

SECTION 15

DESIGN DATA BASE

This section describes the basic data used in the POGO conceptual plant design, and how they were used.

Data for some of the process steps were limited. In some instances, the data were for laboratory runs at conditions differing from those required by the design. Extrapolations were made on what was considered to be the most realistic basis.

15.1 HYDROLIQUEFACTION DATA BASIS

The Tacoma, Washington, pilot plant has operated successfully on the SRC II process for as much as 61 days continuously. Product with sulfur content in the range of 0.3 to 0.4% was produced.

Table 15-1 presents the design dissolver balance on which the SRC portion of POGO is based. This balance was calculated from Tacoma pilot plant data.¹⁸

Tacoma has reported successful operations with solvent-to-coal ratios of 2 or less, with solvent being defined as the total weight of the recycle streams, including both liquids and solids. This design is based on a more conservative total solvent-to-coal ratio of 3. Reduction of the solvent-to-coal ratio to a value of 1.5 would be expected to reduce the fixed capital investment and required product selling prices by 3 to 5%.

Concurrent with the development of the conceptual design reported here, the DOE Tacoma, Washington, pilot plant was operating using the SRC-II mode of operation.¹⁹ Comparisons of the POGO design with recent pilot plant results were made. The recent pilot plant results are primarily concerned with Unit 12, Coal Dissolving. This unit represents 10 to 15% of the total fixed capital investment (FCI); analysis shows that changes to this unit can result in changes to the product required product selling price of + 5%.

Illustrative comparisons of the POGO design with recent pilot plant experience are:

<u>Item</u>	<u>POGO Design</u>	<u>Recent Pilot Plant Experience</u>	<u>Economic Impact</u>	<u>Remarks</u>
Coal Dissolver	37 lb coal/hr-ft ³	23-28 lb coal/hr-ft ³	Increase FCI	Maximum coal feed rate yet to be determined
Solvent-to-Coal Ratio in Coal Dissolver Feed	3:1	2:1	Reduce FCI	
Dissolver Operation	Inlet T=700°F Outlet T=850°F no H ₂ quench gas injection	Inlet T=800°F Outlet T=850°F H ₂ quench gas injection for cooling	Increase FCI	
Hydrogen Consumption in Coal Dissolving	5.3 wt% on coal	3.8 wt% on coal	Reduce FCI	
Product Composition	Summarized in Report	Slightly less net products	Increase FCI to maintain total product quantity	

The results of the comparison indicate that the effects are counterbalancing and the net change in fixed capital investment, and required product selling prices, is essentially zero when the POGO design is adjusted to incorporate the recent pilot plant results.

Pilot plant tests are continuing. It is possible that the results will show that the coal feed rate to the dissolver should be increased and that both the coal feed rates and the dissolver feed solvent-to-coal ratios used in the POGO design are conservative; the result would be reduction in fixed capital investment and required product selling price.

15.2 FLASH PYROLYSIS

The efficiency and economics of a number of alternatives were analyzed before the combination of SRC hydroliquefaction process and pyrolysis was selected as the final design configuration of POGO.⁸ The addition of the pyrolysis process to the SRC hydroliquefaction process has the advantage of inexpensively producing additional liquids, gas, and char from coal. The char can be gasified to generate hydrogen required for hydroliquefaction of coal in the dissolver and for upgrading liquids in the hydrotreating units of the complex. The heavy oil fractions and unreacted coal from the SRC process can be pyrolyzed to produce additional gas, tar, and char, avoiding at the same time the costly and troublesome filtration procedure. The concurrent pyrolysis of coal and coal tar would also result in increased yield of volatile matter.⁸ No credit has been taken for this enhancement of yield when oil and coal pyrolysis are simultaneously effected.

