TECHNOECONOMIC MODELLING OF COAL CONVERSION PROCESSES FOR LIQUID FUEL PRODUCTION

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Doctor of Philosophy

THE UNIVERSITY OF ASTON IN BIRMINGHAM
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SUMMARY

Since the oil crisis of 1973 considerable interest has been shown in the production of liquid fuels from alternative sources. In particular processes utilizing coal as the feedstock have received considerable interest. These processes can be divided into direct and indirect liquefaction and pyrolysis. This thesis describes the modelling of indirect coal liquefaction processes for the purpose of performing technical and economic assessment of the production of liquid fuels from coal and lignite, using a variety of gasification and synthesis gas liquefaction technologies.

The technologies were modeled on a 'step model' basis where a step is defined as a combination of individual unit operations which together perform a significant function on the process streams, such as a methanol synthesis step or a gasification and physical gas cleaning step.

Sample results of the modelling, covering a wide range of gasifiers, liquid synthesis processes and products are presented in this thesis. Due to the large number of combinations of gasifier, liquid synthesis processes, products and economic sensitivity cases, a complete set of results is impractical to present in a single publication.

The main results show that methanol is the cheapest fuel to produce from coal followed by fuel alcohol, diesel from the Shell Middle Distillate Synthesis process, gasoline from Mobil Methanol to Gasoline (MTG) process, diesel from the Mobil Methanol Olefins Gasoline Diesel (MOGD) process and finally gasoline from the same process.

Some variation in production costs of all the products was shown depending on type of gasifier chosen and feedstock.

Key Words: Coal; Gasification; Modelling; Economics; Fuels

DEDICATION

To my parents, Peter and Dorothy Anders.

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Finally, Eusélia, from whom I acquired a taste for cold coffee!

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CHAPTER 1
INTRODUCTION

1.1 Introduction

Coal is the most abundant of the fossil fuels[1] and as the other fuel resources begin to dwindle, it may become necessary to utilize coal for many of the applications that the other fossil fuels are at present used for. These include gas production for domestic and industrial use, power generation and the topic of this thesis, liquid fuels production.

The precise nature of the future of fuels use and production is by no means an easy subject to predict, with global ecological and environmental criteria likely to be applied to various aspects of life and commerce towards the end of this century and into the next. Already ecological motivations have enforced the use of lead free petrol in many countries such as the UK. With the as yet unproven but widely accepted greenhouse effect potentially threatening many of the premises upon which modern industrial society is based, the impact of possible future legislation against various forms of energy use cannot be underestimated or at this stage easily accounted for. A possible example of this would be a tax imposed on fuels in proportion to the amount of carbon dioxide placed in the atmosphere per unit of energy[2]. This would favour natural gas usage rather than coal or oil which contains less energy per carbon atom than natural gas.

Liquid fuels are likely to be required for the foreseeable future for transport purposes, solid fuels are undoubtedly safer then liquids, but are far less convenient to transport and less convenient in their final use. Gaseous fuels are also inconvenient for transport fuels, for example refueling may require the removal and refitting of a pressurized gas tank, which is more time consuming than simply filling the petrol tank at a petrol pump.

On the premise that liquid fuels will be required and that non-renewable sources are an acceptable source of energy in the future, then coal is likely to be the only large scale source at some point in the future. The questions being at what point in the future will it be economically attractive to utilize coal liquefaction and which technologies and processes will be utilized.

Technology is at present available for the conversion of coal and lignite to produce a variety of liquid fuel products such as methanol, gasoline, diesel or fuel alcohol (C_1 to C_6 alcohols). Direct liquefaction processes are, in contrast, at a less advanced stage of development and cannot produce specific products such as methanol as easily.

The only large scale indirect coal liquefaction plants at present operating are at Secunda and Sasolburg in South Africa, employing technology which has now been superseded by modern developments in gasification and synthesis gas conversion technologies. Modern gasifiers operate at much higher efficiencies than those available when SASOL was built and modern developments in synthesis gas conversion technologies have increased the thermal efficiency and and selectivity of these processes. The combined effect of these improvements to different areas of technology, are that the best possible combinations of gasifier and liquefaction processes that exist, can be expected to provide significantly greater conversion efficiencies then previously obtained such as at SASOL.

Although many technoeconomic assessments have been performed for individual processes, the results of these studies are difficult to compare on a consistent basis due to different assumptions in the studies concerned. To compare the results of different studies, the basic economic criteria such as plant life, throughput, feedstock cost and utility costs must be the same otherwise the results cannot be compared consistently. Studies which have attempted to compare several processes on a consistent basis have tended to oversimplify the assumptions used in the preparation of the mass balances, for example by ignoring the effect of feedstock on process efficiency and hence comparing processes with different feedstocks which as is shown in this thesis can significantly affect the efficiency of the conversion and hence the product cost.

It is the purpose of this thesis to present a comparison of results for alternative technologies for gasification and synthesis gas conversion, on a consistent basis, with the same basic economic and financial criteria with which to provide a meaningful comparison of the combinations of processes.

1.2 Background

Coal was first converted to a substitute oil in 1913 by the Bergius[3] process, which is a direct liquefaction or hydrogenation route and this process was operated until 1945.

A second method was also discovered in Germany at around the same time and the process was patented in 1925 by Fischer and Tropsch, based on the result that an oil like substance was formed by passing a gas containing carbon monoxide and hydrogen over a cobalt catalyst. This, together with the gasification of coal, is known as indirect coal conversion. The primary products of the conversion using the cobalt catalysts were found to be more suited to chemicals production and paraffin wax and lubricating oils became high value products from the process. The first commercial scale plant was built in 1936 and produced 70 000 tonnes per annum of primary products. By 1945, encouraged by wartime constraints, nine indirect conversion plants existed in Germany, with a combined capacity of 4 million tonnes per annum. Indirect conversion plants also existed in Japan, Manchuria and France under license from Ruhrchemie[4].

Most of the Fischer-Tropsch plants in existence in the 1930's and 1940's obtained the synthesis gas from coke ovens. By the time that the first SASOL plant was constructed at Sasolburg South Africa, Lurgi had developed the dry ash Lurgi gasifier which had many advantages for inclusion in a Fischer-Tropsch plant. These were pressurized operation and a more suitable gas composition, which did not require steam to shift its composition. Lurgi also had the Rectisol process for desulphurisation and carbon dioxide removal and the Phenolsolvan process to remove phenols and ammonia from the product gas. Thus producing a gas suitable for feeding to the F-T catalysts at SASOL.

All of these plants as well as the existing direct conversion (Bergius) plants were eventually closed after the second world war due to the availability of cheaper alternatives (crude oil).

A resurgence of interest occurred in 1973 and 1982 when oil prices peaked out at 40.5 $ / barrel (1988 equivalent) in 1982[5], with many organizations developing coal gasifiers for synthesis gas and substitute natural gas (SNG). However many of these gasifiers were abandoned due to poor economics or technical problems as explained in Chapter 3.

Interest in gasification was maintained, however, by a reduced number of organizations for the purpose of providing fuel gas and steam for use in Integrated Combined Cycle Gasification (IGCC) power plants. This has led to the large scale development of several gasification processes, the largest of which can at present gasify 2000 te / day of coal in a single train[6].

1.3 Present Coal Demand and Consumption

As can be seen from Tables 1.1 and 1.2, coal is the most abundant of the fossil fuels accounting for over sixty percent of both the total world resources and economically recoverable reserves. Resources are fossil fuel deposits which have been shown to exist with no account being taken of the economic feasibility of extraction, they may or may not be economically recoverable. Reserves are deposits of fossil fuels which are considered to be economically recoverable under present conditions.

At present rates of consumption, coal has an estimated world reserve of 218 years[7], the only other fossil fuel approaching this is oil shale most of which is at present uneconomic to extract. It can, therefore, be assumed that fossil fuel use will become more biased towards coal as the economically extractable reserves of the other fuels become exhausted.

Table 1.1 World Total Resources *in situ* of Fossil Fuels[8]

Fuel	Quantity ($t \times 10^6$, except for natural gas)		Energy content ($J \times 10^{18}$)	Energy content (% of world total)
Crude oil	257 500		11 134	2.8
Natural gas	281 743	$\times 10^9 m^3$	10 509	2.6
Oil shale	2 511 600	(as oil)	108 602	26.9
Tar sand	364 155	(as bitumen)	15 746	3.9
Peat	222 378		1 861	0.5
Coal	11 769 779		255 246	63.3
Total			403 098	100.0

Table 1.2 World Economically Recoverable Reserves of Fossil Fuels[9]

Fuel	Quantity ($t \times 10^6$, except for natural gas)		Energy content ($J \times 10^{18}$)	(% of world total)	Reserves/Production (Years)
Crude oil	85 00		3 675	15.2	37
Natural gas	81 147	$\times 10^9 m^3$	3 027	12.5	58
Oil shale	29 540	(as oil)	1 227	5.1	-
Tar sand	27 312	(as bitumen)	1 181	4.9	-
Peat	23 417		196	0.8	-
Coal	690 672		14 823	61.4	218
Total			24 129	100.0	

1.4 Coal Conversion Technologies

1.4.1 Introduction

The conversion of coal into liquid fuels may be accomplished by one of three basic conversion routes, which are:

- Indirect conversion by gasification and synthesis of liquid fuels;
- Direct liquefaction;
- Pyrolysis and synthesis of liquid fuels.

A comparison of the parameters in each technology are summarized in Table 1.3.

Table 1.3 Comparison of Coal Conversion Technologies

PARAMETERS*	Pyrolysis	Gasification	Liquefaction
Temperature, °C	400-900	700-2000	375-475
Pressure, bar	0.1-100	up to 100	100-300
Maximum throughput, to date (te/day/train)	24	2 200	400

* Figures quoted are typical, and can vary considerably according to technology and operating conditions.

Significant effort spent on coal liquefaction research has centred around the direct liquefaction by hydrogenation route. This is because direct conversion is more thermally efficient at around 65 to 70 %, whereas SASOL One operates at between 38 and 55 %[10] (although this is in part due to the production of methane containing tail gas which has no local use). There are disadvantages, however, with direct conversion which are not present in indirect conversion. Coal quality is more critical for direct conversion which limits the flexibility in choice of feedstock. Direct conversion may also produce heavy fractions which require hydrotreating to convert them to the premium products which are available from indirect liquefaction processes[11].

1.4.2 Indirect Liquefaction

The indirect conversion of coal to liquid fuels is accomplished by first the gasification of the coal with oxygen and steam followed by synthesis of liquids from the resulting synthesis gas. The heat for gasification is normally supplied by the partial oxidation of the coal with oxygen. Steam may be used for temperature moderation and this has the effect of adjusting the CO : H_2 ratio. The products synthesized include alcohols such as methanol or fuel alcohol and conventional hydrocarbons such as gasoline or diesel.

1.4.3 Direct Liquefaction

Direct liquefaction is the conversion of coal into liquid fuels without passing through a synthesis gas stage. Typically the coal is pulverized and mixed with an organic solvent at high temperature and pressure and then the resulting mixture is hydrogenated to give a crude synthetic oil which can undergo conventional refinery operations. Direct liquefaction is beyond the scope of this thesis.

1.4.4 Pyrolysis

Thermal decomposition of coal in the absence of oxidizing agents, or with insufficient oxidant for complete gasification, gives solid, liquid and gaseous products. This process is referred to as pyrolysis and is considered to differ from liquefaction in that there is no solvent and lower pressures and higher temperature are employed. Hydropyrolysis is a variation in which pyrolysis is carried out in an hydrogen atmosphere to produce a product with an improved C:H ratio.

The liquids may be collected and refined to a hydrocarbon fuel by conventional processing of hydrotreating and refining. A more recent proposal is to directly convert the hot pyrolysis vapours to hydrocarbons over zeolite catalysts, in an analogous process to biomass pyrolysis conversion[12].

Pyrolysis is not considered an attractive method for producing liquid fuels from coal due to the low amount of volatiles produced and the difficulty experienced in upgrading the pyrolysis tars to a marketable product as well as the production of large amounts of char which requires further processing (for example by combustion or gasification)[13].

1.4.5 Scope of Project

The purpose of this thesis is to select gasification technologies at an advanced stage of development and compare their performance in economic and technical terms for producing a range of liquid fuel products via several synthesis gas conversion routes. This was accomplished by constructing a robust computer simulation package that models all the steps in a complete coal liquefaction process as summarised in Figure 1.1.

