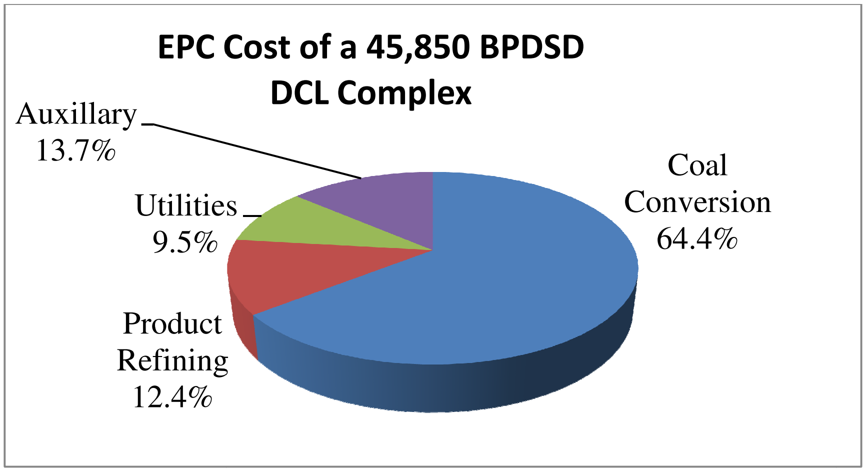
6.1 Plant Cost Estimates

Capital cost of the DCL Unit was estimated by sizing major equipments from the conceptual design. These equipment costs were estimated based on in-house database which is being kept up to date by utilizing information from commercial projects and published inflation index. For this study the cost basis was adjusted to February 2010. The installed cost of the major equipment is then calculated by multiplying the inflation adjusted equipment cost by an average factor of 2.64. This installation factor composes of the following cost elements:

1. Labor for equipment installation
2. Piping material & installation
3. Structure steel & installation
4. Electrical & Installation
5. Civil (Building, Earthwork, and Concrete)
6. Instrumentation
7. Misc (Paint, Insulation, Fireproofing)
8. Detail Engineering (Design and Procurement)
9. EPCM Contractor’s home office costs
10. Insurance & Bonds

EPC costs for the Unit 2000 are summarized in Table 6.1. EPC for Unit 3000 was provided by Axens, which that of other units were estimated based on their capacity using a power factor of 0.68.

The total EPC cost is estimated to be $2,002.27 million. Majority of the cost (64.41%), $1,289.75 million, is for the coal conversion and raw coal liquids/solvent hydrogenation units (Unit 2000). The cost of the Product Refining Unit (Unit 3000) and the remaining process units (Units 1000 and 4000) is $248.57 million (12.41%) and $274.09 million (13.69%). The remaining capital cost is for utilities and buildings, which totals to $189.86 million (9.38%).



6.2 Operating Cost Estimate

Feedstock and Utilities Costs

Illinois coal is priced at $42.99 per metric ton or $39.00 per short ton, while the catalyst/chemicals cost is at $2.50/bbl of distillable product.

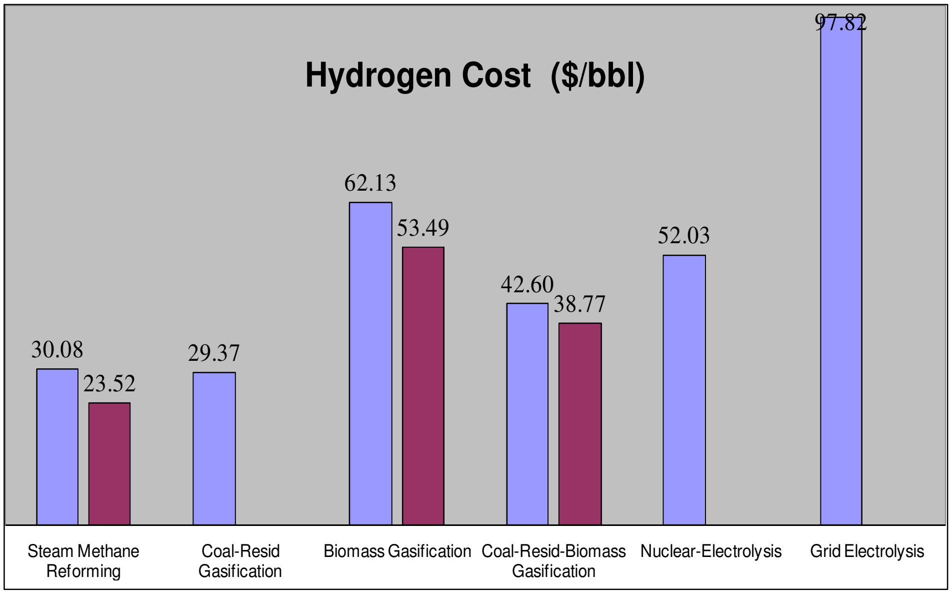
Other operating variable costs are:

