APPENDIX 4.   LIQUIDS FROM COAL BY PYROLYSIS.

Pyrolysis of coal involves   low temperature carbonisation whereby coal is decomposed into gases, liquids and char.   Three such processes have been developed: the TOSCOAL, Garrett and COED processes.   The TOSCOAL process was developed by The Oil Shale Corporation as an extension of a process for retorting oil shale in which the energy for pyrolysis is supplied by circulating hot ceramic balls.   The Garrett flash pyrolysis process requires rapid heating of coal in order to maximise the production of gas while producing tar oil and char.   Hot recycled char provides heat for coal devolatilisation.   Most information has been published about the COED process and it will be considered in the greatest detail in this report.

The COED (Char Oil Energy Development) process was developed by the FMC Corporation under contract to the Office of Coal Research of the U.S. Department of the Interior.   The process is a multi-stage fluidised bed pyrolysis producing oil, gas and char.   Dried, crushed coal is treated in four fluidised bed stages at successively higher temperatures until a major fraction of the volatile matter of the coal is evolved.   Heat for this pyrolysis is obtained by burning a portion of the char with oxygen in the last stage.   Hot gases from the last stage then flow countercurrently to the coal and constitutes the fluidising gas and heat supply for the third and second stages.   Hot char from the fourth and third stages is recycled to supplement the heat from the gases.   The first stage fluidising medium is supplied by burning a portion of the char or gas with air.   Gas and oil are recovered by cooling the volatiles from pyrolysis.   Catalytic hydrogenation of the oil product yields a synthetic crude oil suitable as a refinery feedstock.   Product gas can be reformed to hydrogen (for use in hydrotreating oil) or pipeline gas.   The char can be burned as a boiler fuel for power generation (but is likely to contain substantial amounts of sulphur) or can be gasified to pipeline gas in the Cogas process.   A more detailed description of the COED process is given elsewhere[1].

A pilot plant processing 33 tonnes of coal/day was built and operated
successfully with continuous runs of up to 29 days. A unit hydrogenating
oil was also successfully operated using COED-derived oil. About 90%
of the oxygen, nitrogen and sulphur in the feed oil was removed. In
addition, the C:H ratio of the oil was reduced and some cracking of
heavier molecules occurred. Solid particles in the oil were removed by
pressurised filtration which reduced the solid content of the oil from
about 8.6% to less than 0.5% by weight. Oil recoveries in filtration
were greater than 95%. Using highly volatile bituminous Colarado coal,
the average oil yield was 18.5% by weight and char yield was 59.5% by
weight.

Because of the probable low value of char (although the calorific value
of char is only slightly less than that of the parent coal, it contains
about the same amount of sulphur and may not be suitable for burning in
power stations on environmental grounds) it seems reasonable to consider
a scheme where char is converted to a more saleable product such as gas.
Based on results from FMC's pilot plant, Shearer[2] has produced a
conceptual design and economic study for a plant which combines the COED
pyrolysis process with a low-pressure version of the Kellogg molten salt
process to gasify char. The scheme proposed by Shearer will be used as
the basis of this analysis.

For comparison a second scheme was considered where char was not further
processed but was sold as such, presumably to a utility for electricity
generation. By eliminating the gasification process, the total plant
energy requirements are reduced, and, because of the convention adopted
whereby all plant energy requirements are apportioned to the products
according to calorific value, GER and NER of synthetic crude will be reduced.
In order to investigate the magnitude for this effect, a scheme suggested
by Eddinger et al[9] was considered.

4.1. PYROLYSIS WITH CHAR GASIFICATION.

4.1.1. INPUTS

4.1.1.1. Coal

In Shearer's scheme the pyrolysis plant is self-sufficient in energy using only coal for fuel and generating electricity and meeting the requirements for plant fuel, hydrogen and oxygen on-site.[2]

Shearer estimated that a plant producing $7.08 \times 10^6 m^3$ of pipeline gas and 27,275 bbls of synthetic crude oil per stream day would require a daily coal input of 28,455 tonnes of Illinois No. 6 coal (as received i.e. 10% moisture) having a calorific value of 26,040 MJ(th)/tonne. Of this mass of coal 5,461 tonnes would be used by on-site facilities (together with flue gas) in producing process steam, feed water for boilers and electricity. The total electrical power requirement of the plant was estimated as 362.817 Mw, equivalent to a primary energy requirement of 1.045×10^8 MJ(th) or 4013 tonnes of coal equivalent per stream day. A further 895 tonnes of coal would be burnt in a furnace supplying heat for coal drying and for the first pyrolysis stage. The remaining 22,099 tonnes of coal would be fed to the coal dryer and thence to the first pyrolysis stage. 1818 tonnes of oxygen are required per stream day for the combustion of a fraction of the char to provide process heat (from estimated power requirements of the oxygen plant one can calculate the energy requirement of oxygen as 2.45 GJ(th) of primary energy/tonne). Hydrogen requirements were estimated at 344 tonnes ($\approx 3.8511 \times 10^6 m^3$) per stream day for the hydrogenation of the 2500 bbls of raw oil produced by pyrolysis per day. Shearer's estimate of hydrogen requirements of the plant ($154 m^3$/bbl) is 50 to 100% higher than measured hydrogen consumptions from pilot plant and process development unit[1, 3]. Hydrogen would be produced by steam reforming of product gas.