Table 15-1 - Design Dissolver Balance

Input, lb								
Composition	C	H	N	S	O	Ash	Total	HHV
MF coal	71.52	4.91	1.36	3.91	9.28	6.32	97.30	
H ₂ O w/coal		0.30			2.40		2.70	
H ₂		4.86					4.86	
Total	71.52	10.07	1.36	3.91	11.68	6.32	104.86	
Output, lb								
C ₁	3.64	1.22					4.86	
C ₂	2.42	0.61					3.03	
C ₃	3.28	0.72					4.00	
C ₄	1.62	0.33					1.95	
CO ₂	0.30	-			0.80		1.10	
H ₂ S	-	0.17		2.57	-		2.74	
NH ₃	-	0.04	0.21	-	-		0.25	
H ₂ O	-	0.61	-	-	4.86		5.47	
Light oil	5.31	0.96	0.02	0.02	0.41		6.72	
Wash solvent	6.20	0.83	0.05	0.02	0.50		7.60	
Process solvent	13.17	1.45	0.18	0.05	0.94		15.79	
SRC	32.94	2.82	0.61	0.17	1.46		38.00	
Mineral residue	2.64	0.31	0.29	1.08	2.71	6.32	13.35	
Total	71.52	10.07	1.36	3.91	11.68	6.32	104.86	
Composition								
MF coal	73.50	5.05	1.40	4.01	9.54	6.50	100.00	13,245
Light oil IBP-400°F	79.01	14.29	0.30	0.30	6.10	-	100.00	19,894
Wash solvent 400-500°F	81.58	10.92	0.66	0.26	6.58	-	100.00	18,139
Process solvent 500-950°F	83.41	9.18	1.14	0.32	5.95	-	100.00	17,377
SRC 950°F+	86.68	7.42	1.61	0.45	3.84	-	100.00	16,930
Mineral residue	19.78	2.32	2.17	8.09	20.30	47.34	100.00	3,070
Heat of Reaction - 215.3 Btu/lb AR Coal								

15.2.1 DATA BASIS

Flash pyrolysis offers the simplicity and relatively low cost required for a rapid commercialization of a coal liquefaction process. The reaction time in the pyrolyzer at pyrolysis temperature is short (less than a second) and therefore the liquid yields obtained are relatively high. The pyrolysis is conducted at 500 psig in order to avoid the expensive step of pressurizing the char to the gasifier.

Yields and properties of volatile products and char from flash pyrolysis of coal at 500 psig and 110°F were developed on the basis of data from two processes:

- (1) Occidental Research and Development Flash Pyrolysis Process
- (2) COED Fluid Bed Pyrolysis Process

Both processes operate at essentially atmospheric pressure. Since flash pyrolysis at elevated pressure reduces liquid yields,²⁰ estimates were made to reflect the change in liquid yield with increased pressure. The following procedure was used to develop the design yield structure:

- (1) Yields from Flash Pyrolysis - The Occidental Research Process uses finely ground Kentucky bituminous coal, which is similar to the Illinois No. 6 base coal, used as the base case in the POGO plant design. The coal is exposed to a high temperature (1100°F) for a short period of time (1 second).²¹ The high heating rate of the particles and rapid quench of products result in liquid yields significantly higher than those observed in the COED process, or in yields that would be predicted from standard tests of the volatile matter content of the coal.

It has been assumed that the basic yield pattern from flash pyrolysis of coal at elevated pressures is the same as that at atmospheric pressure, but that, due to vapor pressure considerations, only a part of the liquid product may be vaporized during pyrolysis. The remainder of the liquid is essentially coked in-place on the coal particles. Thus, the problem of estimating pressurized flash pyrolysis yields becomes one of performing a liquid flash vaporization, and then estimating coking yields from the remaining liquid. We judge this to be a model that agrees with the effect of pressure on carbonization yields reported in the literature,^{20,22} and it should predict actual pressurized process yields.

- (2) Since relatively little data were presented on tar properties from the Occidental process, COED data were used for a tar distillation curve. A split of the tar distillation curve was made for the process conditions of 500 psig and 1100°F. Light ends were assumed to be a direct or primary product, and heavy ends were subject to coking conditions. Gas,

liquid, and solid yields from coking of this heavy cut were based on standard correlations²³ and the coking products were assumed for convenience, to have the same properties as the primary gas, tar light ends, and char. Coking products were then added to the primary products.