The comparison has been performed by adapting the main structure of a program constructed for biomass liquefaction[14] and adding computer models of coal handling, coal gasification and the full range of synthesis gas processing steps. A dedicated computer model was necessary because commercially available programs containing libraries of items of equipment and process plant do not contain models of the specific process plant (for example specific gasifiers) required for this project, nor do they include procedures for calculation of the process economics.

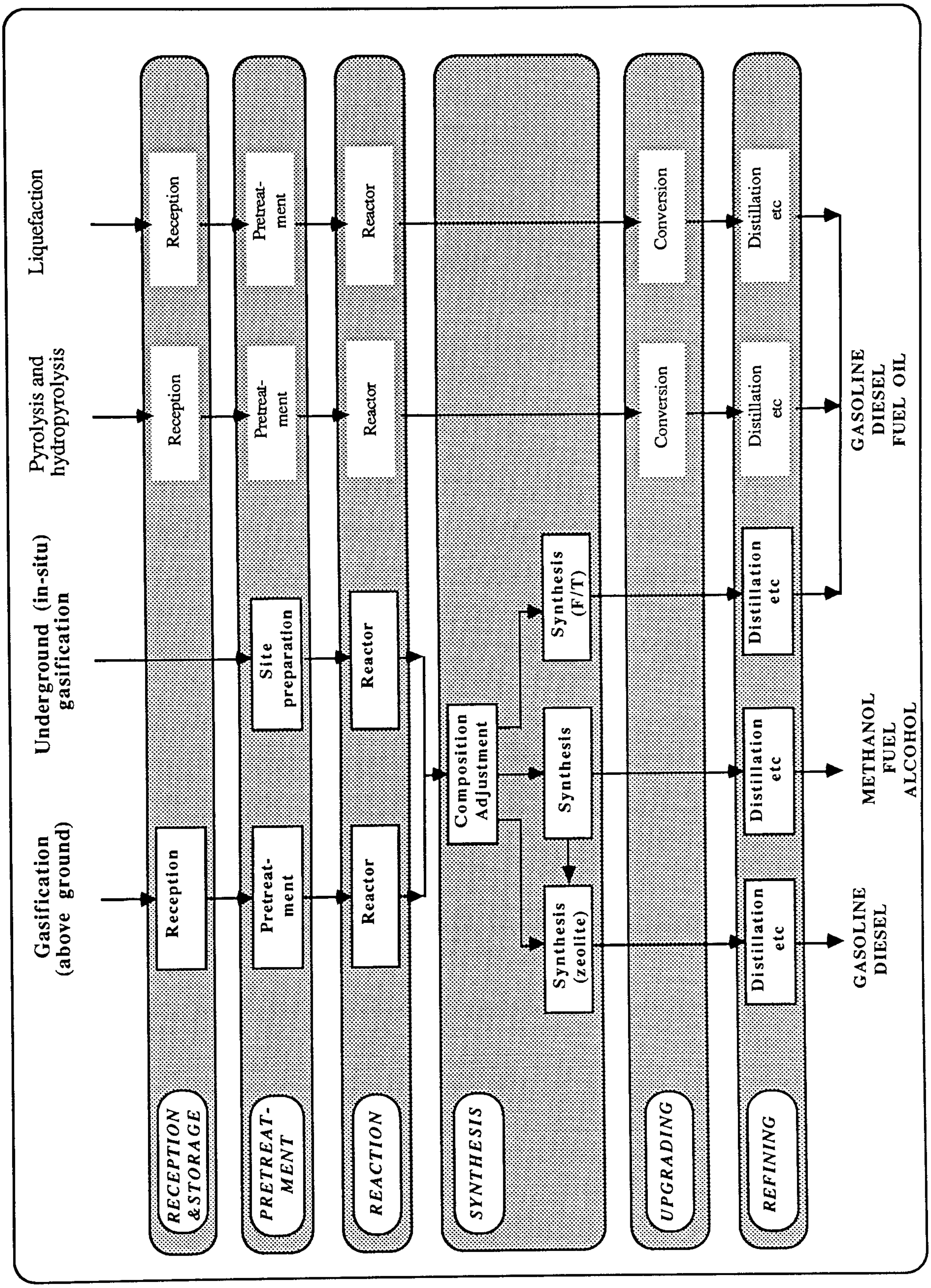

Figure 1.1 An Overview of Coal Liquefaction Technologies

CHAPTER 2
GASIFICATION TECHNOLOGIES

2.1. Introduction

Gasification of coal occurs when carbon in the coal is converted, by the action of a reactant gas, to carbon monoxide, carbon dioxide, methane or less usually higher order hydrocarbons such as ethane and ethene. The reactant gas may be oxygen, steam or hydrogen and inert gases may be present such as nitrogen. If hydrogen is the main reactant gas the process is more usually described as hydro-gasification.

Many alternative methods exist for contacting the feed coal with the reactant gases under different conditions and which produce different product gas compositions. The alternative basic methods, or technologies, for gasifying the coal are described in this chapter. Descriptions of the specific gasifiers included in the modelling are also given.

The gasification processes are here classified according to reactor type, exceptions being made in the special cases of underground gasification and gasification using nuclear process heat which although not included in the modelling are described separately.

Table 2.1 shows a comparison of eight gasifiers in terms of steam and oxygen usage, maximum temperature of the gasifier and the gas exit temperature, also the cold gas efficiency is given for comparison. Table 2.2 gives typical gas compositions for the same eight gasifiers based on Illinois No.6 coal, if applicable, or an alternative feedstock if Illinois No. 6 is not suitable for the gasifier.

Table 2.1 Comparison of Gasifier Conditions

Gasifier	Steam Usage kg/te coal	Steam Produced kg/te coal	Oxygen Usage kg	Max Temp. ℃	Exit Temp. ℃	Cold Gas† Efficiency
Lurgi	2576	1450	541	1000	500	80 %
BG/Lurgi	379	333	630	1500	700	88 %
Shell	32	853	889	2000	1300	80 %
Texaco	0	111	960	1500	1300	77 %
KRW	678	2883	756	1010	1000	81 %
HTW**	221	1790	618	1060	1060	82 %
PRENFLO	-	-	880	2200	1350	80 %
Dow*	0	1367	859	1500	1050	76 %

Illinois No.6 coal all cases except:-
* Western Sub-bituminous Coal
** Lignite

† Defined as heat content of sulphur free gas / heat content of coal.

Table 2.2 Comparison of Typical Gasifier Gas Compositions

	Gas Vol % (dry)							
Gasifier	H_2	CO	CO_2	CH_4	H_2S	C_2'S	N_2/Ar	NH_3
Lurgi	42.1	15.2	30.9	8.6	1.3	0.8	0.3	0.8
BGL	31.5	55.0	3.5	4.5	1.3	0.5	3.3	0.4
Texaco	35.5	49.3	12.3	0.4	1.3	0.0	1.0	0.2
Dow	41.4	38.4	18.5	0.1	0.1	0.0	1.5	0.0
Shell	31.0	61.5	1.6	0.0	1.2	0.0	4.6	0.1
PRENFLO	31.5	61.0	1.8	0.0	1.3	0.0	3.3	0.0
KRW	31.9	43.2	17.5	5.8	0.5	0.0	1.1	0.0
HTW	33.7	53.1	9.0	3.1	0.4	0.0	0.7	0.0

2.2. Selection of Gasification Processes

Gasification processes have been selected for inclusion in the overall model according to the following criteria:

A The product gas must be suitable for use as, or conversion to, a synthesis gas suitable for the indirect liquefaction processes considered, this essentially excludes gasifiers that operate with air as the gasifying agent, as the large volumetric content of nitrogen in the resulting synthesis gas would render any conversion process which contained recycles, inefficient. Synthesis gas conversion processes are possible which operate on a once through basis (such as the Chem Systems Methanol Process[15]) and which may therefore utilize the gas produced by gasifiers using air or enriched air as the gasifying agent. However as no recycle exists, a large part of the feed gas is unconverted and must be used as fuel gas, for example to produce electricity. These processes are considered outside the scope of this thesis due to the production of large quantities of fuel gas and hence co-generation of electricity or other use for which the fuel gas must be found. Therefore, for this thesis, gasifiers unable, or not proven, to run on >99 % pure oxygen are excluded.

B The gasifier must be in one of the following categories:

- Those in current commercial use;
- Those currently being demonstrated at a commercial scale;
- Those at a large scale of development and which offer potential advantages over existing commercial processes;
- Other processes which offer potential advantages over existing processes and for which large demonstration projects are planned in the near future;

Table 2.3 shows the gasifiers to be included in the modelling, and Table 2.4. gives specific reasons for inclusion for particular gasifiers.

Table 2.3 Gasification Processes Selected for Inclusion

Gasifier	Status	Gasifier Output Nm^3/h (dry)	Typical End Product	Planned Developments
Dry Ash Lurgi	Commercial	(55 000) *	Fischer-Tropsch fuels	
Texaco	Commercial	(80 000)	MeOH, Power	
Dow	Demonstration	(≈170 000)	Power	
BG/Lurgi	Demonstration	(45 000)	eg Power	IGCC
HTW	Demonstration	(41 000)	Methanol	Possible IGCC
Shell	Pilot plant	(15 000)	Power, MeOH	250 MW IGCC -
PRENFLO	Pilot Plant	(≈3 500)	Power, MeOH	150 MW IGCC
KRW	Pilot Plant	(≈3 500)	Power, MeOH	60 MW IGCC
U-Gas	Pilot Plant	(≈3 500)	Power, MeOH	30 MW IGCC

* Alternative gasifier sizes are in use commercially

Table 2.4 Reasons for Gasifier Selection

Technology Represented	Gasifier	Reason for Selection
Fixed bed Non-Slagging	Lurgi	Most commercially successful gasifier to date
Fixed bed Slagging	BG/L	Improved design based on Lurgi and at large scale
Entrained flow Slurry feed	Texaco	In use commercially at large scale
Entrained flow Slurry feed	Dow	Largest single train gasifier to date and improved efficiency with low rank coals for wet feed system
Entrained flow Dry feed	Shell	Very wide feed range, high throughput
Entrained flow	PRENFLO	Pressurized version of commercial Koppers-Totzek gasifier
Fluidised bed Non-slagging	HTW	Development of commercial Winkler gasifier
Fluidised bed Ash agglomerating	KRW	Offers wider feed range and improved efficiency over other fluidised gasifiers
Fluidised bed Ash agglomerating	U-Gas	Offers wider feed range and improved efficiency over other fluidised gasifiers

The Koppers-Totzek[16,17] gasifier was not included in this thesis, as no new gasifiers have been built in recent years[18]. The two dry fed entrained flow gasifiers included in this thesis, and which were developed from the atmospheric pressure Koppers-Totzek gasifier offer advantages over the original gasifier in terms of specific throughput and efficiency[19,20].

The Winkler gasifier was not included due to the High Temperature Winkler gasifier, which is included, superseding it in terms of specific throughput, efficiency and feed range[21]. Several other gasifiers exist or are under development in countries such as Japan[22] and communist block countries[23]. These are however technically similar to those included in this thesis and are therefore excluded.

The gasifiers included in this thesis were also chosen to cover the basic technologies available for coal gasification, except for underground gasification[24], which is too site specific to compare easily in a project of this type, and gasification by nuclear process heat[25], the economics of which is dependent on the cost of steam from nuclear process sources and is considered beyond the scope of this thesis.

2.3. Fixed bed (moving bed).

Fixed bed gasifiers are characterized by a large bed of coal which moves slowly down the gasifier and passes through several zones in which the processes of drying, devolatilisation, gasification and combustion take place[26]. The feed coal is generally a sized feed of the order of 1-4 cms diameter and has undergone little preparation (the coal is not normally dried although it may be screened to remove excess feed fines which would otherwise interfere with the operation of the gasifier). There is normally therefore a large inventory of coal in the gasifier, which slows down the gasifier transient responses but which has safety benefits when compared to other gasifier types[27].