Calorific value of total coal input = $28,455 \times 26,040 = 7.4097 \times 10^8$ MJ(th)/ steam day.

4.1.1.2. Capital equipment

Shearer estimated the cost of his conceputal design plant as $(US 1973) 439m. From US wholesale price indices[4] for the machinery and equipment sector

$(US 1973) 1.0 = $(US 1968) 0.85 and

$(US 1968) 2.4 = £(1968) 1.0

Also Casper et al[5] give the energy requirement of the outputs of a number of heavy engineering sectors as about 220 MJ(th)/£(1968). Thus if the plant is on-stream for 90% of its 20 year lifetime, and 50% of its initial costs are allowed for maintenance, then energy requirement of capital equipment

$$= 1.5 \times 439 \times 10^6 \times \frac{0.85}{2.4} \times 220 \times \frac{1}{20 \times 365 \times 0.9}$$

$$= 7.809 \times 10^6 \text{ MJ(th)/stream day}$$

4.1.1.3. Catalysts and Chemicals

Shearer estimated that the requirement of sodium carbonate (for the molten salt gasifier) would be 564 tonnes/stream day and that the cost of other chemicals and catalyst would be about $(US 1973) 2.45m/year. Harris[6] gives the energy requirement of sodium carbonate as 17.15 GJ(th)/tonne. US wholesale price indices for "chemicals and allied products" gives

$(US 1973) 1.0 = $(US 1968) 0.91 and

$(US 1968) 2.4 = £(1968) 1.0

Casper et al[5] give the energy intensity of 'general chemicals' as 702 MJ(th)/£(1968), and thus, assuming that the plant is on stream for 90% of the time,

energy requirement of chemicals =

$$564 \times 17150 + \frac{1}{365 \times 0.9} \times 2.45 \times 10^6 \times \frac{0.91}{2.4} \times 702 = 11.66 \times 10^6 \text{MJ(th)/stream day}$$

4.1.1.4. Water Requirements

Shearer estimated the maximum water requirement of the plant in his conceptual design as 40,200 US gallons/minute, equivalent to 7.70 tonnes of river water per tonne of coal processed.

4.1.2. OUTPUTS

In Shearer's conceptual design of a COED pyrolysis plant with char gasification, the main products are 27,275 bbls of synthetic crude oil and 7.08×10^6 m^3 of pipeline gas per stream day. In lieu of any specific data, the synthetic crude oil produced by pyrolysis and subsequent hydrogenation will be assumed to be similar to syncrude from oil shales, viz, having a calorific value of 6120 MJ(th)/bbl with 7 bbl/tonne[7]. Shearer gives the calorific value of product gas as 34.31 MJ(th)/m^3. In addition, 1900 bbl/stream day of light hydrocarbons (calorific value of 4120 MJ(th)/bbl), 941 tonnes sulphur/ stream day (calorific value of 9240 MJ(th)/tonne and replacement energy requirement of 400 MJ(th)/tonne[8]) and 36 tonnes/st. day phenols (calorific value ~ 3700 MJ(th)/tonne and replacement energy requirement of 50,850 MJ(th)/tonne)[8] are produced. Thus, apportioning the energy inputs for the plant between the products, the energy requirement of synthetic crude oil (per tonne) is a fraction of the total energy inputs to the plant given by

$$\frac{7}{27,275} \quad \frac{27,275 \times 6120}{27,275 \times 6120 + 7.08 \times 10^6 \times 34.31 + 1900 \times 4120 + 941 \times 400 + 36 \times 50850}$$

$$= 1.020 \times 10^{-4}$$

The thermal efficiency of the process, defined as the ratio of the total calorific value of the products to the total calorific value of the inputs, is calculated to be 57.6%.. The thermal efficiency of pyrolysis would be somewhat higher for a scheme in which the 10,227 tonnes of char (calorific value of 25,635 MJ(th)/tonne) was not gasified, but, as mentioned previously it seems more realistic to consider a process which produces saleable products. Shearer suggested that the thermal efficiency of the COED process producing oil, gas and char may approach 90%. Shearer further suggested that the thermal efficiency of the process (including char gasification) could be raised to about 65% by using a high pressure molten salt gasifier rather than the low pressure process used in his design but no details were presented.

