



Direct Coal Liquefaction Overview Presented to NETL

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Direct Liquefaction Presentation Outline

- What is Direct Coal Liquefaction (DCL)? And How does it Differ from Indirect Liquefaction (ICL)?
- History of U.S./Foreign DCL Processes
- Comparison of Results from DOE DCL Technology Support
 - EDS; H-Coal; HRI
- Overall Findings
- DOE Previous DCL Designs and Potential Vendors
- Environmental Considerations/Fuel Specifications
- Current DCL Technology Developments
 - Shenhua; Accelergy
- LTI Thoughts and Comments/Recommendations
 - Analysis
 - R&D

Details are found in supporting presentations

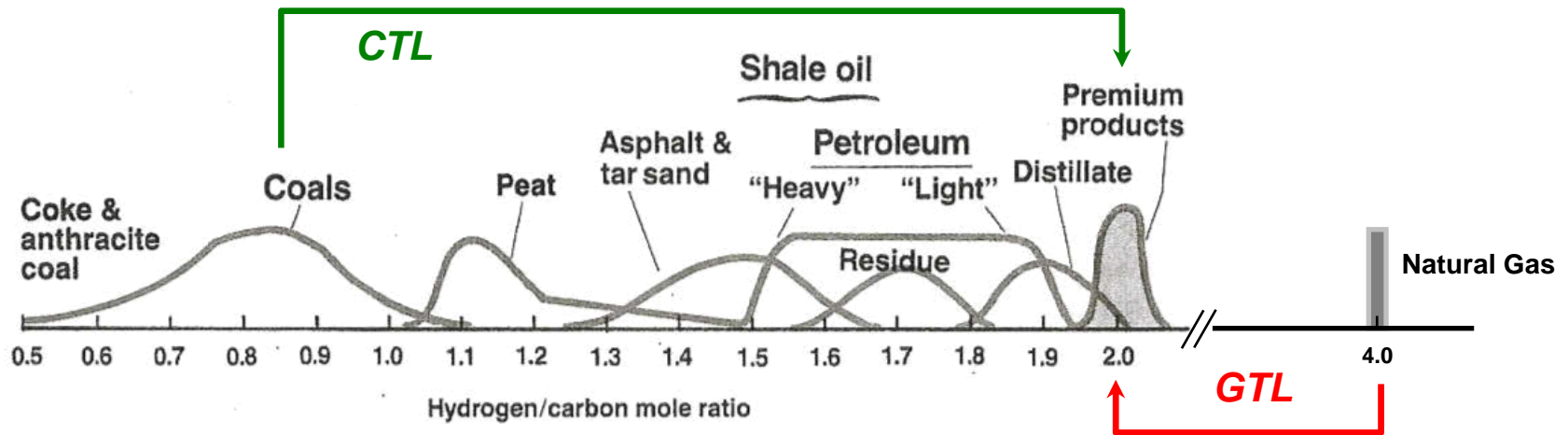
Direct Liquefaction Presentation Summary

- DOE support for direct coal liquefaction occurred mainly over the period 1976-2000.
 - About 90% of total DOE funding of \$3.6 billion was spent for the large scale demo program (1976-82) referred to as Phase I, which showed the overall engineering feasibility and applicability of direct liquefaction to a wide range of coals.
 - Processes demonstrated included SRC (both I and II), EDS and H-Coal. Supporting research paved the way for process improvements
- Three main components:
 - Phase I to accelerate the technology as a short-term response to '70s energy crisis;
 - Fundamental research to develop improvements and identify alternatives;
 - Phase II bench/pilot-scale program to overcome technical and economic deficiencies in Phase I (Lummus, HTI and Wilsonville facility)

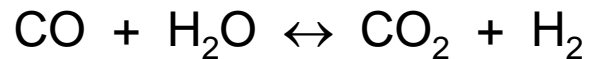
Direct Liquefaction Presentation Summary (2)

- Accomplishments of Phase II
 - Higher distillate yields...naphtha, mid-distillate and gas oil (~ 70% vs. ~50%)
 - Higher quality liquids...no resid and metals and low heteroatom content; naphtha can be processed in conventional refineries
 - Higher hydrogen content and lower product boiling point end point alleviated carcinogenity concerns
 - Applicability to low rank coals and mixed feedstocks ..coprocessing with petroleum resides, heavy oils, waste plastics
 - Valuable chemicals can be produced...cresylics, wax, BTX, argon, krypton; suggests possible advantage of direct liquefaction with IGCC
 - Burke, etal concluded that radical departures from the DOE-supported direct liquefaction program are unlikely to result in substantially improved processes

Fuels H/C Ratios

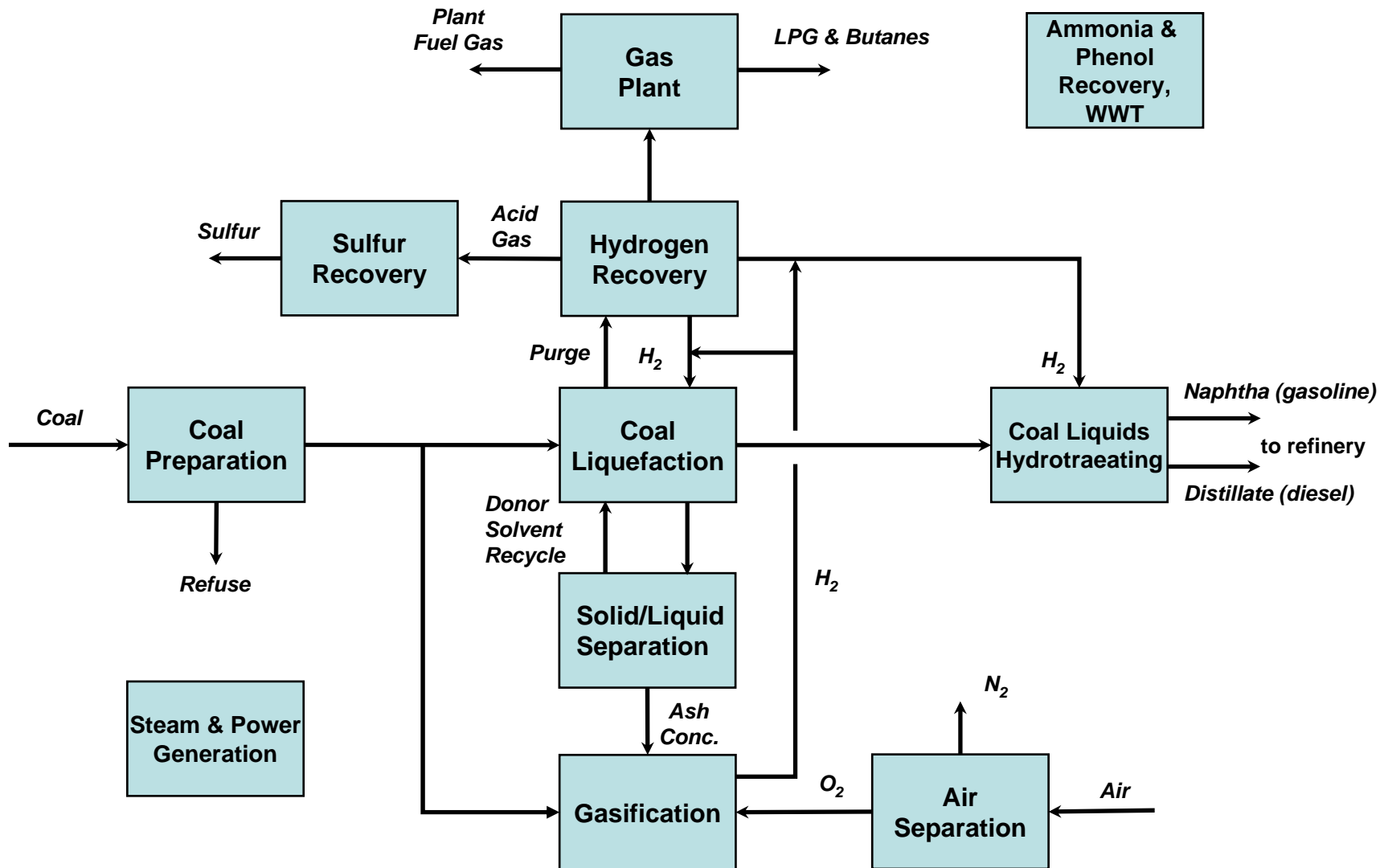


- To make liquid fuels from coal - need to add hydrogen or reject carbon
- To make liquid fuels from natural gas - need to reject hydrogen or add carbon
- Adding hydrogen and rejecting carbon (or vice versa) may be equivalent:



Water Gas Shift (WGS) Reaction

Direct Liquefaction Block Flow Diagram



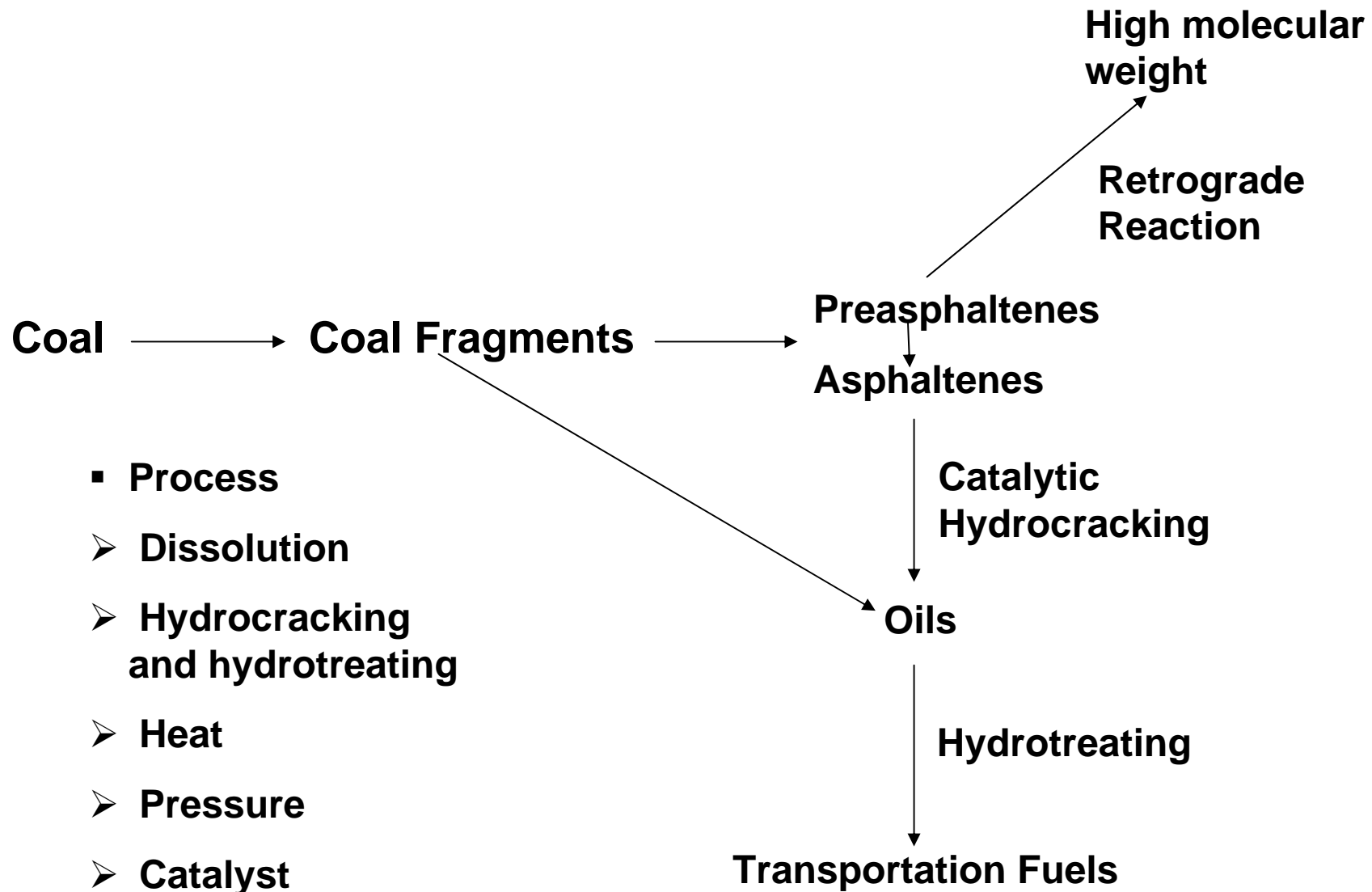
Direct Liquefaction Defined

- Direct liquefaction processes add hydrogen to the hydrogen deficient organic structure of the coal, breaking it down only as far as is necessary to produce distillable liquids.
- Coal dissolution is accomplished under high temperature (~ 400 °C) and pressure (~ 1500 - 3000 psi) with hydrogen and a coal-derived solvent.
- The coal fragments are further hydrocracked to produce a synthetic crude oil.
- This synthetic crude must then undergo refinery upgrading and hydrotreating to produce acceptable transportation fuels.