The product gas is generally characterized by significant methane content and tars and oils are normally produced which increases the difficulty of cleaning the gases[28]. Due to the countercurrent operation, the raw gas from the gasifiers is normally relatively cool (just above the tar dew point) and this reduces the relative amount of energy that may be recovered usefully from the raw gas by steam generation but increases the cold gas thermal efficiency of the gasifier, compared to co-current gasifiers[29]. Figure 2.1 shows a typical fixed bed gasifier (Dry Ash Lurgi)[30]. Advantages of fixed bed gasifiers may be summarized as follows:-

- Potentially complete coal conversion;
- Stable operation;
- High thermal efficiency;
- Low steam and oxygen consumption;
- Minimal feed preparation;
- Inherently safe operation.

Problems normally associated with fixed bed gasifiers are feeding of the coal into the gasifier via the lock hoppers which may become blocked, and with cleaning the tars, oils and dust from the raw gas. The tars and oils represent a problem which is not present with most other types, such as entrained or fluidised bed gasifiers.

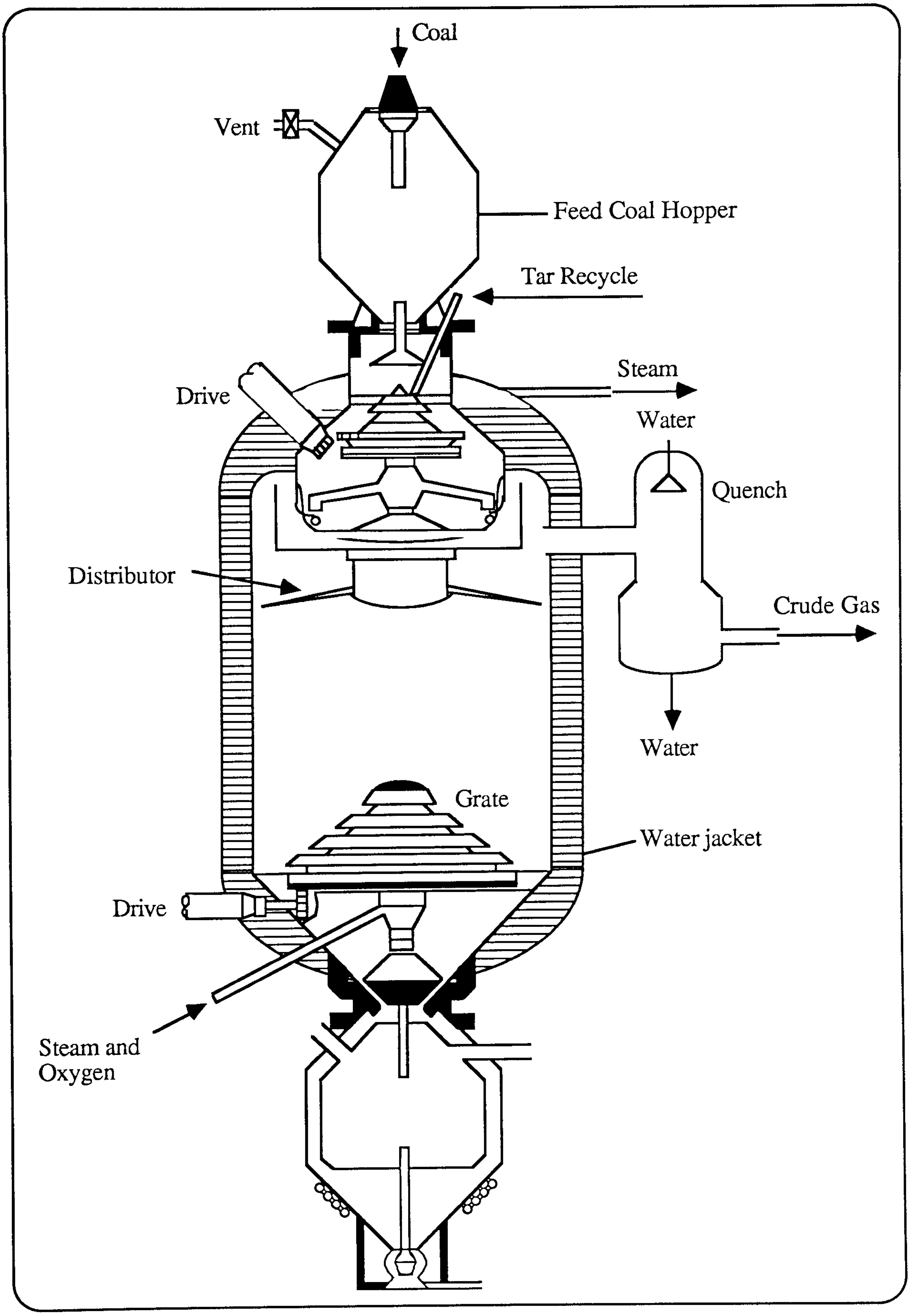

Figure 2.1 A Typical Fixed Bed Gasifier (Dry Ash Lurgi)[31]

For liquid fuel production particularly, the methane content of the gas, although normally considered an advantage (due to increased thermal efficiency of the gasifier) may be considered a disadvantage as it cannot be converted easily to liquids, unless it is first converted to CO and H_2. With the concentrations present in the feed gas for the gasifiers considered in this thesis (<15 %) this is not considered economically attractive[32] and the methane must be passed through the liquefaction processes as an inert gas. This has the effect of decreasing the thermal efficiency of the liquefaction processes, the methane must then be taken off as a purge stream and either used as fuel gas or converted to synthesis gas. This is particularly applicable to gasifiers where there are already high levels of hydrogen, or an excess, in the product gas and for which steam reforming of the methane produces excess hydrogen. In cases where hydrogen levels are low in the gasifier product gas, the additional cost of steam reforming the methane is advantageous, as is shown in section 7.13. Examples of fixed bed gasifiers are shown in Table 2.5.

Table 2.5 Examples of fixed bed gasifiers

Gasifier	Reactant gases	Pressure (bar)	Temperature	Location	Status
BASF	-	-	-	W. Germany	Abandoned
BG / Lurgi	Oxygen/Steam	21	Slagging	Scotland	Current
Chevron	Steam	20-55	Non-Slagging	USA	-
Kerpely	-	-	-	USA	-
Kilngas	Air/Steam	1	Non-Slagging	USA	Current
Leuna / Wuerth	Oxygen/Steam	1	Non-Slagging	-	-
Lurgi	Oxygen/Steam	20-30	Non-Slagging	W. Germany	Commercial
Thyssen-Galoczy	Oxygen/Steam	1	Slagging	-	Abandoned
Riley Morgan	Oxygen/Steam	1	Non-Slagging	USA	-
Ruhr 100 / Lurgi	Oxygen/Steam	Elevated	Non-Slagging	W. Germany	-
Simplex	-	-	-	-	-
Wellman Galusha	Oxygen/Steam	1	Non-Slagging	USA	Commercial
Wellman Incandes.	Oxygen/Steam	1	Non-Slagging	UK	-
Wilputte	Oxygen/Steam	1	Non-Slagging	UK	Abandoned
Woodall-Duc./ GI	Oxygen/Steam	1	Non-Slagging	UK	Current

2.3.1. Dry Ash Lurgi

Sized coal is fed via lockhoppers to the top of the gasifier and is gasified by the up-flowing hot gases as it moves down the gasifier bed. The oxygen and steam required for gasification is fed in at the bottom of the gasifier. The ash is removed after falling through the grate by a lockhopper at the bottom of the gasifier[33], as shown in Figure 2.1.

The gasifier has a relatively low oxygen requirement per tonne of coal (≈550 te of O_2 / te coal, daf) compared to entrained and fluidised bed gasifiers[34]. There is however a large steam requirement, which is necessary to prevent the temperature of the gasifier in the combustion zone from becoming higher than that of the ash melting point[35]. This is necessary to prevent the gasifier from becoming inoperable, as the ash would fuse together and block the gasifier. The steam requirement is greater for higher rank coals.

Disadvantages of the gasifier are the production of tars, oils and phenols which require removal from the gas and disposal which requires additional process plant, increases the complexity of the process and produces additional waste and by-products. Also the H_2 / CO ratio of the gas is too high for several of the modern fuels synthesis processes, many of which require a H_2 / CO of less than two such as the Shell SMDS[36] process and the IFP Fuel Alcohol process[37], the composition of the gas from the dry ash Lurgi gasifier is normally greater than two[38]. This is due in part to the large amount of steam added to the gasifier which increases the hydrogen formation via the water gas shift reaction.

Dry ash Lurgi gasifiers account for the majority of coal gasified in the world today[39], most of this is due to the coal conversion plants in South Africa namely SASOL I, II, and III[40]. Dry ash Lurgi gasifiers are also being used in America in the Great Plains coal to SNG gasification project[41]. Dry ash Lurgi gasifiers in operation are shown in Table 2.6.

Table 2.6 Dry Ash Lurgi Gasifiers in Current Use

Location	Owner	Year of startup	Feed	Throughput net te/d (total DAF)	Gas output 10^3 Nm^3/d	End product
South Africa	SASOL I	1954	Sub-bit	4717	≈8300	Syncrude
South Africa	SASOL II	1974	Sub-bit	17780	≈34000	Syncrude
South Africa	SASOL III	1979	Sub-bit	17780	≈34000	Syncrude
USA	Great Plains Gasif.Assoc.	1981	Lignite	7260	≈14500	SNG
China	China Nat. Tech.Imp.Co.	1982	Anthracite	1000	≈2000	H_2/NH_3

2.3.2. BG / Lurgi

This gasification process is a development of the conventional dry ash Lurgi gasifier. It has a number of advantages in comparison with the dry ash Lurgi gasifier, these include a low steam consumption and higher specific throughput of coal[42].

The essential difference between this gasifier and the dry ash Lurgi gasifier is the removal of the ash in a molten state. This enables the gasifier to be run at higher temperatures, which reduces considerably the amount of steam required for temperature control. This has the added effect of decreasing the H_2 / CO ratio of the product gas[43], making it more suitable for some synthesis gas conversion processes. Methane is produced by the gasifier in significant quantities, although due to the higher operating temperature, in lower amounts than that of the dry ash Lurgi gasifier.

The process has been developed to a throughput of 650 te / day[44] and can gasify a wide variety of feedstocks[45], including some caking coals due to the inclusion of a rotating stirrer to break up the coal. BG / Lurgi gasifiers in operation are shown in Table 2.7. The process is being developed to operate at a pressure of 80 bar with the aim of further increasing the specific throughput[46].

Table 2.7 BG/Lurgi Gasifiers in Current Use

Location	Owner	Year of startup	Feed	Throughput net te/d	Gas output 10^3 Nm^3/d	End product
Scotland	British Gas/Lurgi	1974	Bituminous	300-350	≈600	MBG/Flared
Scotland	British Gas/Lurgi	1982	Bituminous	600	1 206	MBG/Flared

A flow diagram for this process is given in Figure 2.2. Coal below 50 mm is fed through a lock hopper at the top of the gasifier. The coal is gasified with oxygen and steam as it moves downward through the bed. Molten slag is passed through a slag tap hole and is quenched in a quench vessel with water and removed through a lock hopper. Solids entrained in the product gas can be recycled after removal to the top of the gasifier. Tars and oils contained in the product gas may be separated from the gas liquor after gas is quenched and recycled back to the gasifier. Phenolic liquor after tar / oil removal and recycling may be evaporated and incinerated, an alternative to this which is used here is that the phenols are removed from the liquor using the Lurgi Phenolsolvan[47] process and then sold as by-product. Figure 2.3 shows the flow diagram for the tar/oil separation unit. Advantages of the slagging gasifier compared to dry ash gasifiers may be summarized as follows:

- Higher specific throughput;
- Lower steam consumption;
- Higher efficiency;
- Lower aqueous effluent production;
- Increased ability to handle bituminous coals;
- Increased ability to handle coal fines.