4.2.   PYROLYSIS WITHOUT CHAR GASIFICATION.

Eddinger et al[9] have examined the economics of a commercial COED plant in Utah producing synthetic crude oil, pipeline gas and char for sale.   The conceptual design was based on information gained from operation of the process development unit (1 tonne/day) and the pilot plant (33 tonne/day).   The plant is assumed to be sited near the coal mine, which supplies Utah A-seam coal (calorific value of 31400 MJ(th)/tonne of dry coal, moisture content 6% as received).

4.2.1.   INPUTS.

4.2.1.1. Coal.

According to Eddinger's design, the plant would process 3.18×10^6 tonnes of Utah A-seam coal (as received) per year or 9636.4 tonnes/day for 330 operating days/year.   (equivalent to 9091 tonnes dry coal/stream day)

Thus the calorific value of the daily coal input is given by

$$9636.4 \times 31400 \times \frac{100}{106} = 285.46 \times 10^6 \text{ MJ(th)/stream day}$$

Further coal will be required for electricity and oxygen production (cf 4.2.1.2,   4.2.1.3.)

4.2.1.2. Electricity

From the process economics it is possible to calculate the estimated electrical requirements for Eddinger's plant as 574,400 kWhe.   If it is now assumed that this electricity is generated on-site from coal at 30% generating efficiency, the additional amount of coal is given by

$$574,400 \times 3.6 \times \frac{100}{30} \times \frac{1}{31400} = 219.5 \text{ tonnes dry coal/stream day.}$$

4.2.1.3. Oxygen.

Again from the process economics given by Eddinger et al one can calculate the plant requirement for oxygen as 794.3 tonnes/stream day. Harris[6] gives the energy requirement of oxygen as 6.33 GJ(th)/tonne and if it is assumed that this energy requirement can be met from coal, the additional amount of coal required is given approximately by

$$794.3 \times 6330 \times \frac{1}{31400} = 160.1 \text{ tonnes dry coal/stream day}$$

4.2.1.4. Capital Equipment.

Eddinger et al estimated the capital cost of their plant as $(US 1970) 32.70m. From US wholesale price indices[4] for the machinery and equipment sector

$$\text{\$(US 1970) 1.0} = \text{\$(US 1968) 0.93} \quad \text{and}$$

$$\text{\$(US 1968) 2.4} = \text{£(1968) 1.0.}$$

Casper et al[5] give the energy intensity of the outputs of a number of heavy engineering sectors as about 220 MJ(th)/£(1968). Thus if the plant operates for 20 years and 50% of initial costs are allowed for maintenance, then, energy requirement of capital equipment

$$= 1.5 \times 32.7 \times 10^6 \times \frac{0.93}{2.4} \times 220 \times \frac{1}{20 \times 330}$$

$$= 0.63 \times 10^6 \text{ MJ(th)/stream day.}$$

Although the plant envisioned by Eddinger et al is much smaller than that of Shearer (Appendix 4.1.) and the process is considerably simpler, the energy requirement for capital equipment calculated above seems to be rather low. However since it represents only a small input to overall energy requirements, no attempt will be made to refine the estimate.

4.2.1.5. Water.

Eddinger et al estimated that their plant would require 8000 gallons/
min of cooling water, 1300 gallons/min of process water and 370
gallons/min of boiler feed water, equivalent to a total water requirement
of 6.6 tonnes of water /tonne of coal processed.

4.2.2. OUTPUTS

Eddinger et al estimated that a plant processing 9091 tonnes of dry
Utah A-seam coal per stream day (with an additional 379.6 tonnes of
coal for electricity and oxygen requirements) would produce 14,200 bbls
of synthetic crude oil ($\equiv$ 2028.6 tonnes with calorific value of 43000
MJ(th)/tonne), 4781.8 tonnes char (calorific value 19520 MJ(th)/tonne[10])
and 1.10×10^6 m^3 of gas (calorific value of 21.46 MJ(th)/m^3). It will
be noted that no hydrogen is required in this scheme, nor is any sulphur
or ammonia produced. Most of the impurities in the parent coal occur in
the product char. As before, by partitioning the plant requirements
between the products according to calorific values, the fraction which
must be apportioned to the production of synthetic crude oil is given by

$$\frac{2028.6 \times 43,000}{2028.6 \times 43000 + 4781.8 \times 29520 + 1.10 \times 10^6 \times 21.46}$$

$$= \quad 0.346$$

The thermal efficiency of the process can also be calculated, and if
the coal assumed to be used for electricity and oxygen needs is
included, the thermal efficiency of this COED pyrolysis scheme without
char gasification is 84.7%. This is considerably higher than the
57.6% thermal efficiency of Shearer's scheme (Appendix 4.1.2.). However
the largest product of Eddinger's scheme is the high sulphur char which,
as mentioned before, may be of little use as such, on environmental grounds.