Comparing Direct and Indirect Liquefaction

- **In Direct Liquefaction (DL) pressure, heat and catalyst are used to crack the coal to make liquids**
 - theoretical efficiency can be high...roughly 70-75%
 - “sledge hammer” approach
- **In Indirect Liquefaction (IL) coal is first gasified to form syngas. Syngas is then converted to liquids by means of a catalyst and Fischer Tropsch (FT) chemistry**
 - Synthesis Gas or Syngas – mixture of CO, H₂, CO₂, H₂O
 - theoretical efficiency is lower...roughly 60-65%
 - “engineered” approach

The Direct Conversion Process Basics



Direct Liquids Quality

- **Liquid Products are much more aromatic than indirect**
 - DCL Naphtha can be used to make very high octane gasoline component; however aromatics content of Reformulated Gasolines is now limited by EPA
 - DCL Distillate is poor diesel blending component due to high aromatics which results in low cetane versus U.S. average of about 46
- **Raw DCL Liquids still contain contaminants: Sulfur, Nitrogen, Oxygen, possibly metals and require extensive hydrotreatment to meet Clean Fuels Specifications**

Direct Liquefaction Process

- A single-stage direct liquefaction process gives distillates via one primary reactor. Such processes may include an integrated on-line hydrotreating reactor, which is intended to upgrade the primary distillates without directly increasing the overall conversion.
- A two-stage direct liquefaction process is designed to give distillate products via two reactor stages in series. The primary function of the first stage is coal dissolution and is operated either without a catalyst or with only a low-activity disposable catalyst. The heavy coal liquids produced in this way are hydrotreated in the second stage in the presence of a high-activity catalyst to produce additional distillate.

Direct Liquefaction Benefits

- Direct liquefaction efficiency may be higher than indirect technology. One ton of a high volatile bituminous coal can be converted into approximately three barrels of high quality distillate syncrude for refinery upgrading and blending
- Direct Liquefaction provides high octane, low sulfur gasoline and a distillate that will require upgrading to make an acceptable diesel blending stock
- Development of direct liquefaction technology could lead to hybrid (direct/indirect) processes producing high quality gasoline and diesel
- The NCC, others suggest that direct liquefaction may have a better carbon footprint than indirect technology

Direct Liquefaction Challenges

- **Uncertainty in World Oil Prices**
- **High Capital Costs**
- **Investment Risk**
- **Technical Challenges**
 - First technology (since 2nd World War) is being commercialized in the PRC (Shenhua) – need other first-of-kind large scale operation (with carbon management) to verify baselines and economics
 - R&D activity should focus on remaining process issues such as further improvement in efficiency, product cost and quality, reliability of materials and components* and data needed to better define carbon life cycle
 - The timelines for demonstration and development of direct liquefaction technology and carbon capture and storage must be integrated.
 - Hybrid technology needs development including integrated demonstration
- **Environmental Challenges**
 - CO₂ and criteria pollutants
 - Water use
- **Concerns with increased coal use in U.S.**

* The Shenhua commercial plant will provide new information on reliability and performance

U.S. Direct Liquefaction Process History

<u>Year</u>	<u>Process</u>	<u>Coal Capacity</u>
1945-1953	Bergius – Louisiana, MO	100 tons/day
1962-Early 1980s	Solvent Refined Coal (SRC) – Pott-Broche	50 tons/day
1963-1972	Consol Synthetic Fuels (CSF) – Two-Stage, Catalytic	20 tons/day
1970s-Early 1980s	SRC-I and SRC II (Gulf Oil Fort Lewis) – One-Stage, Non-catalytic	50 tons/day
1965-Early 1980s	H-Coal (Catlettsburg KY, HRI) – One-Stage, Catalytic	250 tons/day
Late 1960s-Early 1980s	EXXON Donor Solvent (Baytown, TX)	250 tons/day
Early 1980s-Late 1980s	Integrated Two-Stage Liquefaction (ITSL) – Lummus – Wilsonville (Southern Company) – HRI	6 tons/day
1990-1995	Multi-Stage Slurry Phase Liquefaction HTI	3 tons/day Proof-of-concept

Non-U.S. Direct Liquefaction Processes

<u>Country</u>	<u>Facility</u>	<u>Capacity Tons/Day</u>	<u>Status</u>
Germany	BOTTROP Plant – I.G. Farben Variant	200	Shut Down
Japan	Brown Coal Liquefaction Plant – ITSL Variant – Victoria, Australia	50	Shut Down (~1990)
Japan	Nedol Plant – ITSL Variant – BIT. and SUBBIT. Coals	150	Shut down (Late 1990s)
U.K.	Point-of-AYR Plant – ITSL Variant	2.5	Shut Down (~1990)
China	Inner Mongolia	7,000	Start-up 2008

Comparison of Results for DOE Direct Liquefaction Program

DOE Sponsored Programs 1968-1995

- **Phase I processes**
 - SRC-II
 - Exxon Donor Solvent (EDS)
 - H-Coal
- **Phase II process campaigns**
 - Lummus Integrated Two-Stage Liquefaction (ITSL)
 - Wilsonville Two-Stage Liquefaction
 - HRI/HTI Catalytic Multi-Stage Liquefaction (CMSL)
 - U. Ky./HTI/CONSOL/Sandia/LDP Advanced Liquefaction Concepts (ALC)

EDS Process

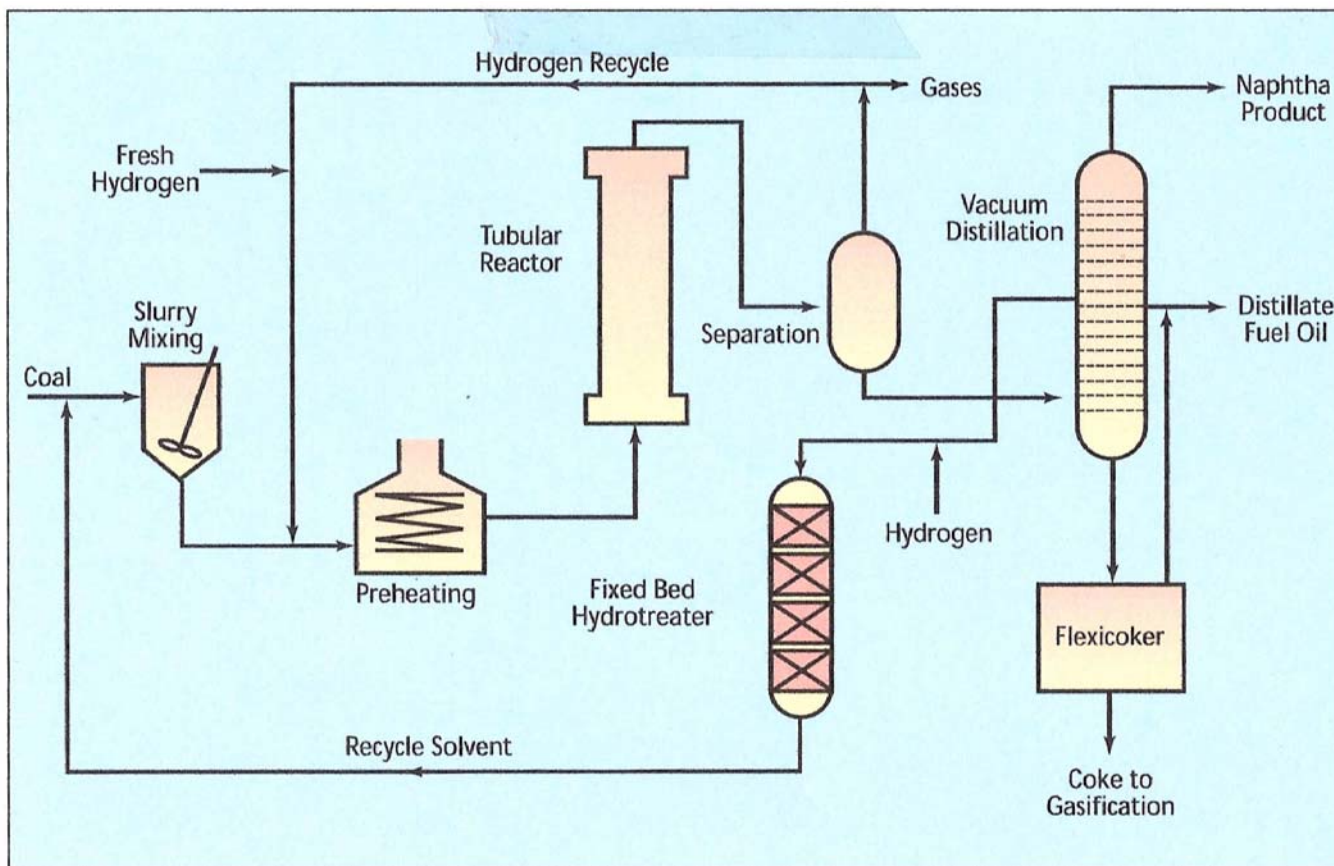
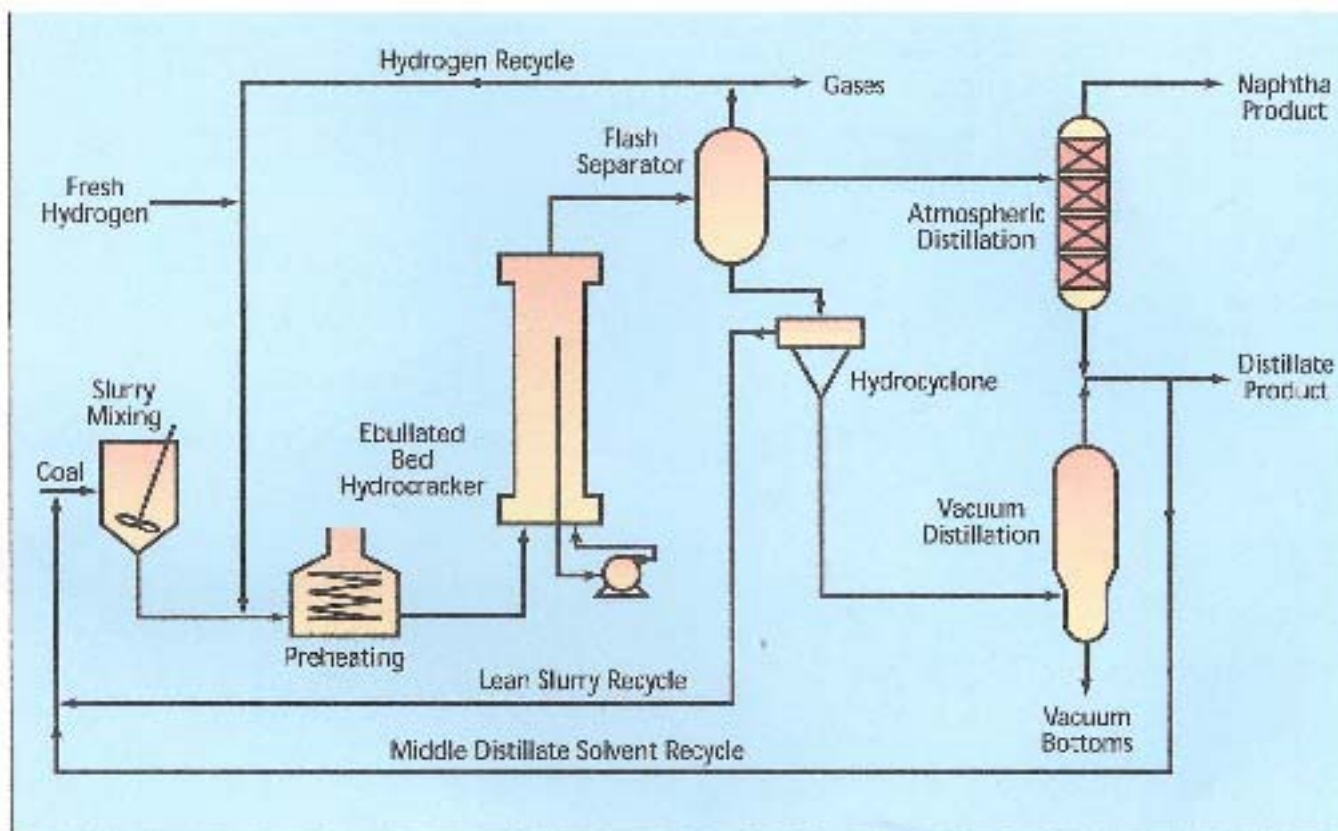