- (3) Finally, an elemental balance was performed for the complete flash pyrolysis process. Occidental product compositions were used as guidelines to compositions of the pressurized flash pyrolysis process products. In some cases, small adjustments were made in yields and analysis to allow closure of the elemental balances. Final yields and elemental balances for pressurized flash pyrolysis are given in Table 15-2. Standard heats of combustion and calculated heats of combustion (Dulong formula) were used to calculate the heat of reaction. Slight readjustments of Dulong heat-of-combustion values were used to give an overall heat-of-reaction of 500 Btu/lb of volatile products, reported in the literature.⁵
- (4) In the POGO plant, both the condensed pyrolysis tar and the SRC liquid product are subjected to atmospheric and vacuum distillation, leaving a vacuum bottoms stream containing solids. This stream is also fed to the pyrolysis reactor, producing additional gases, liquids, and solids. The yields from the flash pyrolysis of this slurry feed were calculated by applying coking correlations, as before, to the liquids, and calcining the solid portions of the feed. Elemental and heat balances were also performed (as above) with adjustments to give the same heat of reaction. Table 15-3 summarizes the vacuum slurry bottoms conversion.

The above procedure for estimating yields from pressurized flash pyrolysis is based on what is believed to be a satisfactory model of such a process. Flash pyrolysis at elevated pressure is considered a viable process. It is believed that the proportions of products may vary as much as $\pm 20\%$ from the predictions developed here. This in turn would affect the overall plant balance, which must balance hydrogen needs for SRC and hydrotreating (which includes hydrotreating pyrolysis liquids) with hydrogen generating capability from char gasification. Swings in pyrolysis yields have double effects on the hydrogen balance, since greater liquid yields would occur simultaneously with lower char yields, and vice versa. However, these swings are expected to affect less than 15% of the hydrogen required for the calculated plant balance, with about 85% being unchanged. Therefore, the effect on overall economics should be slight, and the single-point design is expected to be representative of the proposed process scheme economics within reasonable limits of uncertainty.

A recommendation was made to ERDA (DOE) to obtain experimental data on coal pyrolysis at the conditions selected for the POGO design. A small scale laboratory program is underway under DOE sponsorship at Oak Ridge National Laboratory. Very preliminary initial results indicate general corroboration of the yields employed in this design. Pilot plant data are advisable for an optimum commercial plant design.

Table 15-2 - Pressurized Flash Pyrolysis Yields for Coal Feed

Basis: 10,000 Tons Per Day Feed Coal (2.7% moisture)
All Figures are Tons Per Day.

Feed/Yield	Composition						
	C	H	N	S	O	Ash	Total
Stream Feed Coal	7152.00	491.00	136.00	391.00	928.00	632.00	9730.00
Water in Coal	-	30.21	-	-	239.79	-	270.00
Total	7152.00	521.21	136.00	391.00	1167.79	632.00	10,000.00
Products							
H ₂	-	26.25	-	-	-	-	26.25
CH ₄	249.09	83.62	-	-	-	-	332.71
C ₂ H ₄ ^a	25.69	4.31	-	-	-	-	30.00
C ₂ H ₆	40.61	10.23	-	-	-	-	50.84
C ₃ H ₆	39.72	6.67	-	-	-	-	46.39
C ₃ H ₈	36.21	8.10	-	-	-	-	44.31
C ₄ H ₁₀	11.16	2.34	-	-	-	-	13.50
CO	29.16	-	-	-	38.84	-	68.00
CO ₂	64.95	-	-	-	173.05	-	238.00
N ₂	-	-	19.00	-	-	-	19.00
H ₂ S	-	5.56	-	88.44	-	-	94.00
H ₂ O	-	50.69	-	-	402.31	-	453.00
Tar	1911.12	172.92	22.06	42.93	222.97	-	2372.00
Char	4744.29	150.52	94.94	259.63	330.63	632.00	6212.00
Total	7152.00	521.21	136.00	391.00	1167.79	632.00	10,000.00

^aOlefins estimated from COED data.

Table 15-3 - Pressurized Flash Pyrolysis Yields from Vacuum Bottoms Slurry Feed

Products	Yields Wt%
H ₂	0.17
CH ₄	2.84
C ₂ H ₄	0.08
C ₂ H ₆	0.51
C ₃ H ₆	0.18
C ₃ H ₈	0.49
C ₄ H ₁₀	0.07
CO	0.46
CO ₂	1.30
N ₂	0.41
NH ₃	0.16
H ₂ S	0.50
H ₂ O	1.30
Tar	4.79
Char	<u>86.74</u>
Total	100.00

15.2.2 OTHER DESIGN FACTORS

Other flash pyrolysis design factors are:

- (1) Flash pyrolysis is accomplished in an entrained-type bed upflow reactor operating at 1100°F and 500 psig. Residence time in the reactor is 0.7 seconds.
- (2) The ratio of recycle carrier gas to solids in the pyrolyzer is 1:7 (weight basis). Solids are defined as the total weight of oil slurry and coal. Linear velocities at the bottom and the top of the pyrolyzer are 78 ft/sec and 44 ft/sec correspondingly.