Operating Variable	Unit	Cost
Water	$/1000 gallon	
Cooling Water	$/1000 gallon	0.31
Process/Portable water	$/1000 gallon	13.55
Boiler Feed Water	$/1000 gallon	14.20
Plant Air	$/1000 SCF	0.56
Instrument Air	$/1000 SCF	0.56
Nitrogen	$/1000 SCF	1.07
Fuel Gas	$/MMKcal	29.76
Electric Power	$/MWh	60.00

Hydrogen price is based on each H_2 production options discussed in Section 5 above. Hydrogen price is adjusted to a purity of 99.5 vol% (or 93.4 wt%).

Hydrogen Production Option	H_2 Cost	
	\$/metric Ton	\$/bbl Distillate
Steam Methane Reforming		
Low Cost	1,471.40	23.52
High Cost	1,881.40	30.08
Coal-Resid Gasification	1,837.00	29.37
Biomass Gasification		
Low Cost	3,345.97	53.49
High Cost	3,885.97	62.13
Coal-Resid-Biomass Gasification		
Low Biomass Cost	2,424.82	38.77
High Biomass Cost	2,664.82	42.60
Electrolysis		
Nuclear Power	3,254.20	52.03
Grid Power	6,118.30	97.62

Hydrogen cost ranges from \$23.52/bbl for the case purchasing H_2 from a SMR unit with a low natural gas cost of \$ 5/MMBTU to a high value of \$97.62.bbl from electrolysis using expensive electric power from the grid. Cost of hydrogen increases by 30% when the price of natural gas is increase from \$5.0 to 7.5/MMBTU. Hydrogen from coal-liquefaction residuals costs \$29.37/bbl and is within the cost of the two SMR cases. Substituting part o the coal with 4,000 Ton/day of biomass increases the cost of hydrogen by 45% to \$42.6/bbl, when biomass is priced at \$75/ton.



The 100% biomass cases (@$35/ton & $75/ton) are considerable more expensive than the coal only case (with liquefaction residuals). The unit cost is $53.5 and $62.1/bbl, respectively. It seems that the coal-resid option is a viable option in view of the volatility of natural gas over the past several years. The use of gasification allows the disposal of the liquefaction residuals within the coal conversion complex and there is no need to look for an external market for the liquefaction residuals.

6.2.1 Labor Cost

The total staffing for the plant is 579. A breakdown of staffing requirement by Unit area is given below:

Department	Staffing
Operation:	<u>327</u>
1000 Coal Handling & Preparation	42
2000 Coal Conversion & Raw Product/Solvent HTU	159
3000 Product Refining Plant	36
4000 Sulfur Recovery & Waste Water Treatment	30
Utility Plants	60
Administration/Engineers/Support:	<u>252</u>
1. Management, Engineers & Chemists	94
4. Plant Emergency & Safety Department	65
3. Administration and Support	45
2. Maintenance	48
Grand Total Staffing	**579**

Detailed breakdown is given in Tables 6.2 and 6.3. An average annual salary of $50,000 and an additional burden of 25% on the salary were assumed. The fully loaded labor cost is $62,500 per person.