Figure 6. Schematic diagram of the EDS process

EDS Process Specifications and Conditions

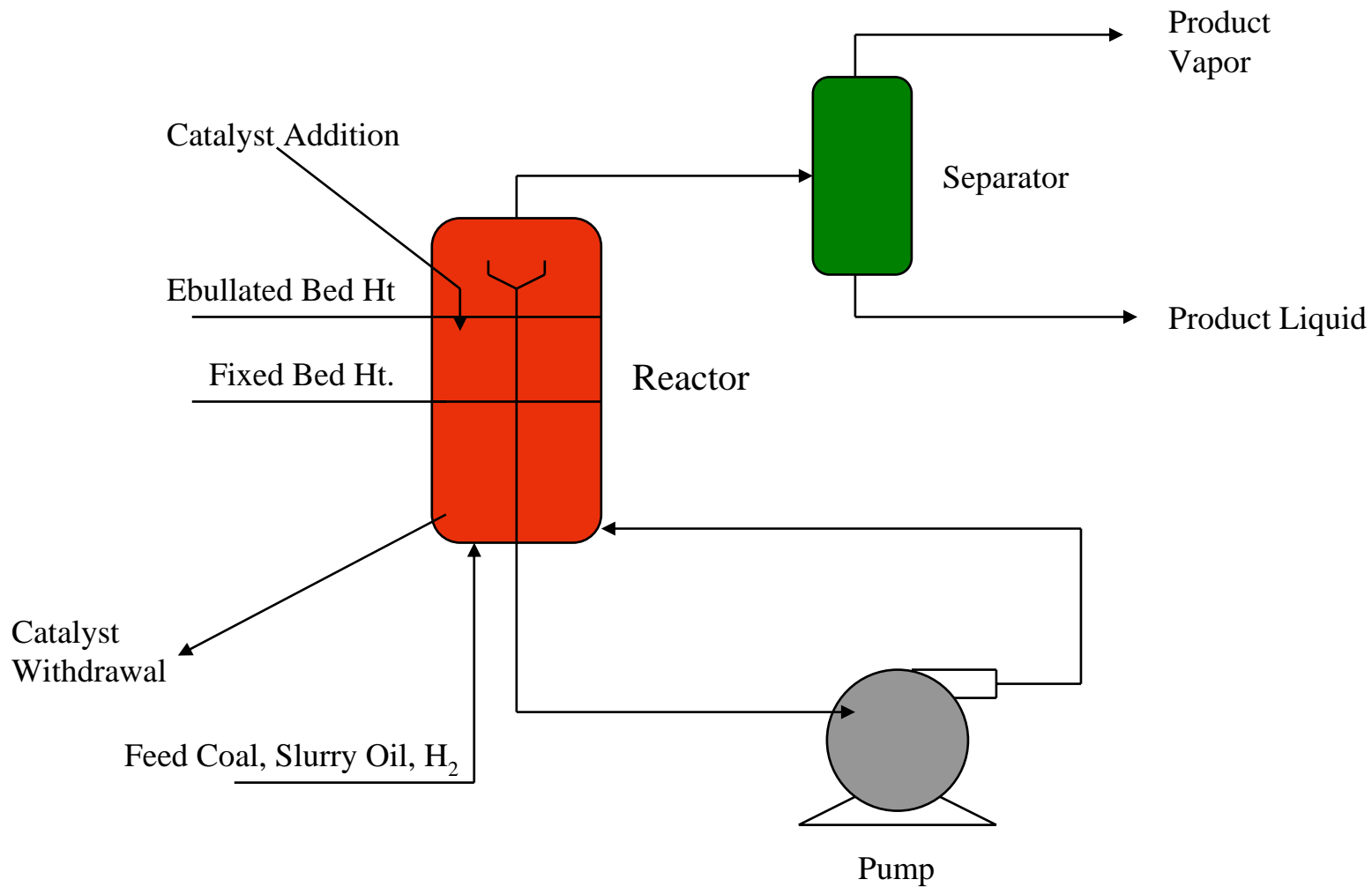
- Coal is slurried with a distillable recycled solvent that has been rehydrogenated to restore its hydrogen donation capacity
- The slurry is mixed with H₂, preheated and fed to a simple up-flow tubular reactor that operates at 425-450 °C and 2575 psig .
- No catalyst is added to liquefaction reactor
- Naphtha and middle distillate products are recovered, although a portion of the middle distillate is recombined with the heavy distillate to form the basis for the recycle solvent.
- Rehydrogenation of the recycle solvent is carried out in a fixed-bed catalytic reactor, using either nickel-molybdenum or cobalt-molybdenum on an alumina support.
- The hydrogenation reactor is operated at conditions in the region of 370 °C / 1600 psig, although conditions are varied to control the degree of hydrogenation of the solvent and thus maintain its quality.
- Yields of up to 47% for lignites, 50% for sub-bituminous coals and 60% for bituminous coals could be achieved.

H-Coal Process Schematic



Schematic diagram of the H-Coal process

H-Coal Ebullated-Bed Reactor



H-Coal Process Specifications and Conditions

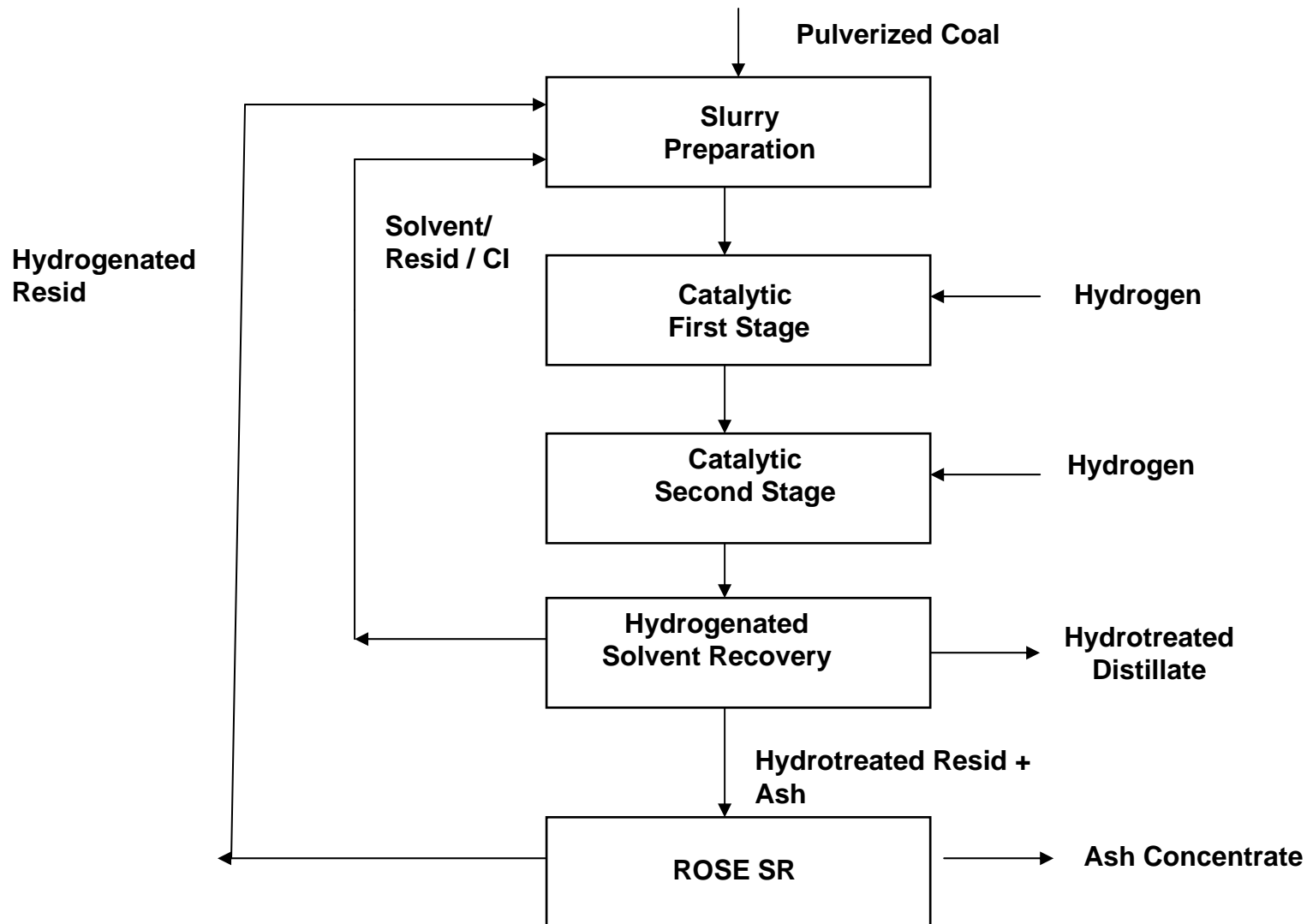
- Coal is slurried with a recycle solvent that consists of a mixture of a solids containing hydrocracker product with heavy and middle distillates obtained by product fractionation.
- H₂ is added and the mixture is preheated and fed to an ebullated bed hydrocracker, which is the distinguishing feature of the process.
- This reactor operates at temperatures of 425-455°C and a pressure of 2900 psig.
- A conventional supported hydrotreating catalyst, either Ni-Mo or Co-Mo alumina is used. The catalyst is fluidized by H₂ and a pumped internal recycle stream, for which the intake is positioned above the upper limit of the expanded bed of catalyst but still within the reactor liquid zone. This recycle stream contains unreacted coal solids.
- The ebullated-bed reactor system offers substantial advantages over fixed-bed reactors - the reactor contents are well mixed and temperature monitoring and control are more easily effected.

H-Coal Process Specifications and Conditions (2)

- Ebullated-bed reactors allow catalyst to be replaced while the reactor remains in operation, enabling a constant catalyst activity to be maintained
- The reactor products pass to a flash separator. Liquids in the overheads are condensed and routed to an atmospheric distillation column, producing naphtha and middle distillate.
- The flash bottoms are fed to a bank of hydrocyclones. The overheads stream, which contains 1-2% solids, is recycled to the slurring stage. The underflow is routed to a vacuum distillation column. Solids are removed with the vacuum column bottoms, while the vacuum distillate forms part of the product for export
- As with other processes, yields are dependent on the coal. >95% overall conversion can be obtained with suitable coals, with liquid yields up to 50% (dry basis).

Wilsonville PDU

Block Diagram of CC ITSL Process



HRI/HTI

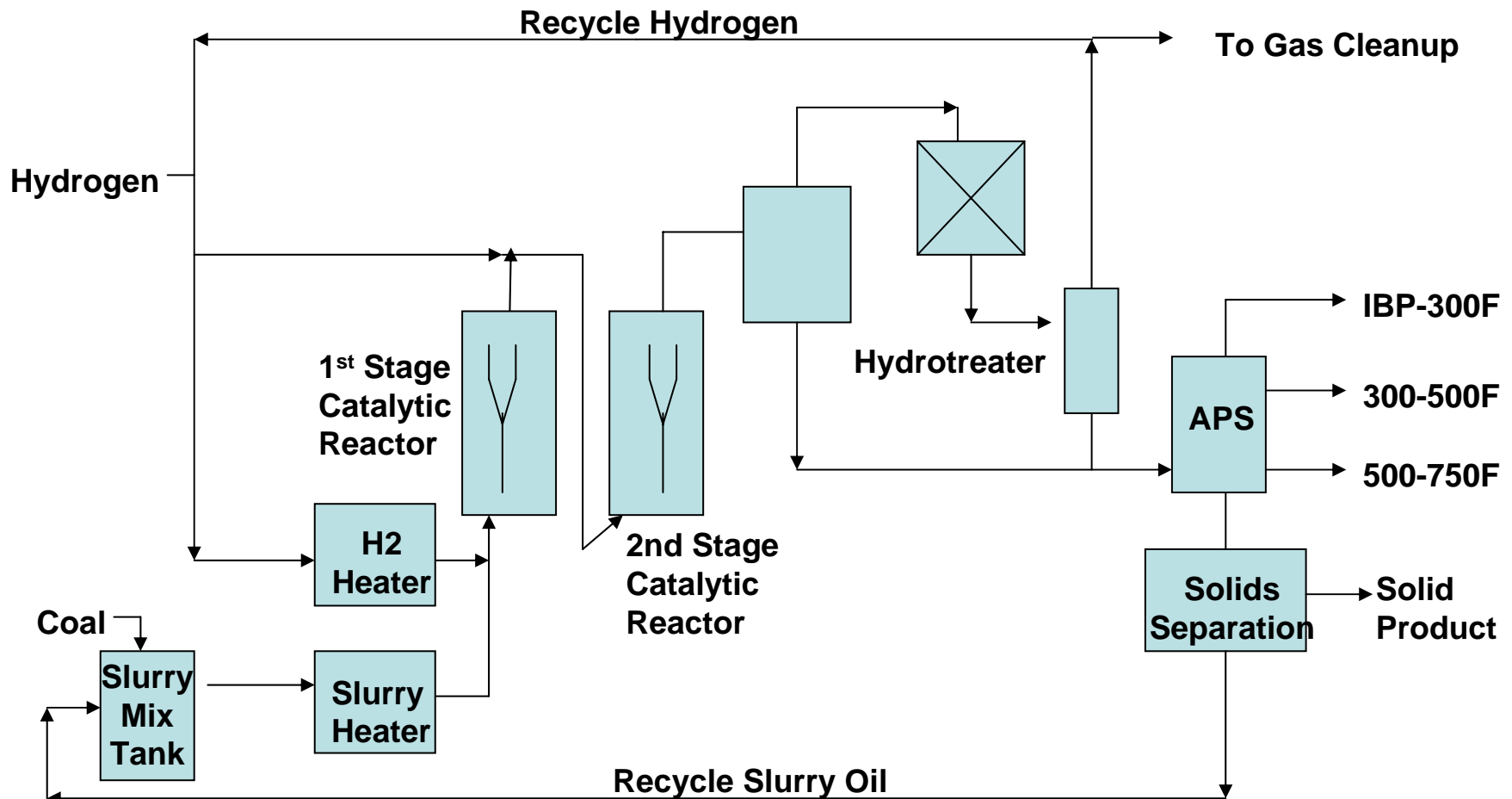
Two Stage Liquefaction

Catalytic Multi-stage Liquefaction (CMSL) System

- In 1993, the two-stage liquefaction system evolved into the catalytic multi-stage liquefaction (CMSL) system.
- In 1993, the Department of Energy awarded HRI a contract to conduct demonstrations of direct coal liquefaction in the 3 t/d PDU. This program was known as the Proof of Concept (POC) Program.
- The PDU was modified to incorporate an in-line hydrotreater, a new second-stage reactor and reactor structure, a ROSE-SR™ solid separation unit, a new pulverized coal storage and handling system, new preheaters, new flare system, and a computerized automated data collection and control system.