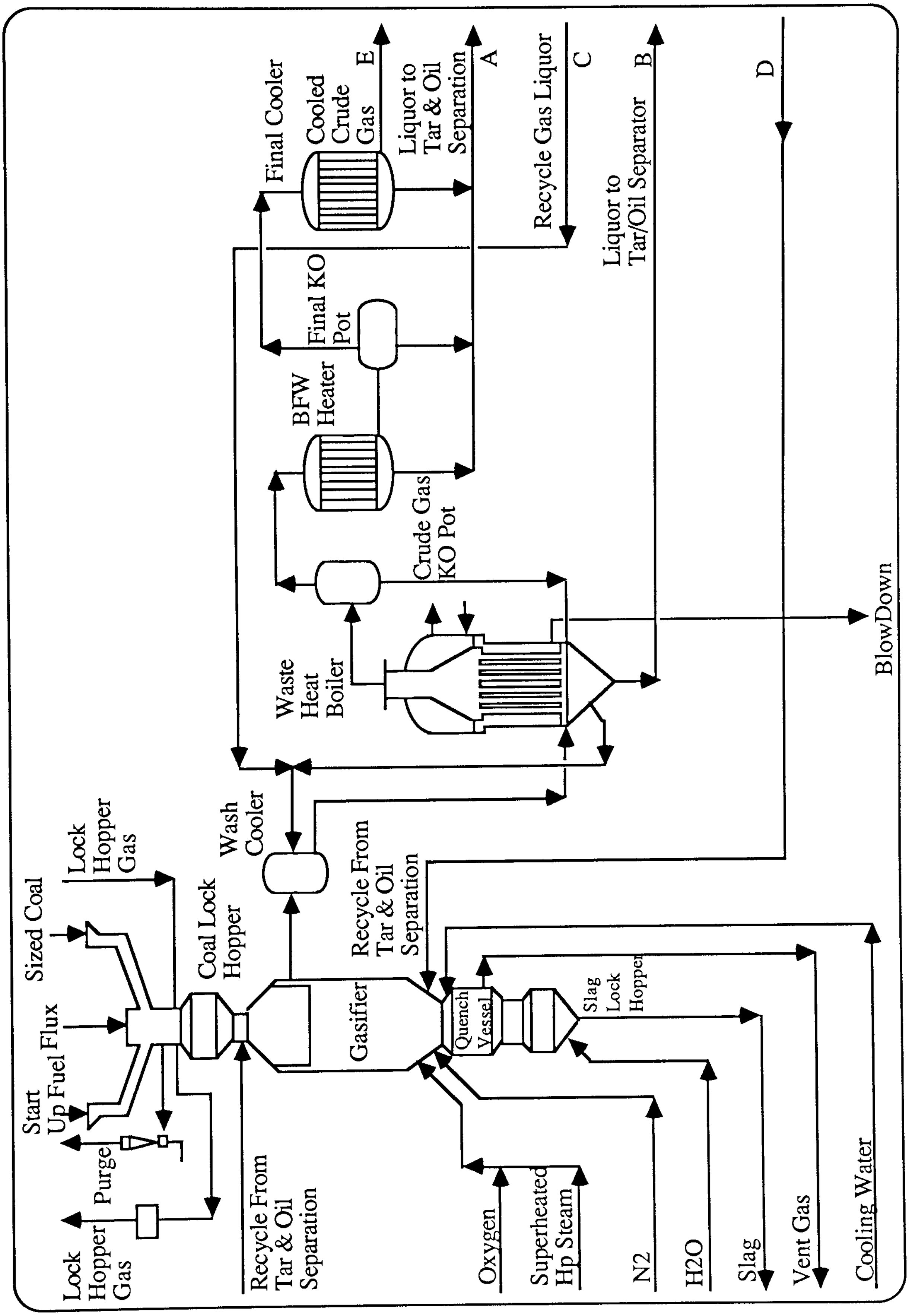

Figure 2.2 British Gas/Lurgi Gasification Process

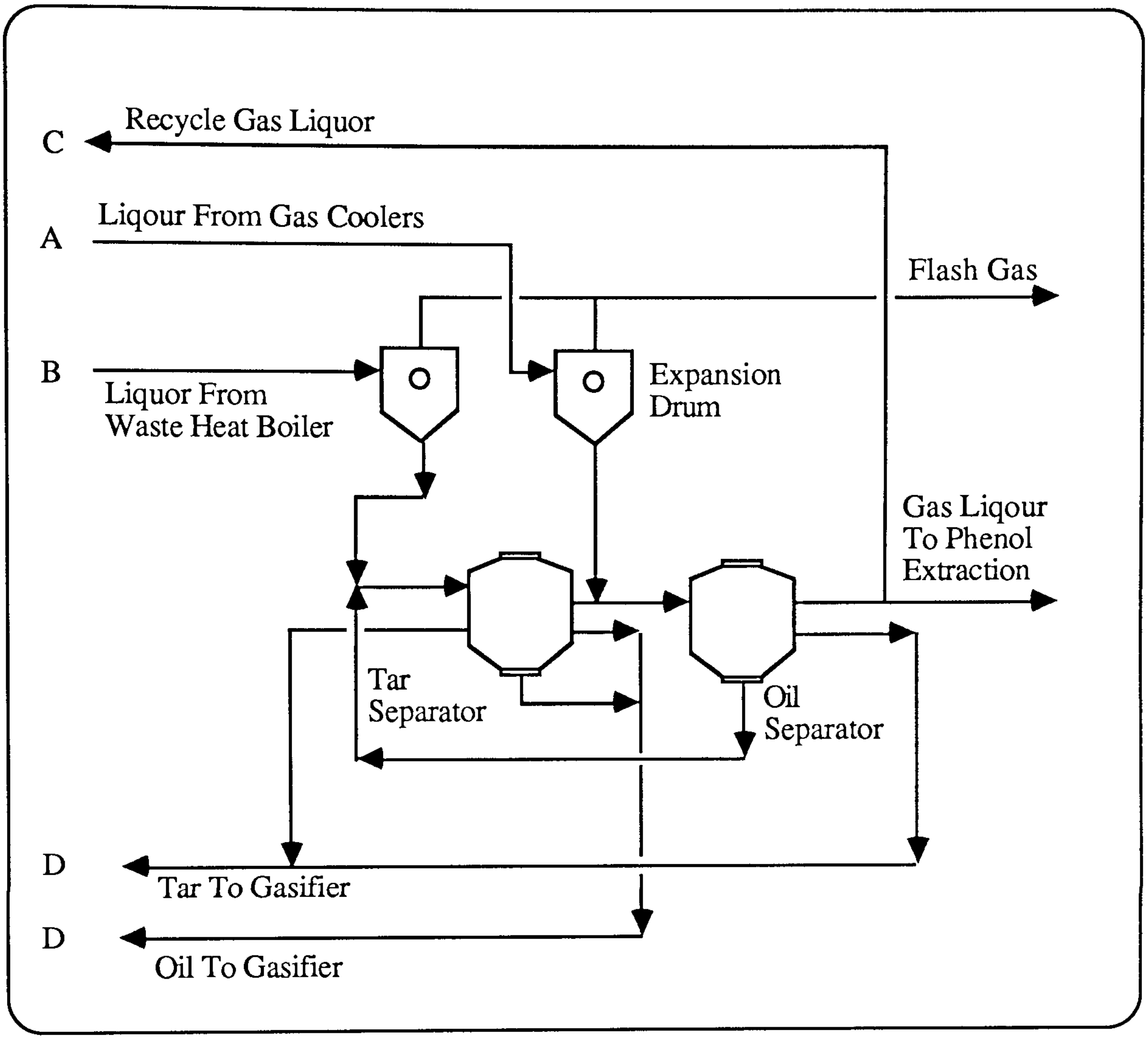

Figure 2.3 Tar/Oil Separation

2.4. Fluidised bed

With fluidised bed gasifiers coal granules and ash particles are suspended in an upward flow of oxygen, steam and recycled synthesis gas. The temperature in the gasifier is kept below the softening point of the ash to prevent a loss of fluidisation by ash agglomeration[48], although some processes use ash agglomeration deliberately as a method of improved ash removal[49]. The ash rich particles are normally removed at the bottom of the gasifier via lockhoppers and fly ash is removed from the product gas stream. An example of a fluidised bed gasifier is shown in Figure 2.6. Characteristics of fluidised bed gasifiers may be summarized as follows:-

- Moderate oxygen and steam requirements;
- Large char recycle;
- Uniform and moderate temperature;
- Difficulty in handling caking coals;
- Difficulty in obtaining very high carbon conversion.

Many varied processes have been developed from the basic fluidised bed configuration involving, for example, using multiple reactors and utilizing char or refractory pellets as heat carriers. Many of these fluidised bed gasifiers have since been abandoned due to unfavorable economics or technical problems[50]. Fluidised bed coal gasifiers have to overcome the inherent problem of removing the ash in the coal whilst removing a minimum amount of carbon, otherwise the efficiency of the gasifier may be significantly reduced[51]. This problem is present to a much lesser extent in most other types of gasifier and attempts to increase the carbon conversion efficiency in fluidised bed gasifiers have in general led to an increase in the complexity of operation of the gasifier. An example of this is the control of the temperature zones which enables the ash to agglomerate together in the Kellogg Rust Westinghouse[52] gasifier. Table 2.8.shows examples of fluidised bed gasifiers.

Table 2.8 Examples of Fluidised Bed Gasifiers

Gasifier	Reactant gases	Pressure (bar)	Location	Status
Coalcon	Hydrogen		USA	Abandoned
Cogas	Steam	3	England, USA	
CO2-Acceptor	Steam	11	USA	Abandoned
Energy Equipment	Oxygen/Steam		UK, Belgium	
Exxon catalytic	Steam	70	USA	Abandoned
Hydrane	Hydrogen	70	USA	Abandoned
HT Winkler	Oxygen/Steam	10	W. Germany	On-going
Hygas	Hydrogen	70	USA	Abandoned
KRW	Oxygen/Steam	20-30	USA	On-going
Synthane	Oxygen/Steam	40-70	USA	Abandoned
Tri gas	Air Steam	Elevated	USA	
U-Gas	Oxygen/Steam	25	USA	On-going
Winkler	Oxygen/Steam	1	Turkey	Commercial

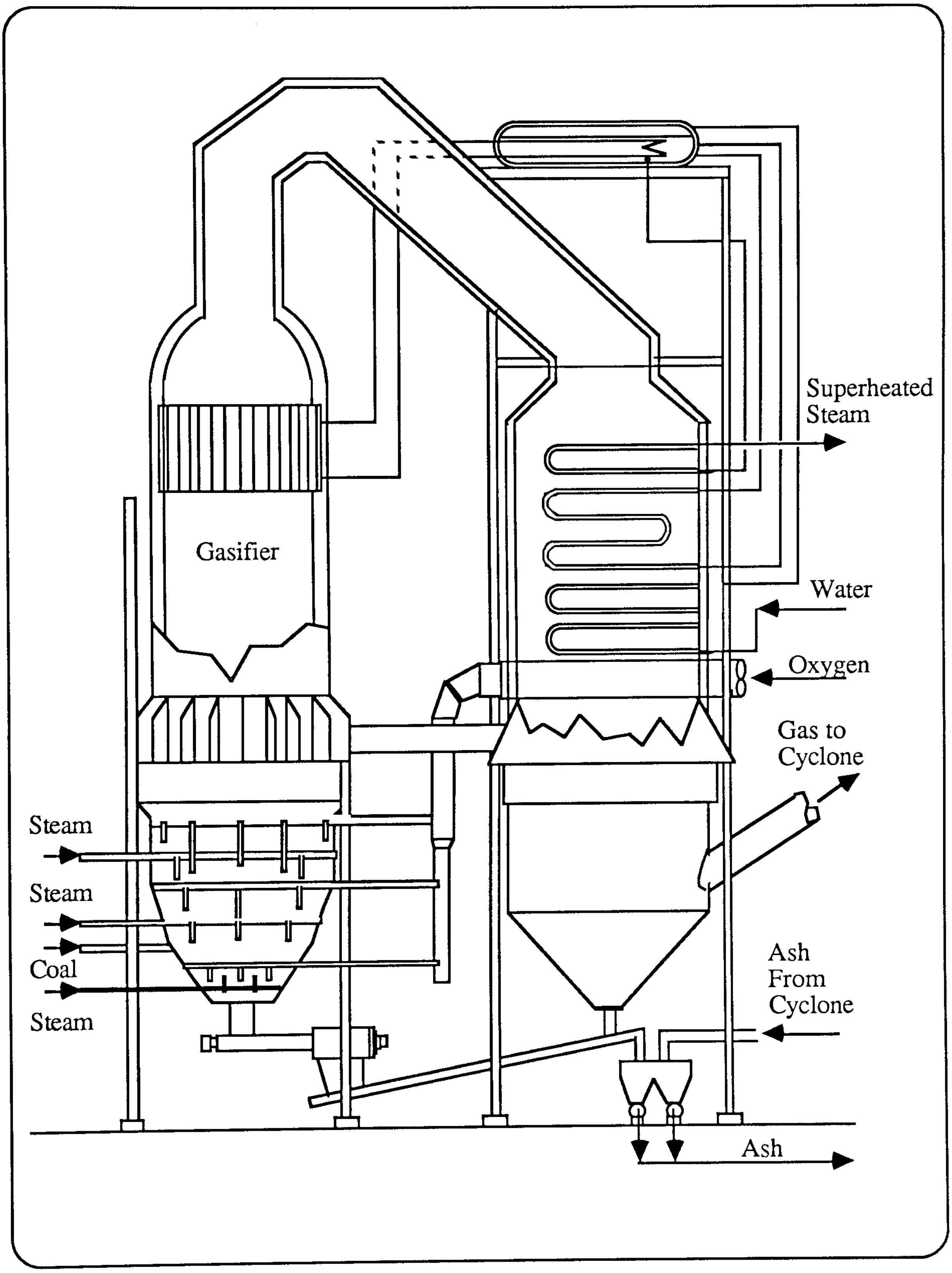

Figure 2.6 Example of a Fluidised Bed Gasifier[53]