6.2.2 Price of Products

Since distillate products from the DCL Complex meet transportation fuels specification, full market pricing can be adapted.

Although the capacity of a 45,850 BPSD DCL plant is considered to be small as compared to a conventional petroleum based refinery, the investment for a DCL plant is relatively high – $43,700 per daily barrel of design capacity. Even though, this price tag does not include investment of the hydrogen plant, this investment is already 1.7 times more than refinery of high complexity. Pricing structure suggests that it is economical to build a simply refining unit attaching to the DCL plant. The refining unit should include only hydrotreating/hydrocarcking and a naphtha reformer. However, the construction of a small FCC unit for processing the gas oil products does not justify the investment. The gas oils will be sold as fuel gas or as FCC feed to an existing refinery.

Product pricing assumptions are given in the table below:

Product/Byproduct	Unit	Price ($)
Product		
LPG	Bbl	83.30
Gasoline	Bbl	82.26
Kerosene/jet fuel	Bbl	84.29
Diesel	Bbl	84.46
Fuel Oil	Bbl	81.66
Byproduct		
Vacuum Tower Residuals	Bbl	51.73
Sulfur	Metric Ton	22.05
HP Steam	Metric Ton	29.13
MP Steam	Metric Ton	21.78
LP Steam	Metric Ton	16.76
Condensate	Metric Ton	3.75

Reference WTI crude oil price = $79.58/bbl.

6.2.3 Overall Operating Cost

The overall operating cost for a case in which hydrogen is produced by coal-liquefaction residuals is shown in Table 6.4. The total operating cost, variable plus fixed costs, is

$52.41/bbl. As anticipated hydrogen is the most expensive component, $$29.37/bbl, of the operating cost with feed coal immediately follows at $10.55/bbl.

6.3 Financial Analysis

The major financial assumptions are listed below:

Variable	Assumption
1. Life of Project	20 years
2. Capacity utilization (on stream time)	330 days/year
3. Equity/(Debt + Equity)	50%
4. Interest rate	7%
5. Debt replacement schedule	20 years
6. Income tax rate	34%
7. Annual Energy Inflation: Annual Non-Energy Inflation	2.5% 1.5%
8. Average labor salary	$62,500 /yr

Other Plan construction related assumptions are:

Variable	Assumption
1. Plant Capacity (distillable products, not including LPG)	45,852 BPSD
2. Construction Period with capital expense schedule of :	4 years
Year 1	15%
Year 2	20%
Year 3	25%
Year 4	40%
3. Capacity Ramp up	
1st Year	60%
2nd Year	80%
3rd Year	100%
4. Contingency in Capital Estimate	20%
5. Other Non-EPC Cost (% EPC Cost)	13.78

The first financial scenario to evaluate is a DCL complex to purchased H_2 from an external source whether via a pipeline or cross the fence. This scenario requires less capital investment but have to rely on a long term H_2 supply contract. The internal rate of return (IRR) for different H_2 supply cost is listed in Table 6.5.

The highest IRR option, 25.3%, is the SMR case with a natural gas cost of $5/MMBTU. This case provides the most favorable scenario – lowest investment cost and lowest operating cost. The second most favorable scenario is shared by the SMR case with a higher natural gas price of $7.5/MMBTU and the case using coal (plus liquefaction residuals) for hydrogen production. The IRR is 22.7 and 23.0%, respectively. This is the balance point ($7.5/MMBTU) above which it is more profitable to switch from natural gas to coal for hydrogen production. This balance point may be lower if the price of liquefaction residuals is lower than the assumed value.

The replacement of part of the coal to the gasifier by biomass will reduced the IRR by 4 to 5%, the higher reduction corresponding to the case of higher price for the biomass ($75/ton). As far as the DCL plant is concerned that is no advantage to use biomass. The plant owner not only has to pay more for the H_2 and there is no CO_2 credit that the DCL plant owner can claim. For the same reason the same comment can applied to the 100% biomass scenario. Also, the hydrogen cost from using 100% biomass as feed is so expensive. The IRR of the DCL plant will drop to a uneconomical value of 3.1 to 10.8 %. H_2 from electrolysis using dedicated power supplying from a small nuclear power generator gives an IRR of 11.7 %. Purchase \price of power from the grid is not practical. It gives a negative IRR.