HRI/HTI

Two Stage Liquefaction (2)



HTI 3 TPD PDU

HRI/HTI

Two Stage Liquefaction (3)

Catalysts

- The role of catalyst in the first stage of the CMSL process
 - promote hydrogenation of the solvent
 - stabilize the primary liquefaction products
 - hydrogenate the primary and recycle resid
- In the second stage
 - promote heteroatom removal and thus product quality improvement,
 - convert resid to distillate,
 - promote secondary conversion to lighter products, and aids in avoiding dehydrogenation.
- Catalyst Types evaluated
 - Supported catalysts (Co/Mo, Co/Ni)
 - Dispersed Catalyst (Fe, Mo)
 - HTI proprietary catalyst (GelCat – iron-based)

HRI/HTI

Two Stage Liquefaction (4)

Proprietary Catalysts

- HTI developed several proprietary dispersed iron catalysts.
- In microautoclave tests with these sulfate-modified iron-based catalysts, coal conversions based on THF solubility of a Black Thunder Mine subbituminous Wyoming coal were greater than that obtained at the same loadings (5000 ppm iron) with a commercially available dispersed iron catalyst (ca. 83- 86 wt % vs 76-81 wt %).
- The addition of a small amount of Mo (100 ppm) improved the conversion further (ca. 87-90 wt %).
- In tests made in the CMSL system with the proprietary catalyst in both reactors (all-dispersed mode of operation) and Mo loadings of 50-100 ppm, coal conversion in the range of 93-96 wt %, resid conversion of 83-92 wt % and C4-524 °C distillate liquid yields of 60-66 wt % were obtained.
- The level of performance achieved was better than that obtained with any other catalyst system.

Sample Process Conditions: One and Two Stage Liquefaction Processes

<u>Process</u> <u>Year</u>	<u>SRC-II</u> 1980	<u>H-Coal</u> 1981	<u>EDS</u> Late 1970's	<u>ITSL</u> 1989	<u>CMSL</u> 1994
Reactor Number	1	1	1	2	2
Reactor Temperature, °F	835-870	800-850	800-932	840-850	755
Reactor Pressure, psig	2000 max	3000	2000-3000	2500	2500
2nd Reactor Temperature, °F				760-810	829-845
2nd Reactor Pressure, psig				2500	2500
Reactor Residence Time, hours	0.75-1.0				
Solids Concentration, wt %	48			33	
Coal Ton per day	30	200	250	~ 6	3
Catalyst	iron pyrite	Co-Mo		Multiple	Multiple

Comparison of One and Two Stage Liquefaction Process Yields

<u>Process</u> <u>Year</u>	<u>SRC-II</u> 1980	<u>H-Coal</u> 1981	<u>EDS</u> Early 1980's	<u>ITSL</u> 1989	<u>CMSL</u> 1994
Yield, wt% MAF Coal					
Heterogases	12.9	11.3	17.4	15.2	15.2
C1-C3 gas	14.5	12.8	19*	5.4	11.4
naphtha	19.3	22.9	22.8	14.5	20.7
middle distillate	25.2	20	17	21.7	39.1
gas oil	4.9	7.6	4.4	29.6	12.5
total distilate	49.4	50.5	44.2	65.8	72.3
H consumption, wt%	5	6	5.9	6	7.5
H efficiency, lb dist/lb H consumed	9.5	8.4	7.5	11	9.7

* C1-C4 gas

Illinois Basin Coal Syncrudes

	H-Coal	ITSL	CMSL	Typical Crude
	1981	1991	1994	
Carbon, %	86.6	85.7	86.6	85.8
Hydrogen, %	10.5	11.5	13.1	13.0
Nitrogen, ppm	5000	4900	44	2000
Sulfur, %	0.19	0.07	0.06	1.00
Oxygen, %	2.13	2.24	0.44	
Vanadium, ppm	nil	nil	nil	200
% 650 °F-	83	79	80	53
% 975 °F+	0	0	0	20
API Gravity	27	22	38	32
Premium	1.00	1.07	1.20	1.00

Comparison of Naphtha Quality Among One and Two Stage Liquefaction Processes

<u>Process</u> <u>Year</u>	Illinois Basin Coal			<u>CMSL</u> 1996	<u>CMSL*</u> 1996
	<u>SRC-II</u> 1980	<u>H-Coal</u> 1981	<u>EDS</u> Late 1970's		
Naphtha Properties					
boiling Point, °F	100-400	180-380	158-392	i.b.p.-350	70-350
°API	39	35	31.1	49.9	53.5
H, wt%	11.5	11.6	10.9	14	14.7
S, wt%	0.2	0.2	0.5	0.04	0.02
N, wt%	0.4	0.31	0.2	0.02	0.002
O, wt%	3.9	3	2.8	0.3	<0.1

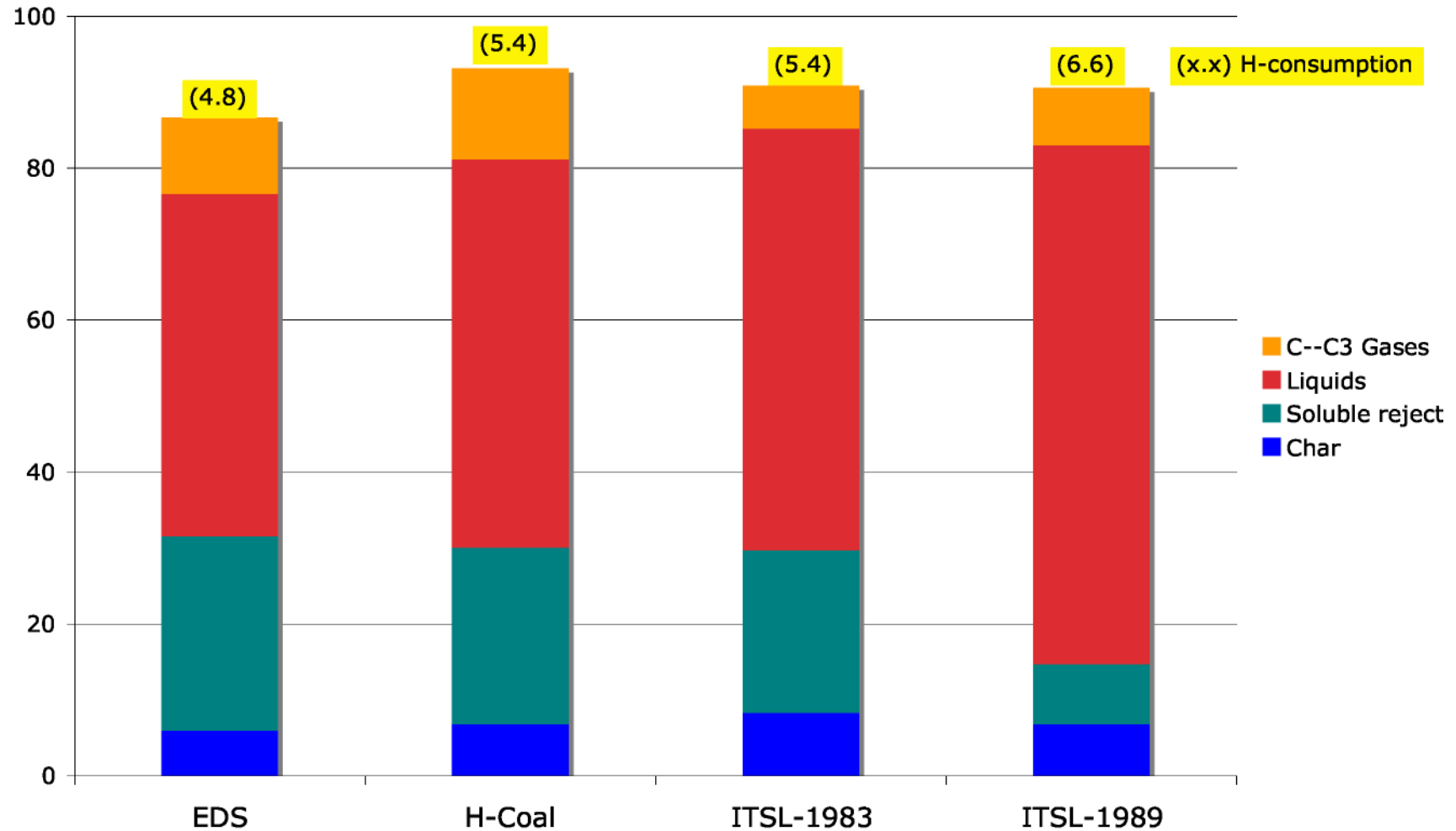
* PRB Coal On-line hydrotreater

Technology Applies to Wide Range of Coals

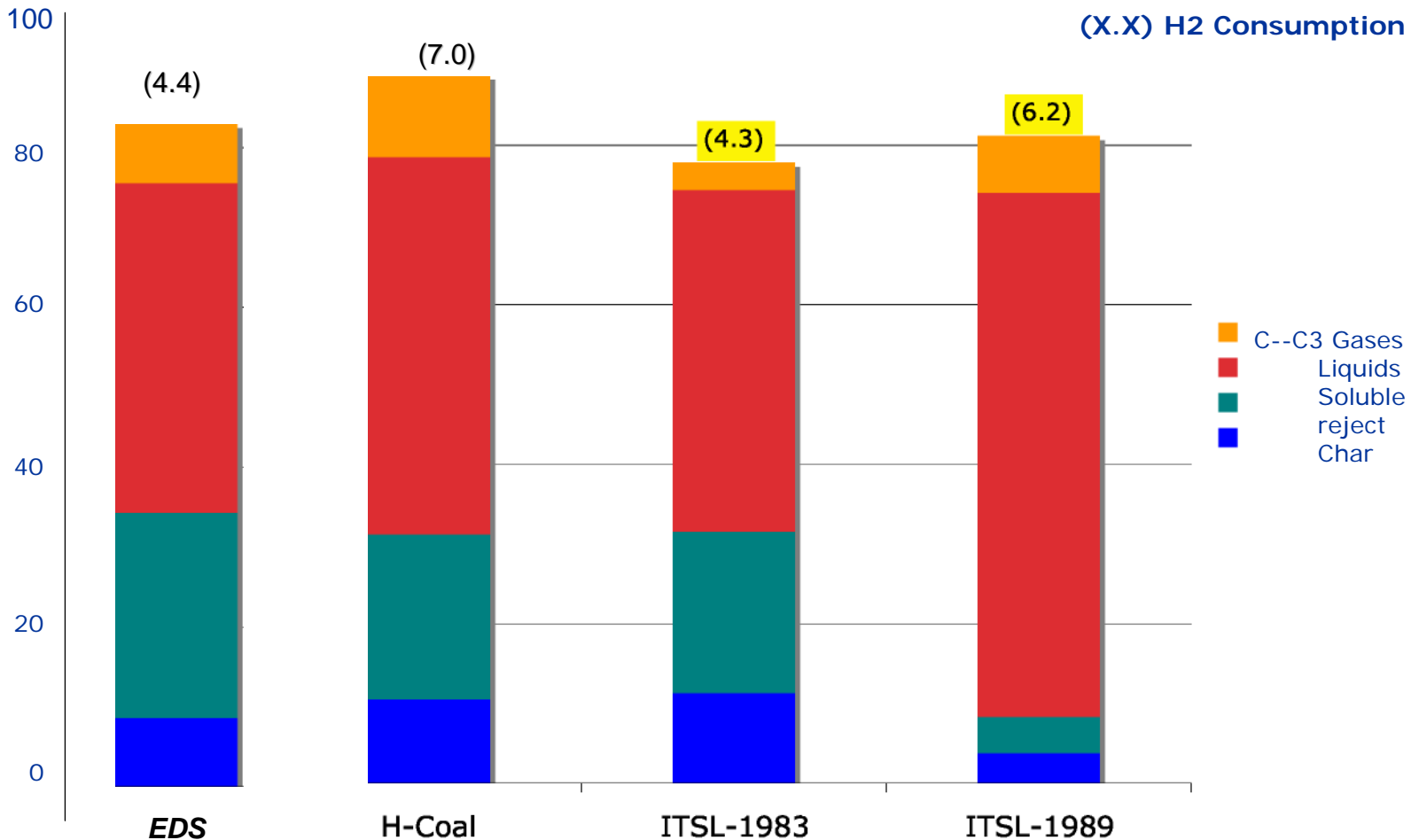
PRB COAL

	H-Coal 1980	ALC/CMSL 1996
Yield, wt % MAF Coal		
C₁-C₃ gas	11.0	12.4
naphtha	24.3	23.0
total distillate	50.7	66.1
H efficiency, lb dist./lb H consumed	9.0	9.7

Liquefaction Product Yields, Illinois # 6



Liquefaction Product Yields, Wyodak



Economic Competitiveness Greatly Improved

ILLINOIS BASIN COAL

	H-Coal	CMSL
	1981	1997
Yield, bbls/day	50,000	51,500
Coal feed, T/D AR	26,370	18,090
Plant cost, \$MM	\$4,592	\$2,914
Coal cost, \$MM/yr	\$178	\$122
Required Selling Price (RSP)	\$63.69	\$38.06
Premium	1.00	1.20
Equiv. Crude RSP	\$63.69	\$31.78

Differences Between Phase I and Phase II Technologies

<u>Issue/Variable</u>	<u>Phase I</u>	<u>Phase II</u>
Minimize reactor volume	Yes	No
Maximize distillate yields	No	Yes
Space velocity	Higher	Lower
Reaction temperature	Higher	Lower
Reactor staging	Generally No	Yes
Dispersed catalyst	Generally No	Yes
Solids recycle	No	Yes
Product recycle	Yes	No
Donor solvent concerns	Yes	No

Overall Findings – DOE Program

- While the H-Coal and EDS programs (Phase I) demonstrated the technical and engineering feasibility of direct coal liquefaction, many issues were not satisfactorily resolved, including those of process yield, selectivity, product quality, and, ultimately, economic potential.
- Process development research had identified a number of options for process improvement that were further developed and demonstrated (Phase II) at the bench and pilot plant scale, principally at Lummus-Crest, HRI (later, HTI) and the Wilsonville facility, during the 1980s and early 1990s.
- Improvements in distillate yields and quality were shown in HTI bench scale program with dispersed catalysts. Low sulfur and nitrogen were achieved with in-line hydrotreating. Need PDU verification, which may have been done.