2.4.1. High Temperature Winkler (HTW)

Although the standard atmospheric pressure Winkler gasifier is a commercially available gasifier, only a few plants have been in recent operation and no new Winkler gasifiers have been built since 1962. However the developmental version of the Winkler gasifier, the High Temperature Winkler, is at an advanced stage of development. This is a high temperature and high pressure version of the Winkler gasifier. Atmospheric pressure Winkler gasifiers in current use are shown in Table 2.9 and HTW gasifiers in current use are shown in Table 2.10.

Table 2.9 Winkler Gasifiers in Current Use

Location	Owner	Year of startup	Feed	Throughput net te/d	Gas output 10^3 Nm^3/d	End product
Yugoslavia	Fabrika Azotnih	1950	Lignite	91	≈80	NH_3
Turkey	Azot Sanyii TAS	1959	Lignite	320	290	NH_3

Table 2.10 High Temperature Winkler Gasifiers in Current Use

Location	Owner	Year of startup	Feed	Throughput net te/d	Gas output 10^3 Nm^3/d	End product
W Germany	Rheinische Braunk. AG	1981	Lignite	708	803	Methanol
Finland	Kemira	1988	Peat	1 100	-	NH_3

2.4.2. Kellogg Rust Westinghouse (KRW)

When compared to the Winkler processes an advantage of both the KRW process and the U-Gas process (see 2.2.3) is their ability to gasify a wide range of coals as well as lignite with relatively high conversion efficiencies. Both processes produce virtually no tar or hydrocarbons (excluding methane). Plans exist to construct a 500 te/d plant for IGCC power production within the next few years. Planned and existing KRW gasifiers are shown in Table 2.11.

Table 2.11 KRW Gasifiers In Operation Or Planned

Location	Owner	Year of startup	Feed	Throughput net te/d	Gas output 10^3 Nm^3/d	End product
USA	KRW	1978	Coal/Lignite	27 (DAF)	≈57	MBG
USA	M.W. Kellogg	Proposed	Coal/Lignite	485	≈800	60 MW

A flow diagram for this process is given in Figure 2.7. Crushed coal (<6 mm) is fed to the gasifier by means of a transport gas, this would normally be recycled synthesis gas for the purposes of this thesis. The bed operates at a temperature of approximately 1 000 °C where the coal is gasified by reaction with a mixture of oxygen and steam. The crude product gas is passed through cyclones where entrained unburnt char is removed and recycled back to the gasifier. High pressure steam is generated in the cooling of the raw gas. The ash agglomerating zone at the bottom of the gasifier operates at a temperature high enough to soften the ash, this then agglomerates until the particles of ash are large enough to sink to the bottom of the fluidised bed, they are then removed by dry lock hoppers. Recycled char is gasified in the ash agglomerating zone. The product gas contains no liquid hydrocarbons but does contain some methane.

2.4.3. U-GAS

A 24 te/d U-GAS pilot plant was built in 1974. The gasifier is a single stage fluidised bed. The coal, which is dried for easier handling and crushed to < 1/4 inch, is pneumatically injected into the gasifier through a lockhopper system. The coal reacts with the oxygen and steam gasifying agents at a temperature of between 955 °C and 1095 °C[54]. The temperature of the bed is controlled to maintain non slagging conditions in the gasifier. The ash eventually agglomerates into small spheres, and these tend to accumulate at the bottom of the bed where a higher temperature is maintained, the particles stick together and when large enough can be removed via the water filled ash hoppers. This ensures that a relatively small amount of carbon is removed with the ash and increases the carbon conversion efficiency compared to other fluidised bed gasifiers. The product gas contains virtually no tars or oils[55]. Table 2.12 gives examples of planned and operating U-Gas gasifiers.

Table 2.12 U-Gas Gasifiers In Operation Or Planned

Location	Owner	Year of startup	Feed	Throughput net te/d	Gas output 10^3 Nm^3/d	End product
USA	IGT	1974	Coal	30	≈50	Flared
USA	Tampella[56]	Proposed	Coal	35-60	≈75	Power

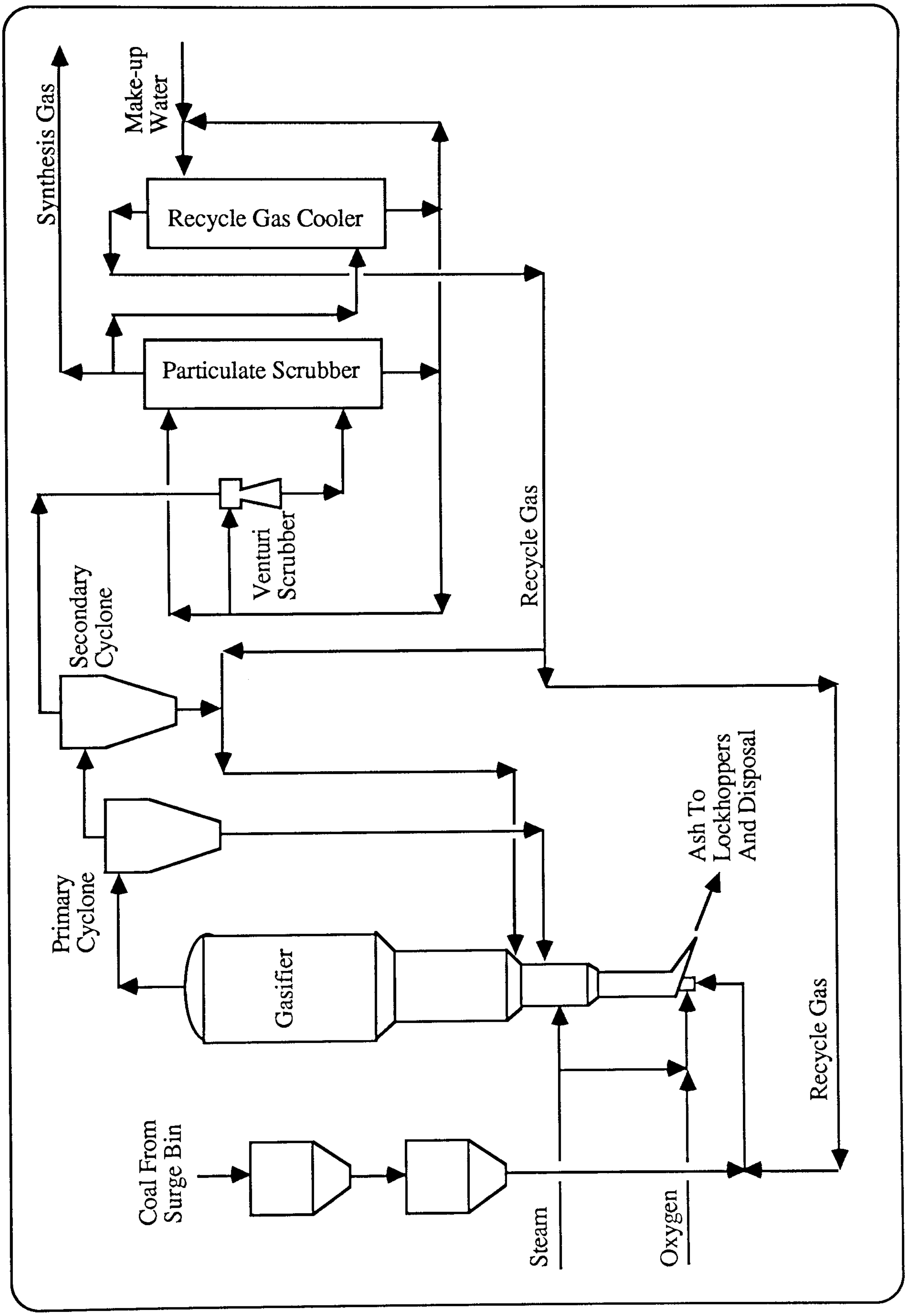

Figure 2.7 Kellogg Rust Westinghouse Gasification Process

A mathematical model of the U-Gas gasifier was constructed and included in the simulation program, however due to the similarity of the gasifier to the KRW gasifier in terms of technology, operating costs, conversion efficiencies, gas quality and plant capital cost, the results of the model where found to be indistinguishable form the the KRW gasifier. Therefore the results for this gasifier may be inferred from the results presented for the KRW gasifier. Both gasifiers are at similar stages of development and comparisons of technical reliability difficult to make from the reported data. For the purposes of this thesis the two gasifiers may be taken as economically indistinguishable.

2.5. Entrained bed.

Pulverized coal is injected into the gasifier with the reactant gases, either oxygen, steam or hydrogen. The gasifiers operate in the slagging mode as high temperatures are required for the reactions to proceed at a rapid rate, necessary for the short residence time characteristic of entrained flow reactors. Figure 2.9 shows a typical entrained flow gasifier. A list of gasifiers identified is given in Table 2.13.

Problems normally associated with entrained flow gasifiers fed with coal powder are with feeding pulverized coal dust under pressure into the gasifier and possible safety problems with coal dust explosions either inside or outside the gasifier[57]. This does not apply to gasifiers which are fed with coal slurry.

Table 2.13 Examples of Entrained Bed Gasifiers

Gasifier	Reactant gases	Pressure (bar)	Location	Status
Babcock & Wilcox	Oxygen	1	USA	Abandoned
Bell Aerospace	-	-	USA	Abandoned
Bigas	Oxygen/Steam	35-100	USA	Abandoned
CS Rockwell	Hydrogen	-	USA	Abandoned
Dow	Oxygen/Steam	30	USA	Commercial
GSP	Oxygen/Steam	30	E. Germany	On-going
Koppers-Totzek	Oxygen/Steam	1	South Africa	Commercial
Prenflo	Oxygen/Steam	30	W.Germany	On-going
Mountain Fuel Resc.	Oxygen/Steam	4	USA	On-going
Occidental Res. Corp.	-	1	USA	Abandoned
Shell	Oxygen/Steam	30	USA	On-going
Texaco	Oxygen/Steam	15-85	USA	Commercial