REFERENCES

(1) Jones, J.F., Schoemann, F.H., Hamshar, J.A. and Eddinger, R.T., 'Char Oil Energy Development', Dec. 1971, 336 pps, available as NTIS reference no. PB-234-168.

(2) Shearer, H.A., 'The COED Process Plus Char Gasification', Chemical Engineering Progress, V69, n3, March 1973, pp 43-49.

(3) Hendrickson, T.A. (ed), 'Synthetic fuels data handbook', Cameron Engineers (Denver, Colorado,) 1975, p.187.

(4) US Department of Commerce, Bureau of the Census, 'Statistical Abstracts of the United States', 96th Annual Edition (1975) pp 418-9.

(5) Casper, D.A., Chapman, P.F. and Mortimer, N.D., 'Energy Analysis of the "Report on the Census of Production, 1968", Open University Report No. ERG 006, Nov. 1975.

(6) Harris, P. (Energy Technology Support Unit, Harwell), personal communication. Calculations made from data obtained from Engelhardt, H.R., Jülich report no. JUL-966-RG, June, 1973.

(7) Hemming, D.F., "Energy Requirement for the Production of Synthetic Crude Oil from Colarado Oil Shales', Open University Research Report ERG 012, May 1976.

(8) Appendix 5.2.2., Table 2.

(9) Eddinger, R.T., Strom, A.H., and Bloom, R., 'A Synthetic Fuels Industry Based on Rocky Mountain Coals', Quarterly of Colorado School of Mines, V65, n4, Oct 1970, pp 183-200.

(10) Lantz, P.M., 'Process Data for Coal Liquefaction Processes-Part I' available on NTIS reference no. ORNL-TM-4789, May 1975.

APPENDIX 5.   FISCHER - TROPSCH PROCESS FOR CONVERTING COAL TO LIQUID
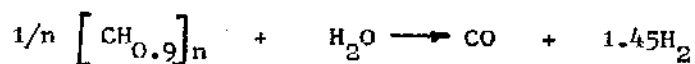
PRODUCTS

Plants based on the Fischer-Tropsch process were successfully operated in Germany during World War II and have been operated commercially at Sasolburg in South Africa for the past 20 years. The process has been investigated in the United States where conceptual designs and economic evaluations have been carried out.

There is an inherent inefficiency involved in the Sasol process whereby coal is broken down to $CO + H_2$ by reaction with steam and then the small molecules are rebuilt to yield mainly liquid products and, solely on the grounds of thermal efficiency it would seem to be an unlikely candidate for the production of liquid fuels from coal on a large scale. However at present the Sasol plant is the only commercial operation in the world, converting about 5000 tonnes coal/day to liquid products and with a known and tried technology it may well be that other Fischer-Tropsch plants will be built.

5.1.   Theoretical efficiency of the Fischer-Tropsch process yielding synthetic petrol.

For the purpose of this exercise it will be assumed that synthetic petrol is represented by n-octane and that it is produced in two separate stages. Synthesis gas $(CO + H_2)$ is first produced and this is then recombined to form the desired product.

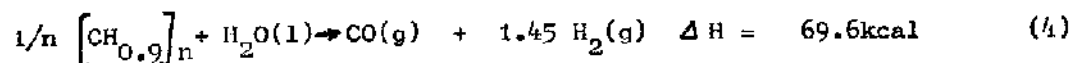The production of synthesis gas from coal can be represented as

$$1/n \left[CH_{0.9} \right]_n + H_2O \longrightarrow CO + 1.45H_2$$

and the heat of reaction can be determined using Hess' law as follows:

$$\frac{1}{n}\left[CH_{0.9}\right]_n + 1.225\ O_2(g) \rightarrow CO_2(g) + 0.45\ H_2O(l) \quad \Delta H = -97.0\ kcal \quad (1)$$
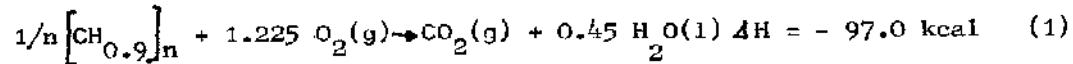
(calculated from calorific value of MAF coal)