Overall Findings – DOE Program (2)

High Yields of Distillate Fuels Demonstrated

- One of the most important accomplishments of the Phase II work was a substantial increase in liquid yields compared to the Phase I processes. High liquid yield is important, because direct liquefaction is capital-intensive. Therefore, increasing liquid yields greatly reduced the capital cost component of the process on a dollars/barrel/stream day basis. Liquid fuel yields were increased from 45% to 50% (MAF coal basis) for Phase 1 processes to about 75% (more than 4.5 bbl/t of MAF coal) for Phase 2 processes, while the yields of less valuable gaseous and non-distillate fuels were reduced commensurately for mid-western U.S. (Illinois Basin) coal.

Overall Findings – DOE Program (3)

High-Quality Liquids Produced

- The liquids made in the Phase I processes were intended to be crude oil replacements, but they were unstable, highly aromatic, and had high heteroatom (sulfur, nitrogen, oxygen) contents. This prompted concern about refinability, storage stability, and human health, principally related to carcinogenicity.
- In the Phase II work, considerable attention was paid to improving liquid fuel quality. The Phase II process produces liquid fuels containing no resid, no metals, and low levels of heteroatoms.
- These primary products can be refined in conventional refineries to meet current specifications for motor and turbine fuels. Product quality evaluations, which were an important element of the Phase II work, ensured that acceptable transportation fuels can be produced by direct coal liquefaction.

Overall Findings – DOE Program (4)

High-Quality Liquids Produced

- The Phase II processes make a quality naphtha that can be processed in conventional refineries into high-quality gasoline.
- No undesirable blending interaction with conventional gasolines and naphthas is expected. Direct coal liquefaction middle distillates can serve as blend stocks for the production of diesel fuel and kerosene.
- The low heteroatom content with accompanying higher hydrogen contents of Phase 2 process products alleviate the carcinogenicity concerns related to Phase 1 process products.

Overall Findings – DOE Program (5)

Process Scale-Up Demonstrated

- The Phase I work demonstrated successful continuous operation of plants as large as 200 t/d of coal feed (Ashland Synthetic Fuels, Inc., Catlettsburg, KY)
- The Phase II processes are sufficiently similar to the Phase I processes, in terms of process equipment and unit operations, that this experience is directly applicable.
- In addition, some of the key process equipment, such as the ebullated bed reactor, is used in petroleum refineries around the world.
- Materials of construction and equipment designs were found to overcome corrosion, erosion, and fouling problems experienced in Phase 1 plants; these new materials and designs were demonstrated to be suitable.
- As a result, we can approach the scale-up of the Phase II processes to commercial scale with reasonable confidence.

Overall Findings – DOE Program (6)

Direct Liquefaction Shown to Apply to a Wide Range of Coals

- One emphasis of the Phase II work was to apply direct liquefaction to low-rank coals. This is important, because it proved that the huge reserves of inexpensive western U.S. subbituminous coals make excellent liquefaction feedstocks.
 - Lignite, subbituminous, and bituminous coals from the eastern, mid-western, and western U.S. were shown to be suitable feedstocks. These represent the vast majority of U.S. coal resources.
- The Phase 2 work showed that direct liquefaction is a flexible process for sub-bituminous and other low rank coals.
- It was shown that direct liquefaction could be applied to a mixed feedstock containing coal and petroleum resids, heavy oil, or bitumen ("coprocessing"), and to coal and waste polymers. This allows a single plant to operate with the most economical feedstock available at a given place and time.

Overall Findings – DOE Program (7)

- Some specific issues that were originally significant problem areas, but that were moderated by improved materials, equipment, or process design during the development program include:
 - Overall plant reliability
 - Deashing
 - Product compatibility with conventional fuels
 - Let-down valve erosion
 - Preheater coking
 - Corrosion in distillation columns

Direct Coal Liquefaction Previous Designs

Direct Liquefaction Design Information

- **During the late 1970's and early 1980's designs were prepared for the one stage liquefaction processes**
 - Pilot Plants: H coal, EDS, SRC
 - Demonstration Plants: SRC-I, SRC-II, H-Coal
- **Baseline Design for Direct Liquefaction Plant**
 - May 1990 to February 1995
 - Bechtel / Amoco Contractors
 - Two Stage Liquefaction based on Wilsonville PDU
 - Plant capacity of roughly 60,000 barrels per day of liquid products plus C1 – C4 gases.
 - Considered both Bituminous and sub-bituminous coals

Direct Liquefaction Design Information (2)

- Development of the cost estimate and economics for
 - the base-line design
 - alternates for the coal liquefaction facility
 - compilation of equipment lists and utilities summary
 - development of scaling factors for equipment size and plant cost
 - development of the estimates for capital equipment, working capital, and owner's costs.
 - The economic analyses includes manpower requirements and operating costs
- Development of mathematical algorithms and models for equipment sizing, scaleup, costing, train duplication for incorporation into the ASPEN/SP simulation program.

Direct Liquefaction Design Information (3)

- **Development of an ASPEN/SP process simulation model of the baseline design.**
 - The model produces complete heat and material balances, elemental balances around each plant and the entire process complex,
 - a major equipment list and outline specifications for the plant sections, utility requirements, capital cost for all plants sections
 - a discounted cash flow economics model for the total complex.
 - The model is suitable for studying technology advances and options in a case study approach. The model does not feature optimization capabilities.

Direct Liquefaction Design Information (4)

Design information beyond Bechtel Study

- HRI Two stage CMSL liquefaction design
- NEDO pilot plant design and operation
- Shenhua Commercial plant design
- Headwaters conceptual designs for India and Indonesia
- Information in public domain is minimal

Comparison of Baselines

Baseline Design Basis:

The baseline design basis is based on the then available pilot plant run data generated at Wilsonville pilot plant facilities (run 257E). This run was deemed to represent the best reliable run with Illinois No. 6 coal.

Improved Baseline Design Basis:

While the baseline study was at the final stage of completion a separate set of data became available which are for a relatively higher space velocity through the liquefaction reactors. These data are based on Wilsonville run numbers 257J, 261B and 261D. In light of these data, the baseline design basis appeared to be rather conservative. Because of the potential favorable economic impact of the higher space velocity, a separate case was studied, and it was designated as the improved baseline design case. The key design basis assumptions for the improved baseline were developed jointly by DOE/PETC, Amoco, Bechtel, and Burns and Roe Services Corporation by utilizing collective experiences and the available data based on the experimental runs mentioned above.

The DCL Process is More Complex Than a Simple Schematic

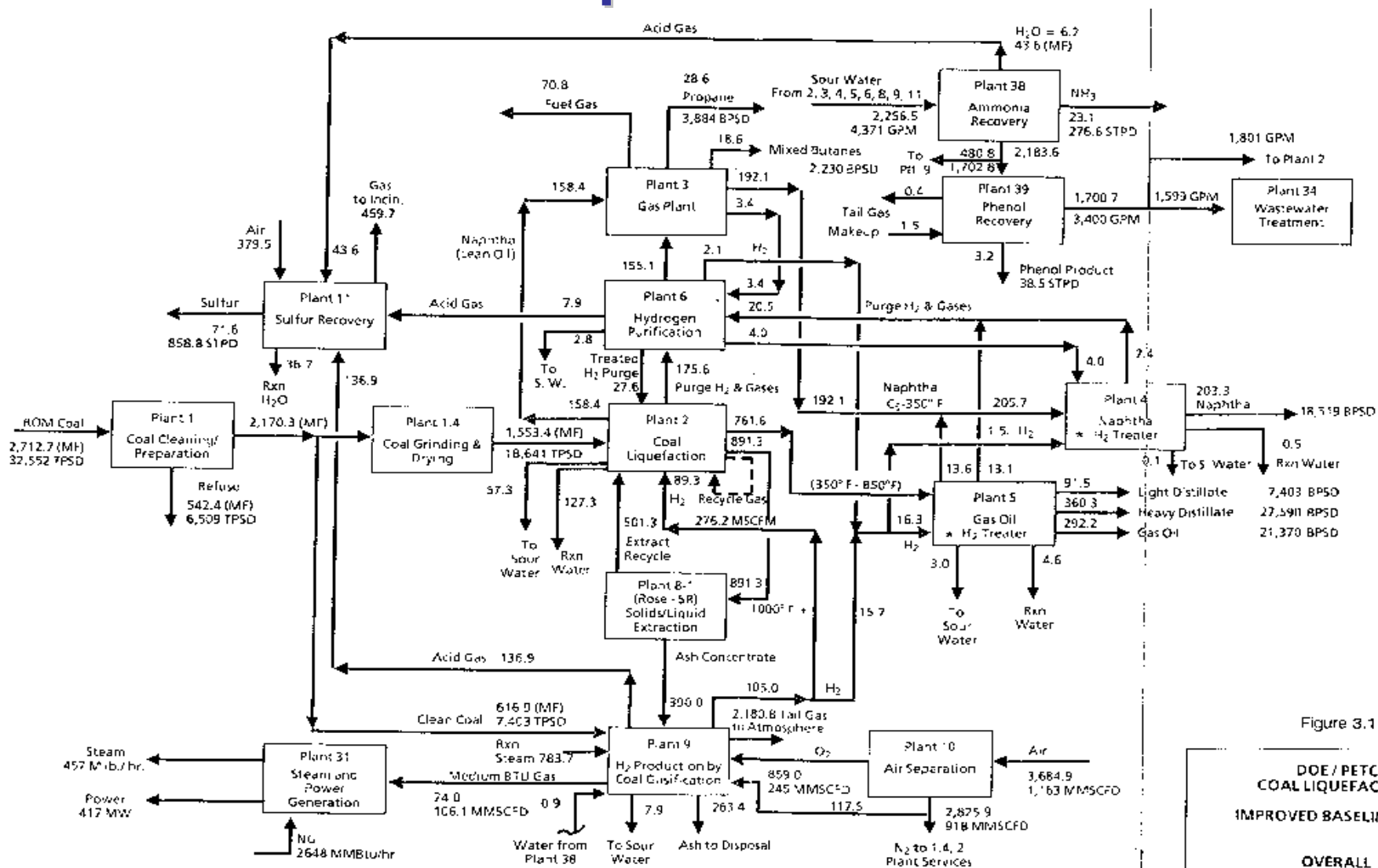


Figure 3.1

DOE / PETC
COAL LIQUEFACTION
IMPROVED BASELINE CASE

OVERALL
MATERIAL BALANCE

Notes:

1. Flow rates are in M³/HR unless noted and on dry basis
2. Minor streams including steam, water, sour water, and make up amine are not shown on this diagram
3. Flow rates around plants #38, 39, 34 are shown on wet basis

* H₂ Treater = Hydrotreater

DCL Reactor Operating Conditions

Key Operating Conditions for the Coal Liquefaction Reactor

	Wilsonville 257-J	Improved Baseline	Baseline
Coal SV, lb MAF/hr/lb Catalyst	2.17	1.95	1.12
Temp, °F			
Reactor 1	809	810	790
Reactor 2	760	760	760
Catalyst addition	3/1.5	3/1.5	3/1.5
Lbs/ ton MF coal each stage			
Solvent/MAF Coal	2.25	2.26	2.46
Resid in Solvent, wt%	50	50	50

DCL Product Yields

Overall Liquefaction Product Yields

Yields, wt%, MAF	Wilsonville 257-J	Improved Baseline	Baseline
H ₂ S + H ₂ O + CO _x +NH ₃	15.1	13.9	14.0
C1 – C3	5.4	5.5	4.8
C4 – 350 °F	14.5	15.8	16.9
350 – 450 °F	7.1	7.3	7.5
450 – 850 °F	44.2	48.1	46.8
C4+ Liquids	65.8	71.2	71.2
Resid	1.2	0.0	0.0
Organics in ash-concentrate	18.5	15.7	16.3
H ₂	(6.0)	(6.3)	(6.2)

Bechtel Capital Cost

Table 6
Nth Plant Capital Cost for the Complex
Baseline

Plant #	No. of Trains	ISBL Plant Field Costs 1000\$	ISBL Plant Adj. with OSBL Costs 1000\$	Installed Plant Costs 1000\$
1	5	91,000	131,000	160,800
1.4	10	87,500	126,000	154,600
2	5	932,200	1343,000	1,647,800
3	1	25,300	36,400	44,700
4	1	15,600	22,500	27,600
5	1	74,000	106,500	130,700
6	1	152,600	220,000	269,800
8	1	42,200	60,800	74,600
9	5	263,700	380,000	465,900
10	5	191,000	275,000	337,700
11	4	46,700	67,200	82,500
38	1	40,100	57,800	71,000
39	1	13,300	19,200	23,500
Total		1,975,200	2,845,400	3,491,200

Capital Cost Mid 1991 dollars

Bechtel Capital Cost (2)

Process Features	Variables	Baseline	Option Number
Coal Cleaning Method	<ul style="list-style-type: none"> • Jig • Heavy Media Separation • Spherical Agglomeration 	X	1 2
Reactor Configuration	<ul style="list-style-type: none"> • Catalytic-Catalytic • Thermal-Catalytic • Catalytic-Catalytic with Vent Gas Separator 	X	3 4
Vacuum Bottoms Processing	<ul style="list-style-type: none"> • ROSE-SR • Fluid Coking ⁽¹⁾ 	X	5
Hydrogen Production	<ul style="list-style-type: none"> • Coal Gasification (Texaco Technology) • Steam reforming of Natural Gas ⁽²⁾ 	X	6

(1) Coke from Coker is fed to Gasifier

(2) In this option the ash concentrate from the ROSE-SR unit goes to a fluid bed combustion unit

Bechtel Capital Cost (3)