In order to take full advantage of integration of the H_2 Production and DCL facilities, a second financial scenario is considered. It is obvious that including the H_2 Production facility will make the project biggest and hence requires a higher investment cost. There will be no transfer pricing between the H_2 Plant and the DCL Facility and both facilities will have the same IRR. Table 6.6 presents the IRR for this scenario. Basically, the conclusion for this scenario is the same as the first scenario. However, the difference in IRR for various cases became smaller. For cases that have an IRR less than 18% under the first scenario, in which IRR was assumed to be 18% for all H_2 Production options, now will have higher IRRs. These cases include biomass only case, and the electrolysis with nuclear generated power. For cases that have an IRR above 18% in the first scenario, the resultant IRR only reduce slightly.

Plant Configuration	**EPC Cost (in Billion Dollars)**					
	SMR	**Coal/ Residuals**	**Coal/ Residuals/ Biomass**	**Biomass (100%)**	**Electrolysis**	
					Nuclear Power	**Grid Power**
DCL Complex	2.00					
H_2 Plant	0.47	1.32	2.02	1.51	2.4	1.37
Total	2.47	3.32	4.02	3.51	4.40	3.37
Ratio	1.0	1.34	1.63	1.42	1.78	1.36

Table 6.1 Breakdown Capital Cost for DCL Complex

Unit No.	Name of Unit	Number of Units	Total Cost (Million $) Feb. 2010
1000	**Coal Preparation Plant**		
1100	Coal Handling & Storage	1	27.27
1200	Coal Pulverization	4	43.20
	Subtotal		**70.47**
2000	**Direct Coal Liquefaction Unit**		
2100	Catalyst Manufacturing	2	10.91
2200	Slurry Feed Preparation	2	164.96
2300	Coal Conversion & Solvent/Product HTU	2	988.26
2400	Slurry Product Fractionation	2	61.77
2500	Gas Plant	1	63.85
	Subtotal		**1,289.75**
3000	**Product Refining Unit**	1	**248.57**
4000	**Other Units**		
4100	Sulfur Recovery	1	31.01
4200	Waste Water Treatment	1	172.61
	Subtotal		**203.62**
	Utilities		
	Oily Water Treatment	1	0.72
	Coal Pile Runoff Treating	1	0.02
	Product Storage Facilities	1	38.59
	Chemical Storage	1	10.36
	Raw Water Treatment	1	3.04
	Boiler Feed Water	1	78.54
	Cooling Water Tower	1	20.85
	Fire Protection Facility	1	5.90
	Portable Water Facility	1	0.45
	Instrument & Plant Air	1	4.46
	Building		26.93
	Subtotal		**189.86**
Grand Total for the DCL Complex		**2,002.27**	

Table 6.2 Plant Operation Staff

Unit	Operating Staff		
	Skill Operator	Non-Labor Labor	Total Operators
1000			
Coal Handling & Preparation	**6**	**36**	**42**
2000 DCL Plant			
Catalyst Manufacturing	3	18	21
Feed Slurry Preparation	3	18	21
Coal Conversion	9	42	51
Gas Plant	3	12	15
Raw Coal Liquids/Solvent HTU	3	18	21
Product Slurry Fractionation	6	24	30
Subtotal	**27**	**132**	**159**
3000 Product Refining Plant	**6**	**30**	**36**
4000			
Sulfur Recovery	3	12	15
Waste Water Treatment	3	12	15
Subtotal	**6**	**24**	**30**
Utility Plants			
Raw Water Treatment	3	12	15
Cooling Water	3	6	8
BFW & Condensate	3	12	15
Storage & Loading	3	18	21
Subtotal	**12**	**48**	**60**
Grant Total Operating Staff	**57**	**270**	**327**