$$CO(g) + \tfrac{1}{2} O_2(g) \longrightarrow CO_2(g) \qquad \Delta H = -67.6\ kcal \qquad (2)$$

$$H_2(g) + \tfrac{1}{2} O_2(g) \longrightarrow H_2O(l) \qquad \Delta H = -68.3 kcal \qquad (3)$$

$$\left[equ\ (1)\right] - 1.45\ x\left[equ\ (3)\right] - \left[equ\ (2)\right] \quad gives:$$

$$\frac{1}{n}\left[CH_{0.9}\right]_n + H_2O(l) \rightarrow CO(g) + 1.45\ H_2(g) \quad \Delta H = 69.6 kcal \qquad (4)$$

Thus it can be seen that the production of synthesis gas is endothermic and heat would have to be supplied (by combustion of coal in <u>oxygen</u> so that nitrogen is not introduced).
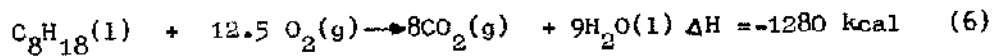
The theoretical energy requirement for synthesis gas can now be estimated. From equ (4) one can calculate that the production of 1 tonne of synthesis gas requires 0.4175 tonnes MAF coal + 9424 MJ(th) of process heat which can be obtained by the combustion of 0.300 tonnes MAF coal. Combustion must be in presence of oxygen (rather than air) so as to exclude nitrogen, and is given by

$$\frac{1}{n}\left[CH_{0.9}\right]_n + 1.225\ O_2 \rightarrow CO_2 + 0.45\ H_2O \qquad (5)$$
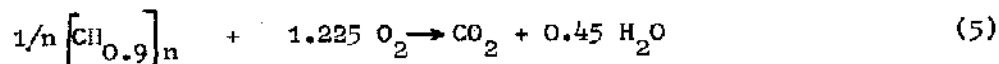
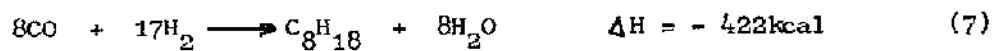from which one can calculate the oxygen required for the combustion of 0.2996 tonnes MAF coal as 0.910 tonnes. Thus the minimum requirements for producing 1.0 tonne synthesis gas are 0.7171 tonnes MAF coal (at 31,460 MJ(th)/tonne) 0.910 tonnes oxygen (at 6330 MJ(th)/tonne[6]) and 0.583 tonnes water, giving a minimum energy requirement of 28.3GJ(th)/tonne. From plant data given elsewhere[9] one can <u>estimate</u> an actual

energy requirement for synthesis gas produced from coal of about 32 GJ(th)/ tonne.

To determine the heat of the reaction synthesising n-octane, a calorific value for petrol of 47000 MJ(th)/tonne has been used. Thus

$$C_8H_{18}(l) \ + \ 12.5 \ O_2(g) \longrightarrow 8CO_2(g) \ + \ 9H_2O(l) \ \Delta H = -1280 \ \text{kcal} \qquad (6)$$

Then, $\left[\text{equ (2)}\right]$ x 8 + $\left[\text{equ (3)}\right]$ x 17 - $\left[\text{equ (6)}\right]$ gives

$$8CO \ + \ 17H_2 \longrightarrow C_8H_{18} \ + \ 8H_2O \qquad \Delta H = - \ 422\text{kcal} \qquad (7)$$

Thus the reaction synthesising n-octane is highly exothermic and this heat must be dissipated and can be used for steam raising.

From equation (14), (5) and (7) it follows that to produce 114 tonnes C_8H_{18} requires:

$$\left.\begin{array}{l} 103.2 \text{ tonnes MAF coal} \\ 144 \text{ tonnes } H_2O \\ 69.6 \text{ x } 8 \text{ x } 10^6 \text{ kcals process heat} \\ 224.9 \text{ tonnes oxygen} \end{array}\right\} \text{ to yield synthesis gas}$$

$$+ \ 10.8 \text{ tonnes } H_2$$

producing 422×10^6 kcal surplus heat in the synthesis reaction.

For Illinois No.6 coal (MAF)   103.2 tonnes = 3.2467×10^6 MJ(th) - excluding energy requirements of mining, crushing, drying etc.

Process heat (supplied at 100% efficiency) = 1.3297×10^6 MJ(th) = 74.05 tonnes MAF coal.