Table 7
Nth Plant Capital Costs for the Complex
for Options

Op. No.	Option Description	Capital Costs \$ MILLION
1	Liquefaction Feed Coal Cleaning by Heavy Media Separation	3,293.2
2	Liquefaction Feed Coal Cleaning by Spherical Agglomeration	3,552.3
3	Thermal-Catalytic Liquefaction Reactor Configuration	3,427.0
4	Catalytic-Catalytic Reactor Configuration with Vent Gas Separation	3,326.7
5	Fluid Coking of Vacuum Bottoms	3,308.0
6	Stream Reforming of Natural Gas plus FBC* Unit for Hydrogen Production	2,782.7
7	Naphtha Reforming	3,345.8

* Fluid Bed Combustion

Bechtel Capital Cost (4)

Table 8
Nth Plant Capital Costs for the Complex
Improved Baseline

Plant #	No. of Oper. Trains	Total No. of Trains	ISBL Plant Field Costs 1000\$	ISBL Plant Cost Adj. with OSBL Costs 1000\$	Installed Plant Costs 1000\$
1	6	6	104,900	1,571,700	182,000
1.4	12	12	96,800	140,000	171,800
2	4	4	854,800	1,236,400	1,517,000
3	1	1	23,600	34,100	41,900
4	1	1	13,600	19,700	24,100
5	1	1	82,900	119,900	147,100
6	1	1	130,000	188,000	230,700
8	1	1	41,700	60,300	74,000
9	6	6	303,300	438,700	538,200
10	6	6	222,500	321,800	394,800
11	5	5	55,100	79,700	97,800
38	1	1	45,000	65,100	79,900
39	1	1	16,000	23,100	28,400
Total			1,990,200	2,878,500	3,531,900

Bechtel Capital Cost (5)

Table 11
Results on Economics

Case	COE \$/bbl
Baseline	38.55
Improved Baseline	33.45
Baseline with H2 from Natural Gas	36.00
Improved Baseline with H2 Production by Natural Gas Reforming	31.00

Bechtel Sub-bituminous Coal

Table 7

**Nth Plant Capital Costs for the Complex
Low Rank Coal Liquefaction with Hydrogen Production by Coal Gasification**

Plant	No. of Trains	ISBL Plant Field Costs, 1000\$	ISBL Plant Cost Adj. with OSBL Costs, 1000\$	Installed Plant Costs, 1000\$
1 & 1.4	10 & 4	186,500	265,000	344,600
2	4	792,400	1,125,900	1,464,200
3	1	19,200	27,300	35,500
4	1	9,500	13,500	17,600
5	1	114,000	162,000	210,600
6	1	232,800	330,800	430,200
8	1	33,400	47,500	61,700
9	5	353,000	501,600	652,300
10	5	184,600	262,300	341,100
11	1	10,200	14,500	18,800
38	1	45,200	64,200	83,500
39	1	17,300	24,600	32,000
Total		1,998,100	2,839,200	3,692,100

Capital Cost 4th Q 1993 dollars

Bechtel Sub-bituminous Coal (2)

Economics

Case	COE \$/bbl
Low Rank Coal with H ₂ Production by Coal Gasification	32.75
Low Rank Coal with H ₂ production from natural gas	33.85

Potential Technology Vendors

EPCs: Bechtel, Fluor, Kellogg, Parsons

Technology	Licensor	Process
Coal Liquefaction	Axens Accelergy Chevron Headwaters/HTI	H-Coal EDS CMSL
Bottom solid-liquid separation	Kerr McGee, ConocoPhillips, Exxon	ROSE™ de-asphalting Delayed Coking Fluid Coking
H2 (NG Reforming)	Foster Wheeler, Kellogg, ICI, Kvaerner, etc.	
H2 (coal Gasification)	GE, ConocoPhillips, Shell, Siemens, Lurgi, Southern Co.	
H2 Purification	UOP	PSA/Membrane
LPG Treating	UOP	Merox
Ammonia Removal	USX	Phosam-W
Phenol Removal	Koch-Glitsch	Dephenolization

Design Thoughts and Issues

- **Bechtel design does not include updated information for HTI PDU activities and post DOE work**
- **Carbon footprint was not considered**
- **Technical information and more recent designs probably done by Headwaters and Axens which would be helpful to update the baseline.**
 - Verification of data may be difficult without independent experimentation
- **Active technology developers Headwaters and Axens (subsidiary of IFP)**
- **Other Technology Developers are working on advanced direct liquefaction technology – not public knowledge**

Environmental Considerations

Illinois No. 6 Coal Analysis

<u>Proximate Analysis</u>	<u>wt.%</u>
Volatile Matter	33.0
Fixed Carbon	38.3
Ash	20.0
Moisture	8.7
<u>Ultimate Analysis</u>	<u>wt.% Dry</u>
Carbon	61.5
Hydrogen	4.2
Nitrogen	1.2
Sulfur	5.1
Chlorine	0.1
Ash	21.9
Oxygen (by difference)	6.0

Illinois No. 6 Coal Analysis (2)

Sulfur Forms

Pyrite	38.3
Sulfitic	20.0
Organic	8.7

Ash Composition

P2O5	0.1
SiO2	43.8
Fe2O3	24.1
Al2O3	17.1
TiO2	0.6
CaO	5.6
MgO	1.0
SO3	4.1
K2O	2.1
Na2O	0.6
Undetermined	0.7

Other Coal Constituents

Besides PAHs, coal also contains many toxic inorganic elements such as cadmium (Cd), arsenic (As), lead (Pb), selenium (Se), and mercury (Hg) that might be carried over into liquid fuel products.

U.S. Fuel Specifications (only a sample)

Spec	Calif. RFG (Average) http://www.arb.ca.gov/enf/fuels/phase3dates.pdf	On-Road Diesel http://0301.netclime.net/1_5/0/H/K/Efect%20of%20Gen49D%20on%20.pdf	JP-8 ConocoPhillips
Sulfur (PPMW)	15	15	3,000
Aromatics (% Vol.)	22	35	25
Benzene (% vol.)	0.7	-----	-----
Olefins (% vol.)	4	-----	-----
Cetane Number (Min)	-----	40(ASTM) (Engine Manufacturers: 42-45)	-----
Flash Point (°F, Min)	-----	-----	100 (JP-5: 140)
Freeze Point (°C, Max)	-----	-----	-47 (JP-5: 46)

Comparison of DCL and ICL Final Products

	Direct	Indirect
Distillable product mix	65% diesel 35% naphtha	80% diesel 20% naphtha
Diesel cetane	42-47	70-75
Diesel sulfur	<5 ppm	<1 ppm
Diesel aromatics	4.8%	<4%
Diesel specific gravity	0.865	0.780
Naphtha octane (RON)	>100	45-75
Naphtha sulfur	<0.5 ppm	Nil
Naphtha aromatics	5%	2%
Naphtha specific gravity	0.764	0.673

Final coal to liquid products meet stringent standards

Environmental Considerations

- **Baseline meets environmental standards as of 1990**
- **Waste streams addressed include:**
 - Solid waste
 - Waste water (organics including phenols)
 - Acid gases
- **Process equipment to meet the environmental standards included in baseline designs**
- **Solid waste and waste water use mainly standard equipment for petroleum processing or coal power plants – some novel processing**

National Coal Council Report

Plant Type	DCL	ICL Recycle	Hybrid
Coal Consumption STPD dry basis	23,044	32,305	25,514
Liquid Products			
Diesel	45,812	47,687	46,750
Naphtha	18,863	22,313	20,591
LPG	5,325	0	2,660
Total	70,000	70,000	70,001
Electric Power			
Import	282		
Export		1,139	45
Overall Efficiency (%)	60.1	47.4	58.7
Plant CO ₂ Generation (lbs/barrel)	783	1,972	1,010

National Coal Council Report (2)

Plant Type	DCL	iCL Recycle	Hybrid	Spec/Typical
				Conventional ULS Diesel
Diesel				
Specific gravity	0.865	0.78	0.821	0.82-0.85
Cetane	42-47	70-75	56-61	> 40
Sulfur (ppm)	< 5	< 1	< 3	< 15
Aromatics (%)	4.8	< 4	< 4.4	< 35
Heating Value (Btu/Gal)	138,100	129,800	133,950	138,700
Naphtha				
Specific gravity	0.764	0.673	0.717	0.72-0.78
Octane (RON)	> 100	45-75	75-95	85-95
Sulfur (ppm)	< 0.5	Nil	< 0.3	< 30
Aromatic (%)	5	2	3.5	< 27
Heating Value (Btu/Gal)	133,000	116,690	124,845	124,800

LTI Review of NCC Data

Preliminary for Discussion only

Plant Type	DCL	iCL Recycle	iCL Once-through	Hybrid
Coal Consumption STPD dry basis	23,044	32,305	37,974	25,514
Liquid Products				
Diesel	45,812	47,687	47,687	46,750
Naphtha	18,863	22,313	22,313	20,591
LPG	5,325	0	0	2,660
Total	70,000	70,000	70,000	70,001
Electric Power				
Import	282			
Export		1,018	1,139	45
Overall Efficiency (%)	60.1	48.4	47.4	58.73
Plant CO ₂ Generation (lbs/barrel)	783	1,557	1,972	1,010
Plant CO₂ Generation with sequestration for gasification	369	217	275	

Current Technology Developments

Shenhua DCL Project

DCL Scale-up and Commercial Development



Lawrenceville, NJ
30 bpd

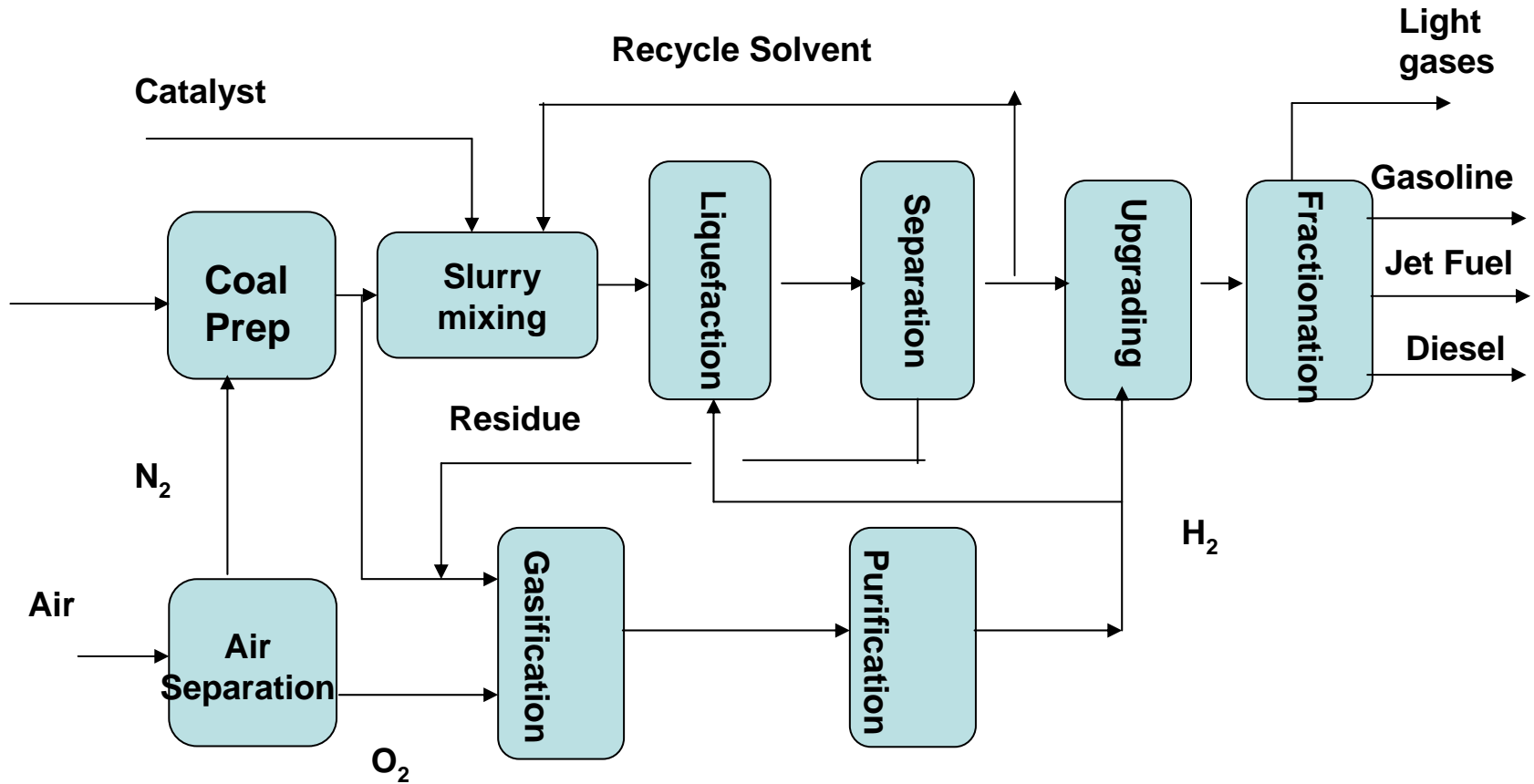


Catlettsburg, KY
1800 bpd



Inner Mongolia, China
17,000 bpd

Shenhua DCL Project



- Shenhua Direct Coal Liquefaction Process
- First Train: 1 MT/a Liquefaction oil

Axens H-Oil and Coal Liquefaction Reactors



H-Oil Reactors in Poland

CTLtec Americas 2008



Shenhua Liquefaction Reactors

Shenhua Plant



Speculations About Shenhua DCL Plant

- **Direct liquefaction**
 - Conversion and hydrocracking to oils
 - Two reactors in series
 - Purpose: conversion and hydrocracking to oils
 - slurry catalyst
 - Expanded bed reactors (probably slurry)
 - Solvent Hydro-treating (?) and upgrading
 - Ebullated Bed (H-Oil)
 - Hydrotreating
 - Recycle solvent hydro-treating (?)
 - Manufactured petroleum catalyst (Co-Mo or Ni-Mo)

Shenhua Patent

- According to a preferred embodiment of the invention, a test of direct coal liquefaction is performed using a low rank bituminous coal as feedstock, and the operation conditions and test results are as follows:
- Test operation conditions:
 - Reactor temperature: 1st reactor 455°C, 2nd reactor 455°C;
 - Reactor pressure: 1st reactor 19.0MPa, 2nd reactor 19.0MPa;
 - Slurry coal concentration: 45/55(dry coal/solvent, mass ratio);
 - Catalyst addition rate: Liquefaction catalyst: 1.0 wt %(Fe/dry coal);
 - Sulfur addition rate: S/Fe=2(molar ratio);
 - Gas/liquid: 1000NL/Kg slurry;
 - Hydrogen in the recycle gas: 85vol %.