Table 6.3 Administration, Engineering and Supporting Staff

Department	**No. of Staff**
1. Management, Engineers & Chemists	
Plant Manager	1
Assistant Plant Manager	3
Chemical Engineers	12
Structural Engineers	6
Electrical Engineers	12
Civil Engineers	6
Instrumentation Engineers	12
Rotary Equipment Engineers	9
Heat Exchanger & Fire Heater Engineers	9
Lab. Technicians	12
Safety & Environmental Engineers	6
Piping Designers & Drafters	6
Subtotal	**94**
2. Maintenance	
Unit 1000	5
Unit 2000	24
Unit 3000	12
Unit 4000	12
Utility Plant	12
Subtotal	**65**
3. Administration and Support	
Manager & Assistant Manager of Admin,	4
Financial	3
Accounting & Payroll	9
Health Care	6
Procurement	9
Marketing	8
Building Sanitary Workers	6
Subtotal	**45**
4. Plant Emergency & Safety Department	
Plant Fire Fighter	24
Emergency Vehicle Drivers	6
Plant Security Guards	18
Subtotal	**48**
Grant total Admin./Engineers/Support	**252**

Table 6.4 Operating Costs – H_2 from Coal/Resid Gasification

Varibale Costs	**$/Unit**	**Units/day**	**$/day**	**$/year**	**$/bbl**
Feed Coal. mT	42.99	11,249.60	483,620	159,594,700	10.547
Catalyst/Chemcials, bbl	2.50	45,852.20	114,631	37,828,065	2.500
Cooling Water, 1000 gallon	0.31	1,867.20	579	191,015	0.013
Fresh & Process Water, 1000 gallon	13.55	2,195.50	29,749	9,817,178	0.649
BFW, 1000 gallon	14.20	555.00	7,881	2,600,730	0.172
Electricity, MWh	60.00	3,009.60	180,576	59,590,080	3.938
Hydrogen, mT	1,837.00	733.10	1,346,703	444,412,067	29.371
Fuel Gas, MMKCal	29.76	402.50	11,978	3,952,872	0.261
Instrument Air, 1000 NM3	20.33	11.87	241	79,635	0.005
Nitrogen, 1000NM3	39.94	5.82	232	76,709	0.005
MP Steam	21.78	897.80	19,554	6,452,848	0.426
Subtotal			**2,195,745**	**724,595,898**	**47.887**

Fixed Costs	**%EPC**	**$/day**	**$/year**	**$/bbl**
Total Labor		109,659	36,187,500	2.392
Plant Maintenance	1.130	68,563	22,625,651	1.495
Contracted Maintenance	0.280	16,989	5,606,356	0.371
Insurnace	0.070	4,247	1,401,589	0.093
Property Tax	0.004	243	80,091	0.005
Legal, acocunting, etc…	0.021	1,287	424,702	0.028
Other (mgmt fees, marketing, etc..)	0.106	6,435	2,123,508	0.140
Subtotal		**207,422**	**68,449,397**	**4.524**
Grand Total Operating Costs		**2,403,168**	**793,045,295**	**52.411**

Table 6.5 Summary of Financial Analysis – Overall Internal Rate of Return for Non-integrated DCL Pant with Cross-the-Fence H_2 Supply.

(Based on Hydrogen Plant IRR = 18%)

	Steam Methane Reforming		**Coal-Resid Gasification**	**Biomass Gasification**		**Coal-Resid-Biomass Gasification**		**Nuclear-Electrolysis**	**Grid Electrolysis**
Feedstock Price Case	**High**	**Low**		**High**	**Low**	**High**	**Low**		
H_2 Cost ($\$$/kg H_2)	1.88	1.47	1.84	3.89	3.35	2.66	2.42	3.25	6.12
DCL Plant IRR (%)	22.7%	25.3%	23.0%	3.1%	10.8%	17.0%	18.9%	11.7%	n/a