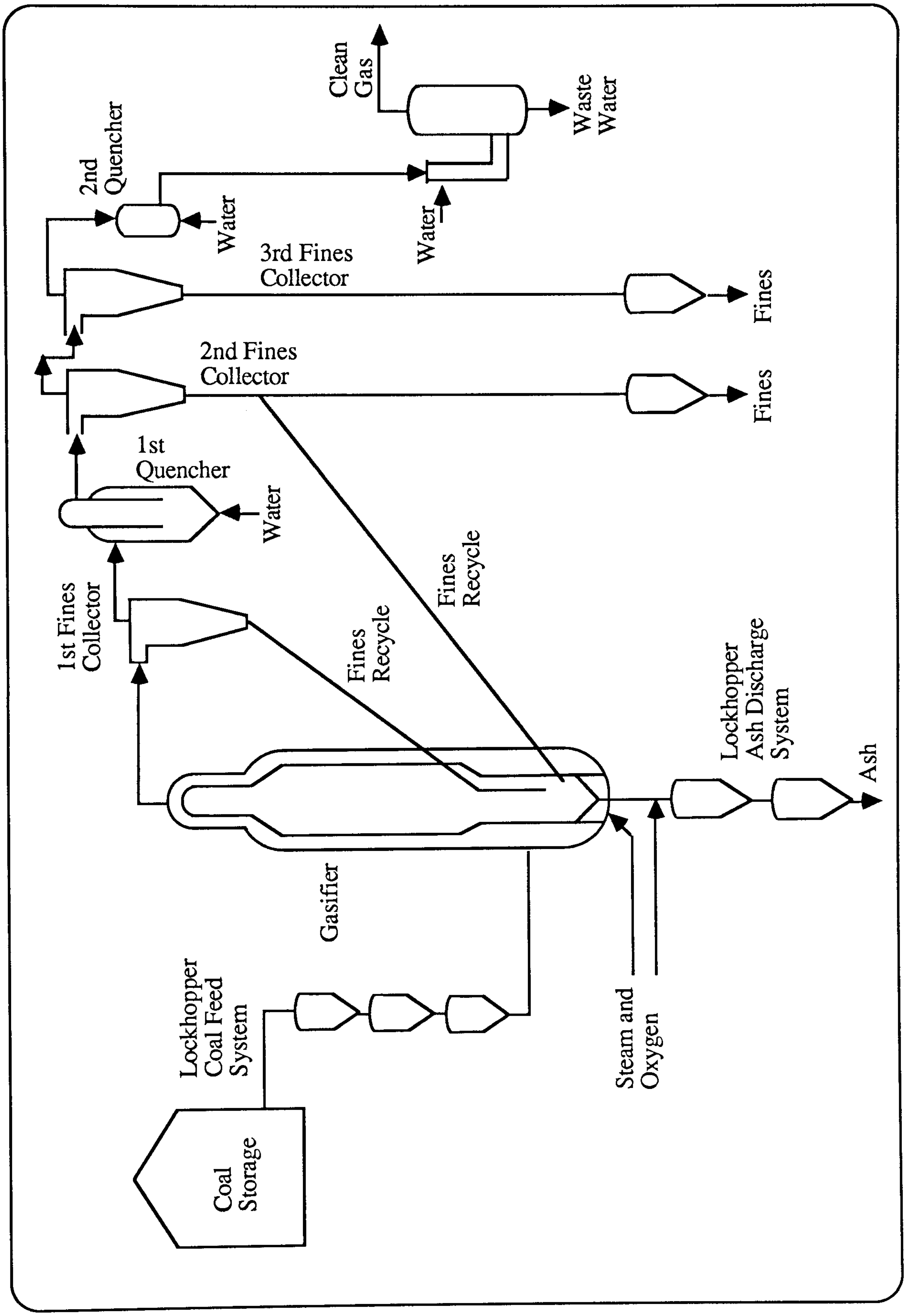

Figure 2.8 **U-Gas Gasifier Flow Diagram**

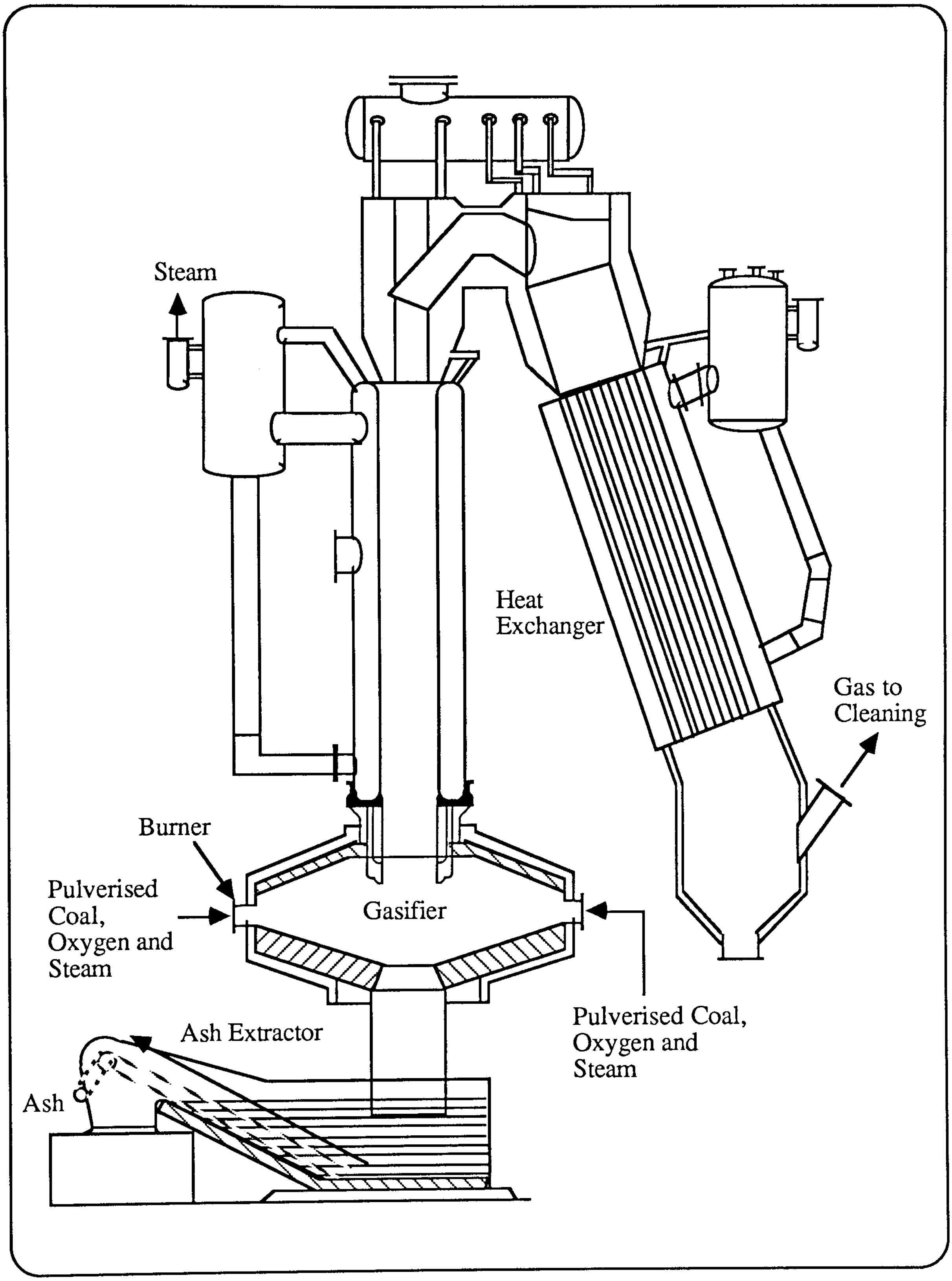

Figure 2.9 An Entrained Flow Gasifier (Koppers-Totzek)[58]

2.5.1. Koppers-Totzek

Many Koppers-Totzek gasifiers have been built to produce, in most cases, synthesis gas for ammonia or methanol production[59]. The most recent plants have been built within the last ten years[60]. Koppers-Totzek gasifiers in current use are shown in Table 2.14.

The gasifier operates at atmospheric pressure and the coal is blown into the gasifier with the oxygen and steam used as the gasifying agents. The reactor is refractory lined and surrounded by a water jacket from which low pressure steam is generated. High pressure steam is generated from the cooling of the product gas. The reactor operates at approximately 1800 °C. A disadvantage of the gasifier is the large quantity of energy which is converted to low pressure steam in the water jacket.

Table 2.14 Koppers-Totzek Gasifiers in Current Use

Location	Owner	Year of startup	Feed	Throughput net te/d	Gas * output	End product
Greece	Nitrogen. Fert. Ind.	1959	Lignite	635	629	NH_3,MeOH
Turkey	Azot Sanayii	1966	Lignite	454	775	NH_3
India	Fert. Corp. of Ind.	1970	Bituminous	2360	4000	NH_3,MeOH
S. Africa	African Expl. and Chemicals Ind.	1972	Bituminous	1360	2150	NH_3,MeOH
Zambia	NCZ Nitrogen Chem.of Zambia	1978	Bituminous	442	214	NH_3,MeOH
Brazil	PETROBRAS	1979	Bituminous	≈850	1500	NH_3
Poland		1980	Bituminous	≈1700	3070	

* 10^3 Nm^3/d

2.5.2. Texaco

The Texaco process has recently reached commercial status with several plants in operation around the world[61]. The gasifier is slurry fed, with the capability to handle a wide range of coal types. The possibility of disposing of a variety of waste materials, from asbestos and spent catalysts to a variety of hazardous organic wastes, by co-gasification with coal has also been proposed[62]. Texaco gasifiers in current use and proposed are shown in Table 2.15.

Table 2.15 Texaco Gasifiers in Current Use

Location	Owner	Year of startup	Feed	Throughput net te/d	Gas output 10^3 Nm^3/d	End Product
USA	EPRI/TEX., etc (Cool Water)	1984	Bitum.	900	1800	Power 110 MW
USA	Tenn. Eastman Co.	1983	Bitum.	820	1340	MeOH/ Ac. Anhy.
Japan	Ube Industries	1984	Bitum.	1500	80	NH_3
Germany	Ruhrchemie /Rurhkohle	1986	Bitum. /Lig.	720	50	NH_3
Sweden	Nynäshamn	Design	Bitum.	4700	350	MeOH, Pow, NH_3
PR China	Lu Nan	Design	Bitum.	380	20	NH_3
PR China	Shougang	Design	-	1000	55	Fuel

A flow diagram for this process is given in Figure 2.10. Coal/water slurry from the previous step (Entrained Flow Feed Preparation) is pumped into the gasifier with oxygen. Gasification takes place at a temperature above the ash melting point of the particular coal at approximately 1 400 °C[63], the temperature being moderated by the slurry water. The product gas contains CO, CO_2 and H_2 traces of methane and no liquid hydrocarbons. Unburned carbon contained in the crude gas can be removed in the quenching operation and recycled back to the slurrying operation in the feed preparation step. Two typical configurations are available for the Texaco gasifier[64], these are the Direct Quench mode, as described here, and applicable to liquid fuels synthesis, and Radiation Gas Cooler mode[65,66] which is more applicable for combined-cycle power plants due to the production of HP Steam. The direct quench mode is so called because the hot gas is cooled directly by contact with water in a water quench. The Radiation Gas Cooler mode cools the gas by radiation loss of the heat, this is used to raise high pressure steam.