For oxygen, energy requirement (@ 6.33 GJ/tonne[6]) of 224.9 tonnes = 1.4238×10^6 MJ(th).

Raising water to steam at $100^{\circ}C$ requires a minimum of 2679 MJ(th)/tonne and this is included in the heat of reaction of equations (3) and (4), but boiler efficiencies are not included.

Thus <u>heat required due to boiler efficiency</u> (say 80%)

$$= \left(\frac{100}{80} - 1\right) \times 144 \times 2679 = 0.0964 \times 10^6 \text{MJ(th)}$$

The theoretical minimum energy requirement for hydrogen is calculated in App 2.1.1.1.1. as being 143,000 MJ(th)/tonne.

Thus <u>energy requirement for hydrogen</u> $= 10.8 \times 143,000 = 1.5444 \times 10^6 \text{MJ(th)}$

If 50% of the waste heat of the synthesising reaction can be recovered for steam raising, the energy requirements would be reduced by 0.8828×10^6 MJ(th).

Thus the minimum theoretical energy requirement for producing synthetic n-octane from Illinois No.6 coal by Fischer-Tropsch reaction, taking into account boiler efficiency and partial heat recovery but assuming zero coal mining costs, 100% conversion efficiency and zero gas losses is given by

$$\frac{1}{114} \left[3.2456 + 2.3297 + 0.0964 + 1.5444 + 1.4238 - 0.8828 \right] \times 10^6$$

$$= 68,040 \text{ MJ(th)/tonne. } \left[\text{thermal efficiency of } 69\% \right]$$

$\left[$If <u>all</u> reaction heat is recovered and no boiler losses, energy requirement of synthetic n-octane $= 47000$ MJ(th)/tonne $\equiv$ calorific value$\right]$.

If one now makes more realistic assumptions about efficiencies such as energy efficiency of coal mining of 96%[1], efficiency of hydrogen production at 60% of the optimum[2] and coal conversion at 70% efficiency[7,8] $\left[\text{due to}\right.$ heat and gas losses$\left.\right]$, then the energy requirement of n-octane is given by

$$\frac{1}{114} \left[\frac{100}{70} \left\{ 3.2456 \times \frac{100}{96} + 2.3297 + 0.0964 \right\} + \frac{100}{60} \times 1.5444 + 1.4238 - 0.8828 \right] \times 10^6$$

$$= 100,090 \text{ MJ(th)/tonne } \left[\text{thermal efficiency } = 47\% \right]$$

5.2   Conceptual Design of a Sasol-type Process for the Production of Motor Spirit from Coal.

Based on actual operating data from the Sasol plant in South Africa, Chan[3] has prepared a conceptual design of a plant producing primarily motor spirit but also a range of other chemicals, and his report has been used in this analysis.

5.2.1. INPUTS

5.2.1.1   Coal

In fueling a plant nominally producing 44,500 bbls/stream day of motor spirit and other hydrocarbon liquids, Chan[3] estimated the coal input as 31,135 tonnes/stream day of Western U.S. coal of which about 40% is used for steam and power generation.   The calorific value of this coal was given as 640.998×10^6 MJ(th).

5.2.1.2   Plant and Capital Equipment

Chan[3] estimated the cost of the Sasol-type plant (including on-site power plant) as $ (US 1975) 533m.

From US wholesale price indices for the machinery and equipment sector[4]

$$\text{\$(US 1975) 1.0} = \text{\$(US 1968) 0.65 and}$$

$$\text{\$(US 1968) 2.4} = \text{£(1968) 1.0.}$$

Casper et al[5] give the energy intensity of the outputs of a number of heavy engineering sectors as about 220 MJ(th)/£(1968).   Thus if it is assumed that the plant is on-stream for 90% of its 20 year lifetime, and 50% of initial costs are allowed for maintenance, then energy requirement of plant and equipment

$$= 1.5 \times 533 \times 10^6 \times \frac{0.65}{2.4} \times 220 \times \frac{1}{20 \times 365 \times 0.9}$$

$$= 7.251 \times 10^6 \text{ MJ(th)/stream day.}$$

5.2.1.3   Catalyst and Chemicals

Chan[3] estimated the annual cost of catalyst and chemicals as $(US 1975) 8m.   Again, using US wholesale price indices[4] for "chemicals and allied products" gives

$$\$(US\ 1975)\ 1.0 = \$(US\ 1968)\ 0.55,\quad and,$$
$$\$(US\ 1968)\ 2.4 = \£(1968)\ 1.0$$