Shenhua Patent (2)

The results of direct coal liquefaction of a low rank bituminous coal in a CFU test unit of the invention is shown in Table 1, wherein the figures in the table are based on MAF coal. The results of the same kind of coal tested in another direct coal liquefaction CFU is shown in Table 2, wherein the figures in table 2 are also based on MAF coal.

Table 1. Direct coal liquefaction results of a low rank bituminous coal in a CFU unit

	Conversion %	Oil yield %	Gas yield %	H ₂ O yield %	Organic residue %	H ₂ consumption %
Process of the invention	91.22	57.17	13.11	12.51	23.99	6.8

Table 2. Direct coal liquefaction results of a low rank bituminous coal in a CFU unit

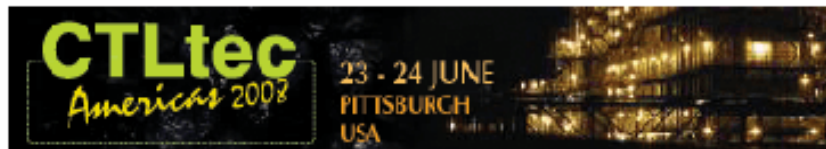
	Conversion %	Oil yield %	Gas yield %	H ₂ O yield %	Organic residue %	H ₂ consumption %
Process of the prior art	89.69	52.84	17.89	7.3	28.1	6.75

Shenhua Information on PDU

- **Coal to liquid fuels product data**
 - Naphtha product: 0.748-0.758 g/cm³
 - N < 0.5 ppm (wt)
 - Jet fuel: smoke point, 25mm, minimum
 - Naphthene < 0.1wt%
 - High density
- **Table of diesel product results**

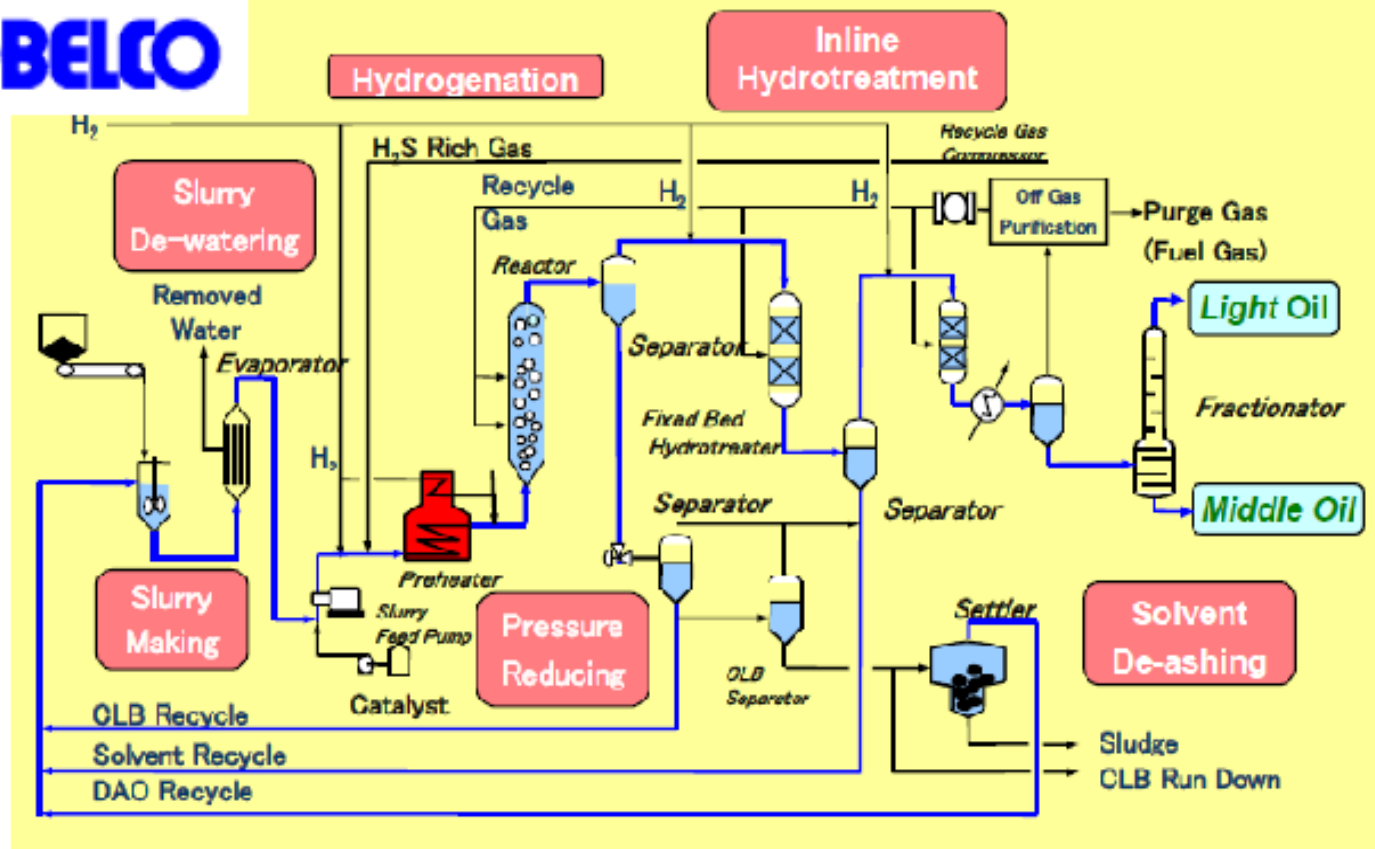
	Diesel A	Diesel B
Density	0.866	0.86
S (mg/g)	1.8 (< 5ppm)	< 5 ppm
Aromatics %	4.5	4.6
Carbon %	86.66	86.67
Cetane #	43.3	43.9

The Brown Coal Liquefaction Process



Improved Brown Coal Liquefaction (BCL) Process

KOBELCO



Brown Coal Liquefaction Process

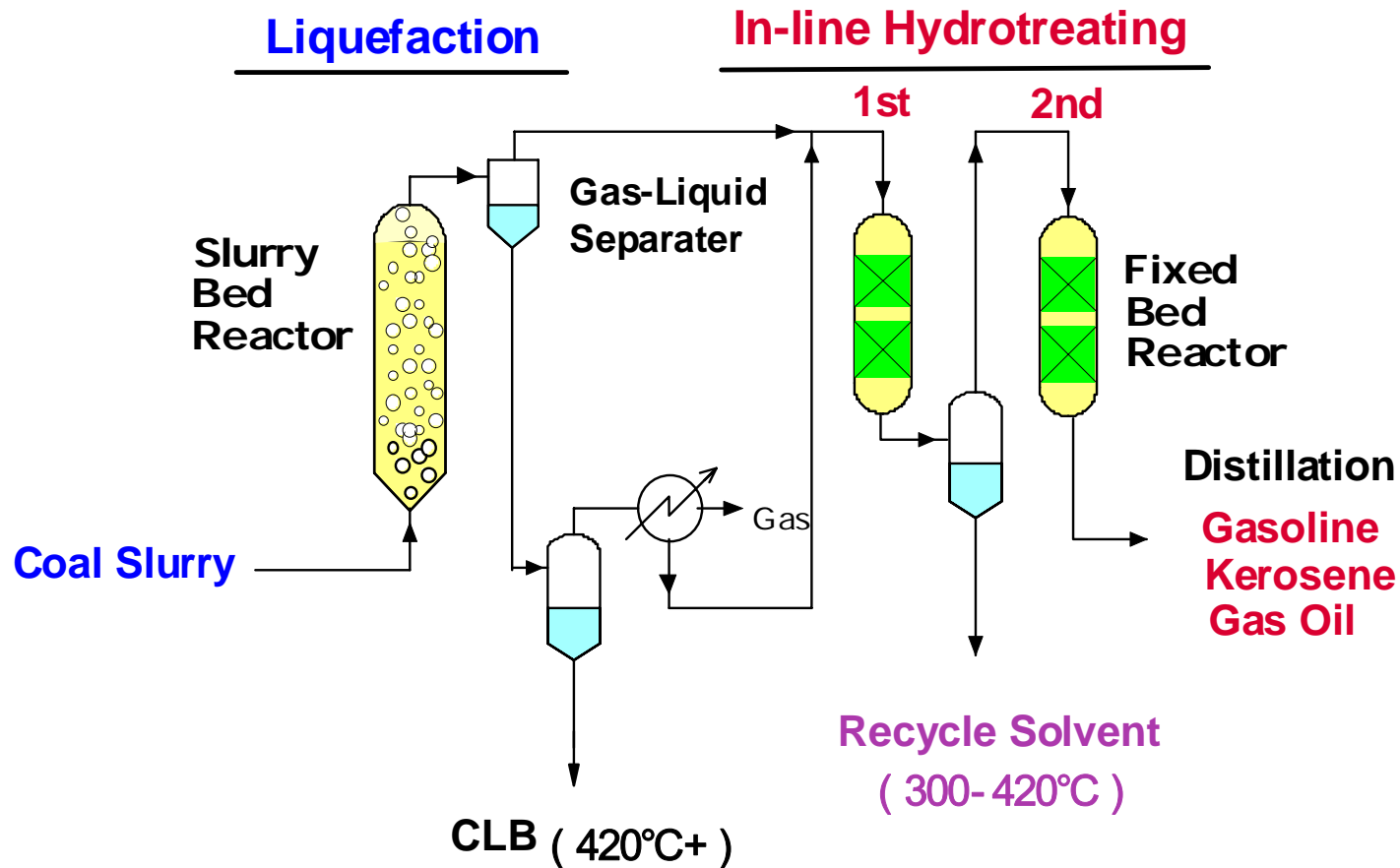


Fig. Conceptual flow of In-line hydrotreating section

Brown Coal Liquefaction Process (2)

- The BCL process was developed by NEDO of Japan to a 50 tonnes/day pilot-plant scale, constructed at Morwell in Victoria, Australia.
- The process is designed specifically to handle very low-rank coals such as those found in the Latrobe Valley of Victoria, which may contain >60% moisture.
- It was operated over the period 1985-1990, processing a total of ~60,000 tonnes of coal. Operations ceased in October 1990.
- The plant was decommissioned in 1991 and demolished in 1992.
- A crucial aspect is the efficient drying of the coal. The 50 tonnes/day rated throughput of the pilot plant required ~170 tonnes/day of raw coal to be processed.
- Following extensive pilot plant operation, R&D using a 0.1 tonnes/day bench-scale continuous liquefaction test facility and related equipment was carried out until 1997 to improve the reliability, economics and environmental compatibility of the coal liquefaction process.