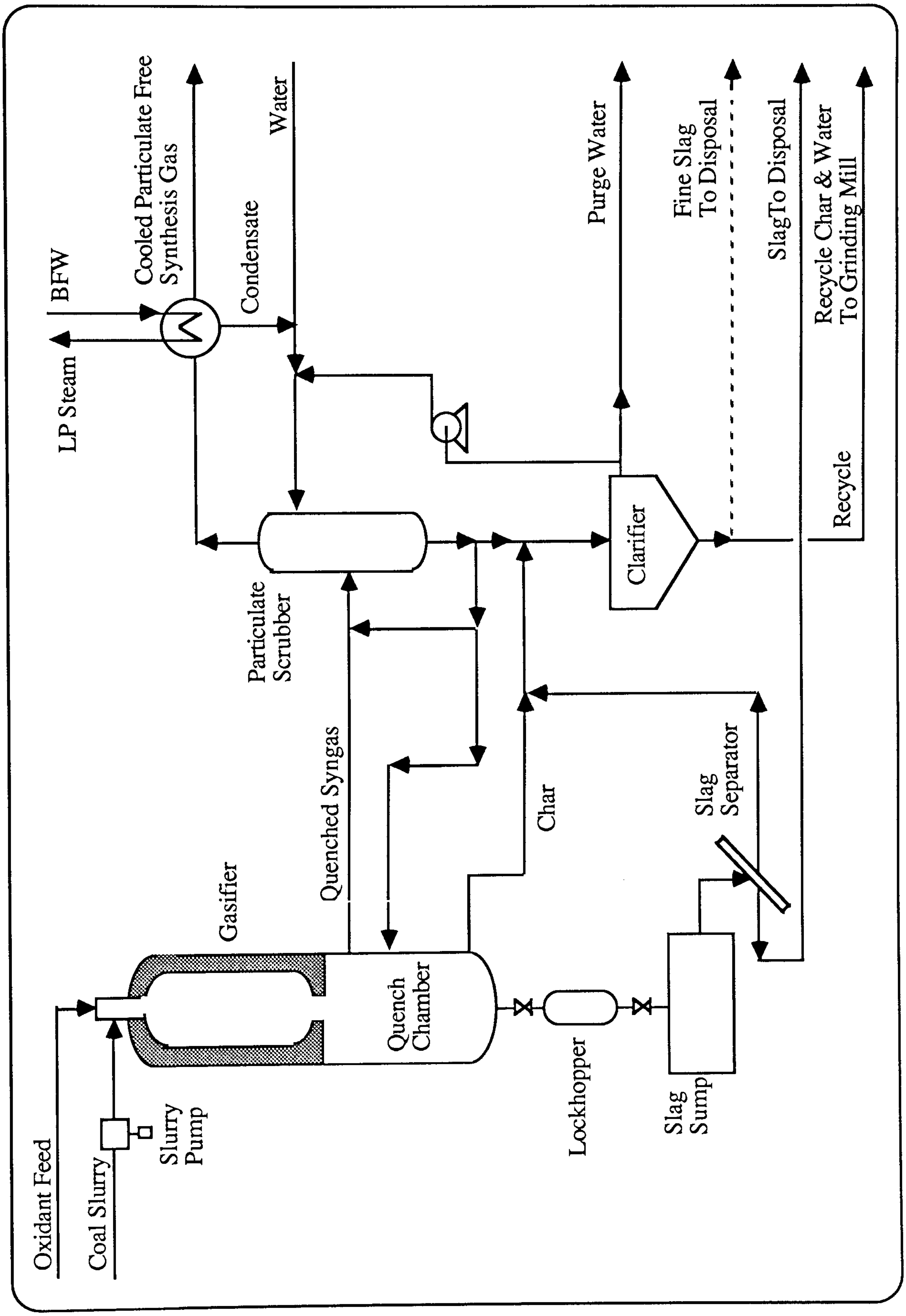

Figure 2.10 Texaco Gasification Process; Direct Quench Mode

2.5.3. Dow

In 1979 Dow constructed a 36 te/d plant and followed with a 1600 te/d plant in 1982[67]. Dow have constructed a 2200 te/d demonstration plant of their process to provide synthesis gas for chemical synthesis and co-generation of heat and power[68]. This plant was commissioned in 1987. The plant has a capacity of 30 Billion BTU/Day of medium BTU gas, making it the largest single train gasifier in the world at the present time. The syngas produced and the co-produced steam are utilized to produce 160 MW of power using modified Westinghouse turbines[69].

The Dow process at present utilizes feedstock with a concentration of typically 52 to 54 % solids in water for subbituminous coal, higher concentrations of solids are reported to be possible with better quality coals, chemical additives or more sophisticated grinding processes than the rod mill in present use[70]. The slurry is pressurized with positive displacement pumps and fed to the gasifier with oxygen to the first stage nozzles. A separate stream of slurry is fed to the second stage of the gasifier where it cools the stream of hot gas leaving the first stage of the process and is itself gasified by contact with the hot gases[71]. The molten ash from the coal is water quenched at the base of the gasifier and crushed, it is the passed through pressure reduction devices to atmospheric dewatering tanks. Water from the slag quenching is recycled.

Char and ash is removed from the hot raw gas in a high temperature cyclone. The char is then quenched with water and depressurized and then fed back to the first stage of the gasifier after concentration. Hot gas from the cyclone enters the high and low temperature heat recovery system.

The Dow gasifier has the advantage that it can utilize low rank coals such as Western Sub-bituminous coal and Gulf Coast Lignite as feedstock and retain the simplicity of a slurry feed system. Dow gasifiers in operation are shown in Table 2.16.

Table 2.16 Dow Gasifiers in Operation

Location	Owner	Year of startup	Feed	Throughput net te/d	Gas output 10^3 Nm^3/d	End product
USA	LGT	1978	Lig./sub-bit	36	≈60	-
USA	LGT	1983	Lig./sub-bit	1 600	≈3 000	-
USA	LGT	1987	Lig./sub-bit	2 200	≈4 000	161 MW

LGT Louisiana Gasification Technology

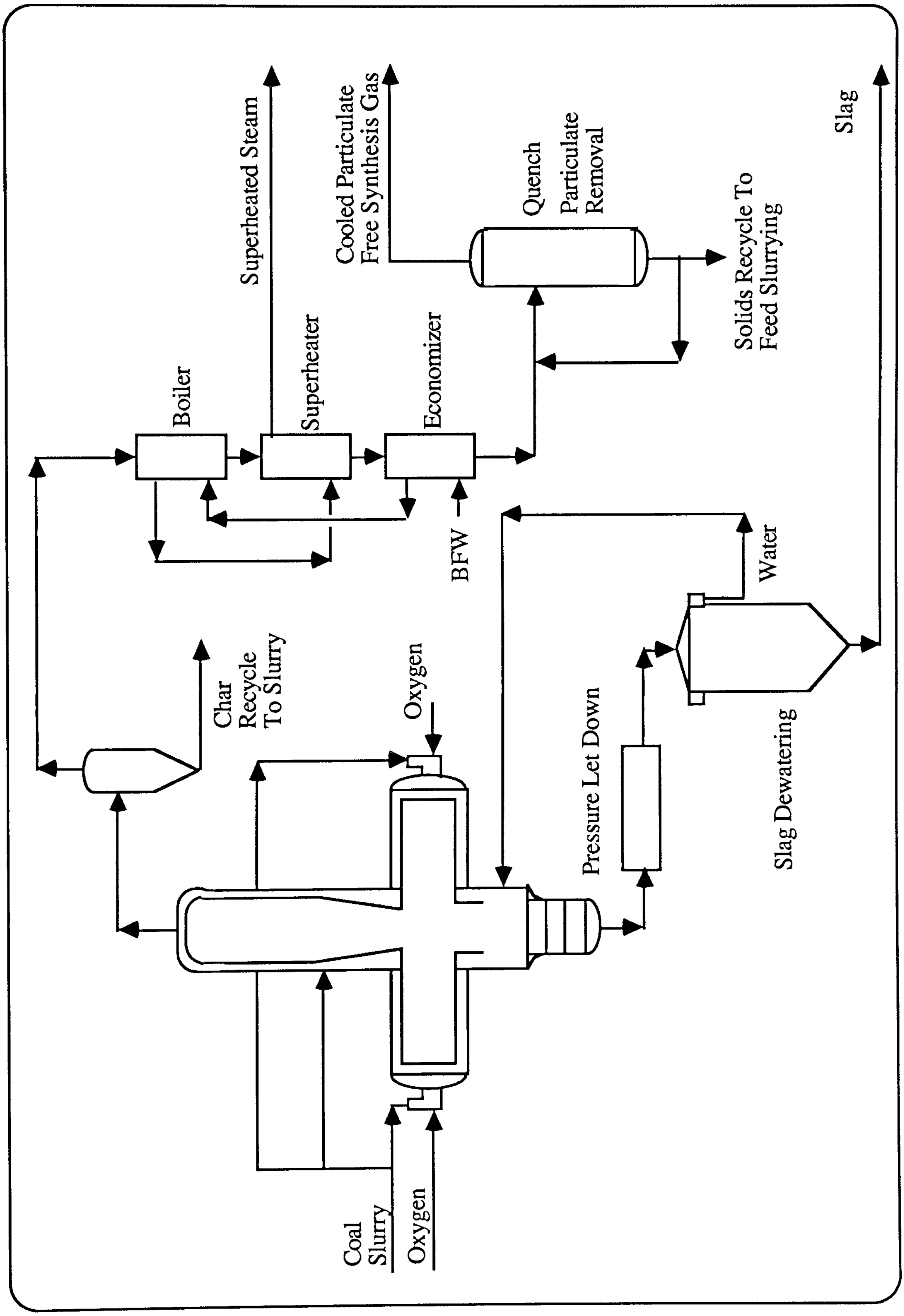

Figure 2.11 Dow Gasification Process

2.5.4. Shell

The feed coal for the gasifier is dried and pulverized and fed from storage pneumatically to the burners where the oxygen and steam (if required) is also fed to the gasifier. The operating temperature of the gasifier is within the range of 1400°-1700°C[72]. The ash melts and is removed from the bottom of the gasifier as slag, it is then quenched and disposed of.

The largest Shell coal gasifier built to date is a 250-400 te/d unit built at Houston Texas, which was commissioned in 1987[73]. The gasifier is dry fed with pulverized coal or lignite. In comparison with the Koppers-Totzek gasifier the Shell gasifier operates at elevated pressures, typically at 30 bar, for liquid fuels synthesis the operating pressure of the gasifier would be increased to up to 60 bar, depending on particular process configurations. Shell gasifiers in operation are shown in Table 2.17.

Table 2.17 Shell Gasifiers in Operation

Location	Owner	Year of startup	Feed	Throughput net te/d	Gas output 10^3 Nm^3/d	End product
W. Germany	Shell	1978	Coal/Lignite	150	≈300	MBG
USA	Shell	1986	Coal/Lignite	250-400	≈350	MBG & 16000 kg/h Steam

A flow diagram for this process is given in Figure 2.12. The Shell gasifier is fed with dried and pulverized coal or lignite, by gas transport, through lock hoppers. It is gasified as it flows upward through the gasifier. The product gas is composed of mainly CO and H_2, little CO_2 negligible methane and no liquid hydrocarbons. The slag runs down the side of the gasifier and into a water bath at the base of the gasifier, where it is removed through lock hoppers. Cold recycle gas is used to quench the product gas and prevent the entrained ash particles from agglomerating. The gas is then cooled in the heat recovery section where high pressure steam is generated before the gas is water scrubbed[74].