- (3) Heat for pyrolysis is obtained by means of a circulating stream of hot pyrolysis char, which transports heat from the process gasifier to the pyrolyzer. This heat transport requires the circulation of 24,000 TPD of char, which is 2.5 times the fresh char production rate of 9,645 TPD.
- (4) The high char circulation rate is also beneficial for preventing: (a) agglomeration tendency in the feed coal, (b) agglomeration tendency of the char due to the effect of coating of char particles with the oil injected in the pyrolyzer.

15.3 PROCESS GASIFICATION

Medium pressure steam/oxygen gasification of pyrolysis char was used to produce a hydrogen-rich synthesis gas to supply hydrogen for dissolving, naphtha hydrotreating, and heavy liquid hydrotreating. In addition, the gasifier supplies heat to pyrolysis through a circulating char stream. The gasifier is an entrainment-type, slagging, two-stage design. The gasifier heat and material balances were calculated using basic kinetic, thermodynamic, and composition data for gasification. The results from this calculation, together with information developed by Bituminous Coal Research (BCR) provided the basis for prediction of the gasifier reaction products and yields.

The gasifier operating pressure of about 500 psig was chosen to facilitate the transfer of char to and from the pyrolysis unit. This circulating char stream is heated to about 1800°F in the second stage of the gasifier. The hot char is separated from the gases and recycled to pyrolysis. Thus, the gasifier operates very similarly to a pebble heater with respect to the circulating char stream.

This system should be piloted in order to confirm the conceptual design and to provide data for an optimum commercial plant design.

15.4 FUEL GAS GENERATION

The fuel gas required for process furnaces and power plant gas turbines is generated by gasifying coal in a medium pressure, slagging, oxygen-blown, two-stage gasifier. This gasifier was designed to operate at a pressure of 400 psig in order to move the gas through the downstream acid gas removal system and to the point of use. Calculations for this gasifier are similar to that for the process gasifier. The process utility balance determined the required coal feed rate of 16,700 TPD.

15.5 PRODUCT POST-TREATMENT

The naphtha from the pyrolyzer and the SRC processes is hydrotreated and reformed to produce the gasoline product. The higher boiling liquids are hydrotreated to produce a low sulfur distillate fuel oil and a residue that is thermally cracked and coked to produce a high quality coke product. These operations are discussed in the following subsections.

15.5.1 NAPHTHA REFORMING

The heavy naphtha (200°F to 400°F boiling range) from the naphtha hydrotreater is reformed to produce a suitable stock for gasoline blending. The reformer operating conditions and yields are based on information supplied by Englehard Industries,²¹ and published information on reforming of coal-derived liquids.⁵

15.5.2 HEAVY LIQUID HYDROTREATING

The total heavy liquid (400°F to 1200°F) from the pyrolysis and the SRC processes is hydrotreated to produce a desulfurized, distillate fuel oil product, and a higher boiling liquid fraction, which is thermally cracked and coked. The operating conditions and yields were based on a previously published design for hydrotreating of coal-derived liquids.^{8,20,24} The distillate fuel oil product contains 0.04% by weight sulfur and less than 0.10% by weight ash.

15.5.3 THERMAL CRACKING

The fractionator bottoms from the fuel oil hydrotreater are thermally cracked to produce gas, naphtha-range material, and thermal tar, suitable for production of coke. The thermal cracking yields are based on information from the Technical Advisory Committee (of the Petroleum Industry War Council), TAC Report TML-16. The unit employs a tubestill process with a reaction chamber. Fuel oil and the gas oil delivered from it, are cracked in two separate heaters and the cracking of the combined outlet streams is completed in a reaction chamber at 930°F and 400 psig. The thermal tar product contains 0.03% by weight sulfur and has a boiling point range and gravity appropriate for a coker feedstock.