Table 6.6 Summary of Financial Analysis – Overall Internal Rate of Return for an Integrated H_2 & DCL Complex

(Based on same Hydrogen Plant and DCL Plant IRR)

	Steam Methane Reforming		**Coal-Resid Gasification**	**Biomass Gasification**		**Coal-Resid-Biomass Gasification**		**Nuclear-Electrolysis**	**Grid Electrolysis**
Feedstock Price Case	**High**	**Low**		**High**	**Low**	**High**	**Low**		
H_2 Plant IRR (%)	21.8%	24.1%	21.2%	12.0%	14.7%	17.5%	18.6%	15.3%	n/a
H_2 Cost ($\$$/kg H_2)	2.01	1.67	2.11	3.23	2.96	2.62	2.48	2.88	-
DCL Plant IRR (%)	21.8%	24.1%	21.2%	12.0%	14.7%	17.5%	18.6%	15.3%	n/a

7. CONCLUSION & RECOMMENDATION

Conceptual design of a 45,850 BPSD direct coal liquefaction facility using Illinois no. 6 coal has been developed. This plant also produces 4,790 BPSP of LPG. Six different options for H_2 production were being looked at. This study also includes a refining study in which a bituminous coal derived syncrude was processed to produce gasoline, kerosene and diesel fuels that meet current transportation fuel specifications. This section summarizes the major finding from the study and outlines areas of further study to further delineate other critical issues that have not been investigated.

7.1 Conclusion

The following major conclusions can be drawn from this study:

Direct Coal Liquefaction:

1. The total installed cost of the DCL block, not including the H_2 production facility, is estimated to be $2.71 billion, which includes financing cost; other non-EPC cost, 13.7% of EPC cost, and contingency, 20% of the EPC cost.

2. Of the six H_2 production options evaluated, SMR and gasification (with coal or coal-biomass co-feed as feed) are the two only economical and practical options.

3. The overall internal rate of return for the integrated facility (including the H_2 Plant) is estimated to be 24% for a SMR-H_2 Plant with natural gas price of $5.00/MMBTU, 21% for a Gasification-H2 Plant with coal as the only feedstock, and 18% for a Gasification –H_2 Plant with a coal-biomass as co-feed (biomass was priced at $75 per dry tons).

4. With 90% carbon capture of the process effluent gas stream, CO_2 emission from the DCL+H2 Plant complex is controlled at 52.3, 61.0 and 50.8 Kg/bbl of liquid fuels (including LPG) for the SMR, Gasification-coal and gasification-coal/biomass case, respectively.

H_2 Production

5. SMR requires the least investment cost ($0.51/kg H_2), which is only 38% of that of the gasification-coal only case – the next lowest investment option.

6. The coal/biomass co-feed gasification case, with 4,000 ton/day of biomass, increases the investment of the coal only gasification case by 24%.

7. The overall H_2 production cost via SMR is equivalent to that of coal gasification, \$1.84/kg H2, when natural gas price is at \$7.30/MMBtu.

8. Co-feeding of 4,000 tons/day biomass (@\$75/ton) with coal results at 45% increase of overall production cost than that of using coal only. However, the Co2 emission (at 90% capture) is reduced by 46%.

Refining and Properties of DCL Liquid Fuels

9. The total installed cost of the DCL complex will be XX% high if the coal liquids are refined to meet transportation specifications.

10. Coal liquids have higher density than petroleum derived liquids of similar boiling point range.

11. Coal liquids can be refined using conventional refining technologies to meet current US and European transportation specifications.

12. Coal derived naphtha reforms easily into high octane gasoline.

13. Conventional cetane index correlation cannot be applied to coal derived diesel. Through a single hydrotreating/hydrocracking step coal distillate can be upgraded to have cetane number of 52.

14. A bituminous coal derived kerosene sample with boiling point of (135 to 250^{o}C) passed all JP-8 specifications without relying on blending with any petroleum distillate. The coal derived jet fuel has a higher heating value (4% higher) and lower freeze point of -77^{o}C.