Brown Coal Liquefaction Process (3)

- Based on the R&D results an improved BCL process was proposed. This comprises slurry de-watering, liquefaction, in-line hydrotreating, and de-ashing, with the following features:
 - use of a high-active and inexpensive catalyst such as limonite ore pulverized in oil
 - use of a heavy fraction solvent (bp 300-420°C)
 - adoption of coal liquid bottom (CLB) bp>420°C recycling
- Compared with the results of the pilot plant, the increase of oil yield, improvement of product oil quality and suppression of scale formation in reactors were proved using the bench-scale unit with <1% (dry ash-free coal) catalyst addition.
- It was estimated that the improved process could decrease the crude oil equivalent nominal price by 24% compared with the BCL process at the Australian pilot plant.
- Yields are stated to be 65% distillate.
- A new cooperation agreement was started between Japan (Sojitz) and Indonesia in 2005 to build a 27,000 BPD plant



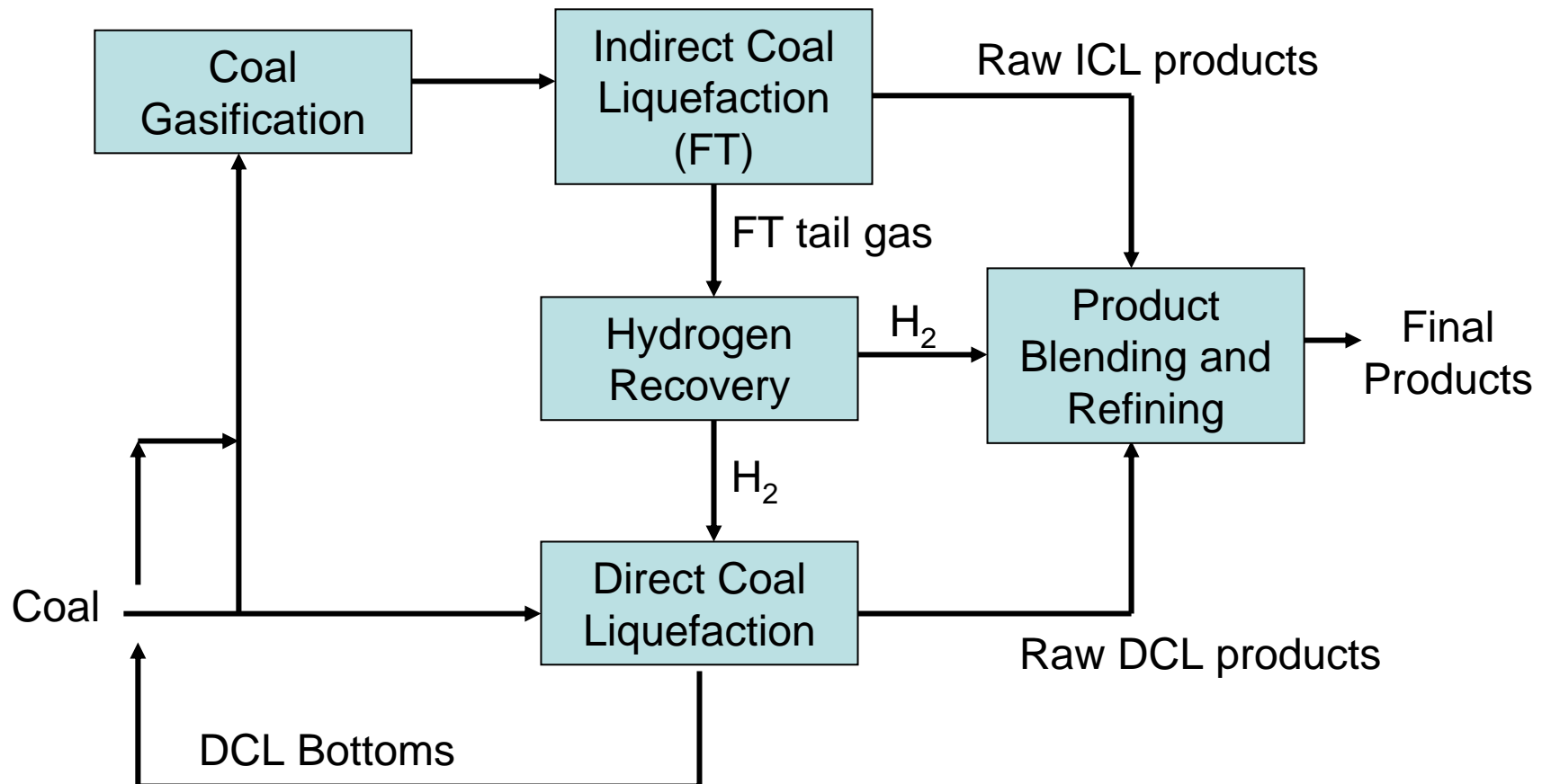
Specification of Products

	Unit	BCL Process Product	Industrial Standard	
			Indonesia	JIS
Gasoline				
Octane Number (RON)		min. 90	min. 88	min. 89
Sulfur Content	wt%	max. 0.005	max.0.2	
Kerosene				
Smoke Point	mm	min. 16	min. 16	min. 23
Sulfur Content	wt%	max. 0.005	max. 0.2	max. 0.015
Gas Oil				
Cetane Number		min. 45	min. 45	min. 45
Sulfur Content	wt%	max. 0.005	max. 0.5	max. 0.2

KOBELCO

Hybrid DCL/ICL Plant Concept

Hybrid DCL/ICL Plant Concept



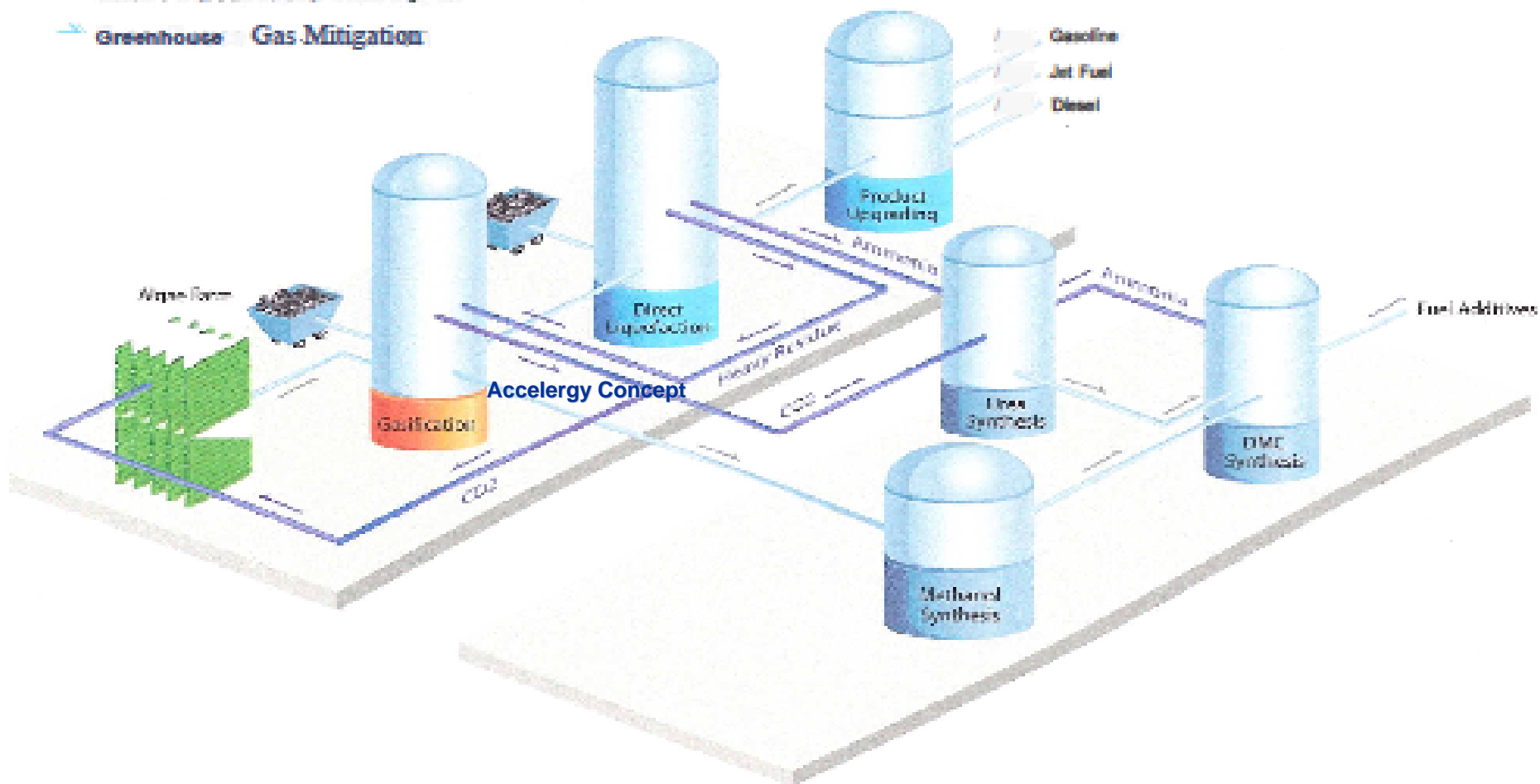
Hybrid Plant Theoretical Product Yields

- **C3-C4** **18 %**
- **F-T naphtha** **19 %**
- **DCL Naphtha** **26 %**
- **F-T diesel** **22 %**
- **DCL distillate** **10 %**
- **DCL VGO** **5 %**

Accelergy Concept

Accelergy Concept

- Microcatalytic Coal Liquefaction to Fuel
- DMC Fuel Additive Production
- Greenhouse Gas Mitigation



LTI

Thoughts and Comments

Potential Merits of Direct Coal Liquefaction

- DCL produces high octane gasoline
- DCL has higher thermal efficiency than indirect liquefaction
- Literature suggests that DCL with no CCS may have a lower carbon footprint
- Opportunity for combined coal and renewable energy processes with improved carbon footprint and carbon management
- Synergistic opportunities
 - Hybrid direct/indirect technology integration
 - Coprocessing with biomass (Hydrogen production)
 - Coprocessing with heavy oil/refinery bottoms/wastes(?)

Thoughts and Issues

- LTI reviewed documents/analyses of direct liquefaction technology, design and current data where available
- General findings and conclusions
 - Review of the past DOE R,D&D program generally agrees with the analysis and findings of Burke, Gray and Winschel, et al (2001)
 - Significant progress has been made in achieving improved yield of distillate and product quality
 - Reliability of operation of components has been increased

Thoughts and Issues (2)

- Operation issues and readiness are still believed to be less than Indirect technologies and are a major concern
- Bechtel design for bituminous and sub-bituminous coals were thoroughly done and are authoritative
 - Were based on Wilsonville data and are still considered reasonably up to date, however:
 - Capital cost and economics must be revised
 - To the extent possible recent HTI and other data should be considered
 - Carbon footprint and carbon management were not considered

Thoughts and Issues (3)

- HTI CMSL data with highest distillate results and later experimentation at the bench scale with coal and coal and other feedstocks (mixed plastics) needs further evaluation at the PDU scale to be considered highly reliable (this may have been done by HTI and others after the DOE program)
- Recent HTI results (for example) would meet current specifications for diesel and gasoline after significant hydrotreating

Thoughts and Issues (4)

- Bechtel Baseline Design (1993) does not include updated information for HTI PDU activities and post DOE work
- Post Bechtel design information particularly CMSL provides hope for increased distillate but this is confounded by the many variables that effect yields and the small scale at which the data was generated
- The low sulfur and nitrogen content of the distillate achieved in the CMSL was due to in-line hydrotreating and lighter distillate
- Technical information and more recent designs probably done by Headwaters and Axens would be helpful to update the baseline.
 - Verification of data may be difficult without independent experimentation
 - Technology developers Headwaters and Axens (subsidiary of IFP) are actively seeking partners for direct liquefaction projects
 - It also appears that Shenhua, Sojitz as well as others are in some stage of planning or marketing their technology

Thoughts on Present Concepts

- There is still competition for what is the preferred direct liquefaction Technology
- NEDO and Accelergy (possibly) are proposing single stage liquefaction through the primary use of a hydrogen donor solvent treated in a separate reactor
- Shenhua is supporting a combination of dispersed catalyst for liquefaction (single stage) and may be utilizing hydrogen donor solvent catalytically hydrotreated in separate reactors (H-Oil)
- HTI (and others?) are supporting two stage liquefaction (separate stages for coal dissolution and upgrading of the resulting oils). The technology likely incorporates use of either manufactured catalyst or dispersed catalyst
- Concepts are either providing a distillate crude for refinery upgrading or producing specification gasoline, diesel, jet fuel products. In either case, in-hydrotreating is being used in current technology.

Thoughts on Present Concepts (2)

- It appears that current direct liquefaction distillate products can meet the existing fuel standards
- Concepts must have a strategy for waste product (liquefaction bottoms) use or disposal
- Configurations with liquefaction, upgrading, hydrotreating and ash separation will produce high yield, good quality products but are complex, highly integrated and capital intensive
- Need carbon management strategy, e.g. capture and sequestration of carbon produced during hydrogen production and/or use of renewable energy for hydrogen production or cofeeding

Thoughts on Present Concepts (3)

- Other technology developers are working on advanced direct liquefaction technology – not public knowledge
- Similar to other complex conversion technologies, EPC contractors are available
 - Need track record in complex and large (multi \$ billion) projects
- Specialized high pressure equipment vendors for reactors and components (slurry pumps, let-down valves) are limited and probably foreign based (India/China)
- Shenhua could be useful source of information – material may not be available to public. WVU could facilitate obtaining information.

Direct Liquefaction Technical Needs

- Advanced concepts
 - Reduce carbon footprint
 - Combination coal and renewable energy concepts
 - Co-feeding concepts
 - Less severe processing
 - Lower capital and process cost
- Product integration with refinery or finished distillate products
- Component material and reliability studies

System Analysis Needs

- Perform carbon LCA for DCL using available data (Bechtel design study, e.g.) and compare with ICL
- Compare carbon LCA for two stage liquefaction with advanced one stage with separate reactor for hydrogenation of recycle hydrogen donor solvent
- Evaluate advanced concepts with reduced carbon footprint
 - Determine the benefits for producing hydrogen from non-carbon producing sources including biomass
 - Determine the benefits of hybrid concepts (combined direct and indirect liquefaction)
 - Determine the direct liquefaction opportunities for carbon capture and storage and other carbon management techniques

System Analysis Needs (2)

- Direct Liquefaction Data Validation
 - Evaluate and confirm direct liquefaction data post DOE program
 - Two-stage liquefaction current concepts
 - Single stage
 - Compare catalyst and reactor types for direct liquefaction
 - Ebullated or slurry reactors
 - Manufactured or dispersed catalysts
 - Verify improved DCL product quality results (beyond that achieved in DOE program)

System Analysis Needs (3)

- Shenhua Plant Operation
 - Confirm process operation (yields & quality)
 - Evaluate component reliability
 - Improve understanding of process configuration
 - Recognize that data may not be available in the public domain

R&D Needs

- Verify by R&D Process and Product improvements
 - Verify improved DCL product quality results (beyond achieved in DOE program)
 - Hybrid Studies
 - Process and product optimization
 - Product characterization and compatibility
- Verify liquid products meet health and safety standards for commercial use
- Explore technologies to reduce water consumption
- Evaluate potential technologies that offer lower life cycle carbon footprint
 - Use of renewable feedstock or energy for hydrogen or synthesis
 - Integration with carbon management techniques

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