Casper et al[5] give the energy intensity of "general chemicals" as 702 MJ(th)/£(1968) so that, assuming the plant is on-stream for 90% of the time,

energy requirement of catalyst
$$and\ chemicals = 8.0 \times 10^6 \times \frac{0.55}{2.4} \times 702 \times \frac{1}{365 \times 0.9}$$

$$= 3.918 \times 10^6\ MJ(th)/stream\ day.$$

5.2.2   OUTPUTS

Based on the Sasol plant in South Africa, Chan's[3] conceptual design of a plant producing motor spirit also produces a wide range of organic chemicals.   The range of organic chemicals.   The range of products are listed in Table 2   with production rates, calorific values and replacement energy requirements.   By convention , the energy requirements of a process producing a number of products are partitioned on the basis of calorific values for fuels and on the basis of replacement energy requirements (i.e. the energy required to produce a material by the usual method) for non-fuel products.   Thus from Table 2 it can be seen that the energy requirement of motor spirit (MJ(th)/tonne) is given by the following fraction of the overall plant energy requirement per stream day:

$$\frac{1}{2862.03} \left[\frac{134.516}{(134.516 + 7.374 + 5.506 + 8.638 + 98.232 + 1.470 + 0.199 + }\right.$$
$$\left.\frac{}{3.391 + 0.360 + 0.430 + 1.261 + 0.284 + 7.580 + 17.468 + 0.060)} \right]$$

$$= 1.6390 \times 10^{-4}\ (\equiv 46.91\%)$$

TABLE 2   PRODUCTS FROM CHAN'S CONCEPTUAL DESIGN OF A

SASOL-TYPE PROCESS FOR MOTOR SPIRIT FROM COAL.

Product	Production Rate (tonnes/stream day)	Replacement Energy Requirement[6] (GJ(th/tonne)	Total Calorific Value $(x10^6$ MJ(th))	Total Energy Requirement $(x10^6$ MJ(th)
Motor Spirit	2862.03	-	134.516	-
Diesel Oil	169.96	-	7.374	-
Waxy Oil	129.24	-	5.506	-
LPG	175.16	-	8.638	-
Tar, Oil Naphtha	1768.08	-	98.232	-
Acetone	28.909	50.85	0.881	1.470
Methanol	3.742	53.08	0.084	0.199
Propanol	52.71	64.33	1.767	3.391
Methyl Ethyl Ketone	7.309	49.22	0.246	0.360
i-Butanol	5.956	-	0.215	0.430*
n-Butanol	17.52	-	0.630	1.261*
n-Pentanol	4.08	-	0.142	0.284*
Phenol	149.07	50.85	0.552	7.580
Ammonia	313.55	55.71	6.995	17.468
Sulphur	150.08	0.40 (mining, crushing)	1.387	0.060

*Since for those alcohols where data was available the energy requirement was of the order of twice the calorific value, these figures were estimated from given calorific values on the same basis.

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APPENDIX 6   PRODUCTION OF METHANOL FROM COAL

Methanol can be produced from coal by gasification followed by
direct methanol synthesis from carbon monoxide and hydrogen.
Three such coal gasification processes have been proved commercially -
the Lurgi, the Koppers/Totzek and the Winkler processes, all of which
require the treatment of coal with steam and oxygen.   These processes
are described in detail elsewhere[1, 2].

Gasification reactions require high temperatures ($900-1400^{\circ}C$).   Higher
temperatures favour the production of synthesis gas while lower
temperatures result in the production of significant amounts of methane.
High pressures also favour the production of methane.   The Lurgi
process operates at substantially higher pressures than either the
Koppers/Totzek or the Winkler processes and produces, in addition to
synthesis gas, substantial amounts of methane (up to 33% of the quantity
of synthesis gas produced), ammonia, naphtha, phenol and tars[3].

In each of the gasification processes, the reaction of coal with steam
is according to the following reaction:

$$C + H_2O \longrightarrow CO + H_2 \qquad \Delta H = + 31.4 \text{ kcal (at } 25^{\circ}C) \qquad (1)$$
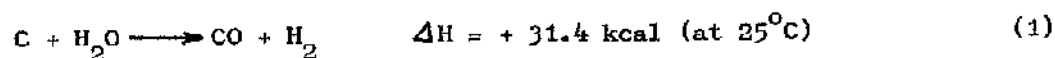
This reaction is very endothermic, and the heat required can be provided
in a number of ways, one of which is the combustion of coal itself (in
the presence of oxygen to avoid the dilution of synthesis gas with
nitrogen if air were used):

$$C + O_2 \longrightarrow CO_2 \qquad \Delta H = 94.1 \text{ kcal (at } 25^{\circ}C) \qquad (2)$$
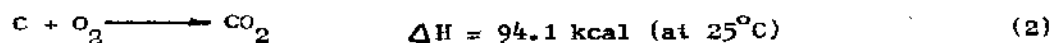
Methanol is then formed according to the following reactions:

$$CO + 2H_2 \longrightarrow CH_3OH(g) \qquad \Delta H = -21.7 \text{ kcal} \qquad (3)$$

$$CO_2 + 3H_2 \longrightarrow CH_3OH + H_2O \qquad (4)$$
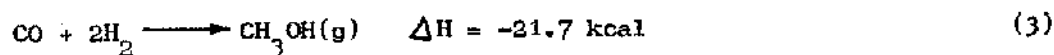
In the original high-pressure process, pressures of 300 atmospheres at
$200^{\circ}C$ were used in the presence of a zinc-chromium oxide catalyst,
and yields of over 60% were obtained.   In 1968, ICI developed a low-

pressure process using 50 atmospheres at 250°C and a highly selective, copper-based catalyst. This process produces much purer methanol, but is much more sensitive to catalyst poisoning by sulphur than the high pressure process.

Chan[4] has prepared a conceptual design of a plant producing methanol from coal via synthesis gas as in the Sasol plant in South Africa. His report has been used in this analysis to estimate energy and material requirements of the process.

6.1 INPUTS

6.1.1 Coal

In fueling a plant producing 10,121 tonnes of methanol/stream day, Chan[4] estimated the total coal input as 28,904 tonnes/stream day of Western U.S. coal having a total calorific value of 594.68×10^6 MJ(th).

6.1.2 Plant and Capital Equipment

Chan[4] estimated the cost of a plant producing 10,121 tonnes methanol/ stream day as $(US 1975) 472m. As before (Appendix 5.2.1.2)

$$\$(US\ 1975)\ 1.0 = \$(US\ 1968)\ 0.65$$

$$\$(US\ 1968)\ 2.4 = \pounds(1968)\ 1.0$$

and energy intensity of capital equipment = 220 MJ(th)/$\pounds(1968)$

Thus, if the plant is on stream for 90% of its 20 year lifetime, and 50% of initial costs are allowed for maintenance,

$$\text{energy requirement of plant and equipment}$$
$$= 1.5 \times 472 \times 10^6 \times \frac{0.65}{2.4} \times 220 \times \frac{1}{20 \times 365 \times 0.9}$$

$$= 6.42 \times 10^6 \text{ MJ(th)/stream day}$$

6.1.3 Catalyst and Chemicals

Chan[4] estimated the annual cost of catalyst and chemicals as $(US 1975)6m and using a similar calculation to that in Appendix 5.2.1.3 gives

energy requirement of catalyst & chemicals = 2.94×10^6 MJ(th)/stream day

6.2 OUTPUTS

The products expected in Chan's[4] conceptual design of a methanol plant based on technology developed at Sasolburg are given in Table By convention[5] the energy requirements of a process producing a number of products are partitioned on the basis of calorific values for fuels and on the basis of replacement energy requirements for non-fuel products. Thus from Table 3 it can be seen that the energy requirement (MJ(th)/tonne) of methanol produced in such a plant is given by the following fraction of the total plant energy requirements per stream day:

$$\frac{1}{10,120.9} \left[\frac{233.609 \times 10^6}{233.609+93.154+3.352+7.240+16.684+0.049) \times 10^6} \right]$$

$$= 6.5187 \times 10^{-5}$$

i.e. 65.97% of plant energy requirements are attributed to the production of methanol.

The calculated thermal efficiency (the ratio of the calorific value of all outputs to the calorific value of all inputs) was given as 56.6%.

TABLE 3   PRODUCTS FROM CHAN'S CONCEPTUAL DESIGN OF A
SASOL-TYPE PROCESS FOR METHANOL FROM COAL.

Product	Production Rate (tonnes/ stream day)	Replacement Energy Requirement[6] (GJ(th)/tonne)	Total Calorific Value ($\times 10^6$ MJ(th))	Total Energy Requirement ($\times 10^6$ MJ(th))
Methanol	10,120.9	–	233.609	–
Tar, Oil, Naphtha	1654.73	–	93.154	
Higher Alcohol + Dimethyl Ether	48.57	–	1.676	3.352*
Phenol	142.39	50.85	0.529	7.240
Ammonia	299.49	55.71	6.681	16.684
Sulphur	123.52	~ 0.40	1.142	0.049

*As before (App. 2.2.2) the energy requirement was assumed to
be of the order of twice the calorific value.

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