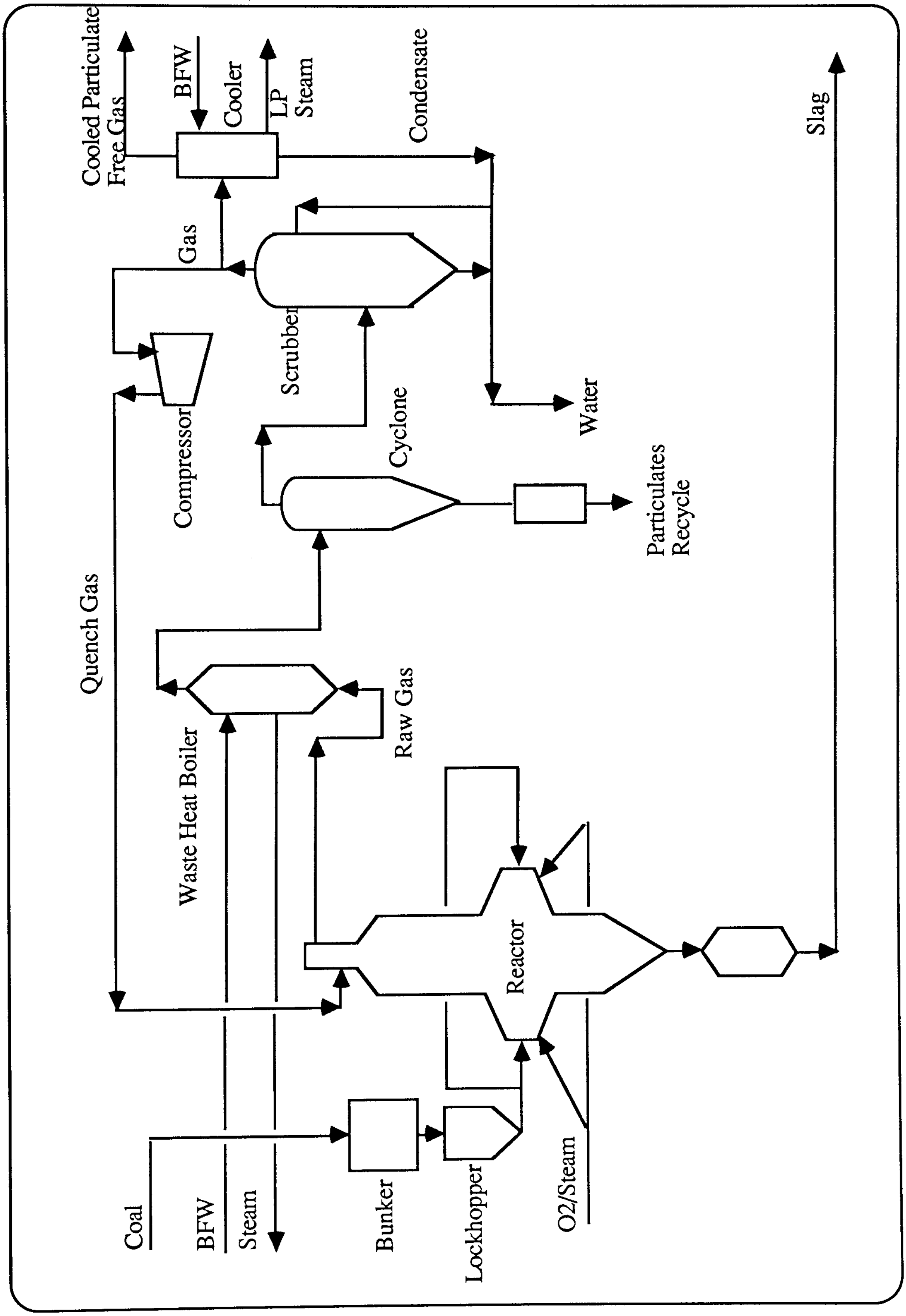

Figure 2.12 Shell Gasification Process

2.5.5. PRENFLO

From 1974 to 1981, Shell International Petroleum Maatschappij (SIPM) B.V. and Krupp-Koppers Gmbh, were developing the Shell-Koppers process jointly[75]. After 1981 the Shell and the PRENFLO processes were developed separately by Shell and Krupp-Koppers respectively. Both processes are pressurized versions of the Koppers-Totzek dry fed entrained flow gasifier. The PRENFLO process currently operates at a throughput of 48 te/day. A 1 000 te/d demonstration plant for power generation is in the planning stage[76]. Table 2.18 shows existing and planned gasification plants.

The PRENFLO process is shown in Figure 2.13. Coal dust is pneumatically conveyed to a cyclone and from there it is transferred by lockhoppers to feed bin which is kept under pressure, from there it is fed to the gasifier burners. Oxygen and steam if necessary is fed to the burners. The coal is gasified at a temperature of over 2000°C at the hottest point[77]. There is reportedly no limitation on the suitability of the feed coal with respect to reactivity, particle size, ash or sulphur content[78].

The reactor is lined with refractory lining which has a hot water re-circulating system which produces high pressure steam. Slag is discharged form the reactor into a water bath and the solid ash particles are removed via a lockhopper system. The raw gas leaves the reactor at between 1400°C and 1600°C. The raw gas temperature is reduced at the outlet by recycled cool clean gas to solidify entrained molten fly ash particles. The gas is then further cooled and de-sulphurised in a manner depending on the application of the gas[79].

Table 2.18 PRENFLO Gasifiers In Operation Or Planned

Location	Owner	Year of startup	Feed	Throughput net te/d	Gas output 10^3 Nm3/d	End product
W. Germany	Krupp-Kopp.	1982	Bituminous	48	≈100	Fuel Gas
W. Germany	Krupp-Kopp.	Proposed	Bituminous	1 000	≈1 480	Power (150 MW)

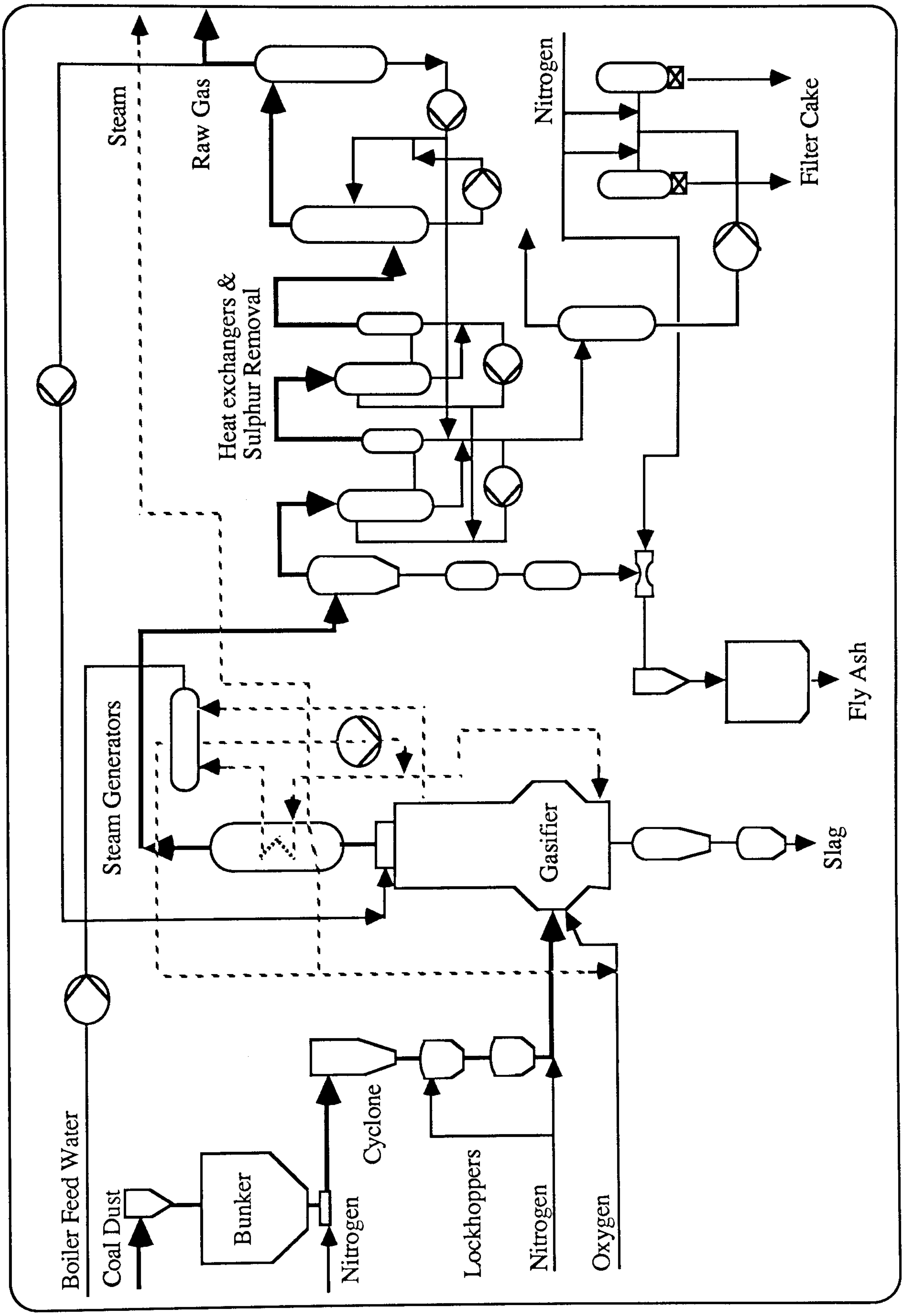

Figure 2.13 PRENFLO Gasifier Flow Diagram

2.6. Molten bath.

In these processes the coal is introduced into a bath of either molten slag, metal or salt with the gasifying agent. The operating temperature is dependant on the type of bath. The molten bath depending on the melt used can increase the rate of gasification of the coal by increasing the rate of heat transfer and by catalysing the gasification reactions. Another advantage is that much of the sulphur in the coal may be removed by absorbing it in the actual melt if molten salts are used or in substances such as limestone which may be added to the bath. A schematic diagram is given in Figure 2.14. Molten bath gasifiers were not included in the modelling due to the complexity of operation and comparatively small scale of development of the gasifiers. The most likely use of molten bath gasifiers would be in smelting iron ore for which the processes of smelting the ore and producing fuel gas to heat the process is combined.

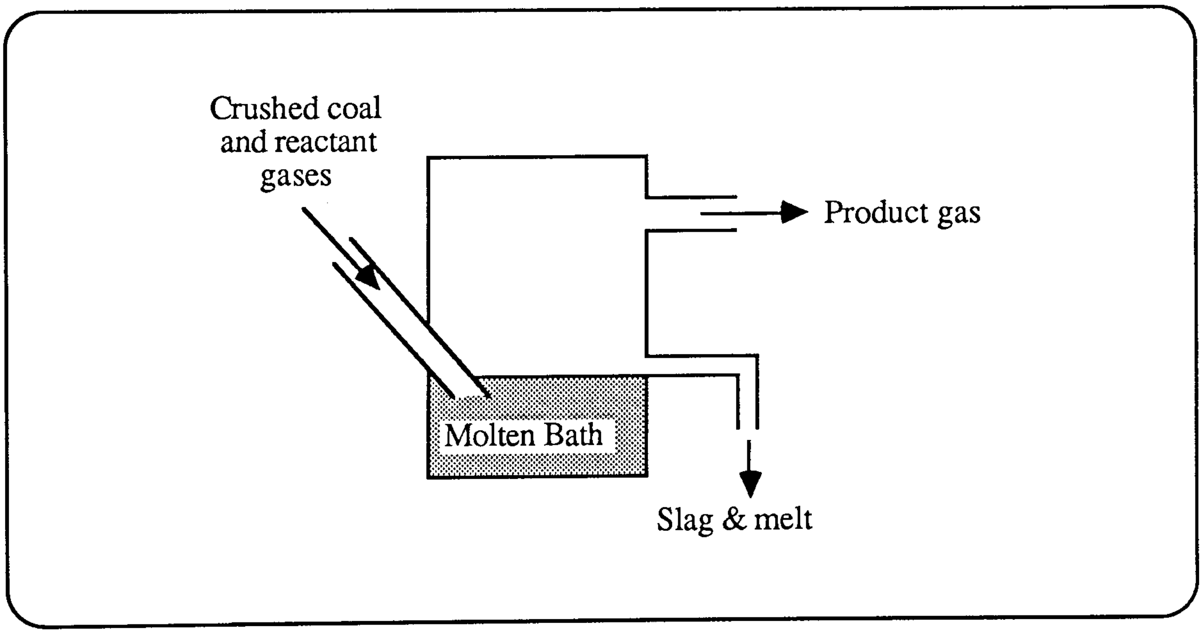

Figure 2.14 Diagrammatic Representation of Molten Bath Gasifier.

Table 2.19 Examples of Molten Bath Processes

Gasifier	Reactant gases	Pressure (bar)	Temperature	Location	Status
Atgas	Oxygen/Steam	4.4	Slagging	USA	A
British Steel				UK	
Humboldt Klockner	Oxygen/Steam	1-30	Slagging	Germany	O
Kellogg	Oxygen/Steam	1-30	Slagging	USA	A
Mitsubishi	Oxygen/Steam	1		Japan	O
Otto-Rummel	Oxygen/Steam	1	Slagging	W. Germany	A
Otto-Rummel 2 shaft	Air/Steam	1	Slagging	W. Germany	A
Rockgas	Oxygen/Steam	1-2	Non -Slagging	USA	A
Saarberg-Otto	Oxygen/Steam	26	Slagging	Germany	A
Sumitomo	Oxygen/Steam	1-30	Slagging	Japan	O
Sun	Steam/Air	1	Non-Slagging	USA	

2.7. Underground Coal Gasification (UCG)

Underground coal gasification (UCG) effectively combines coal mining and gasification into a single process unit, and this may have potential economic advantages over traditional mining and surface gasification methods. However a possibly greater consideration is the potential of UCG to convert otherwise un-mineable coal reserves into useful sources of energy or chemicals. For example it has been estimated that for the USA, UCG could quadruple the countries recoverable coal reserves[80]. UCG has been used in the USSR for many years as a source of LCV fuel gas[81]. Commercial status has not yet been achieved in the western world but plans for the commercial development of an UCG site in the Triunfo Coal area of Brazil, to produce a medium BTU gas, utilizing the Controlled Reverse Injection Point (CRIP) method exist and phase I of a three phase programme for commercialisation has been completed[82] .

Underground coal gasification techniques are site specific and therefore the application of the CRIP method as used at Triunfo, may not be directly applicable to European coals and conditions.

In situ gasification is performed while the coal is still in the coal seam. The site is prepared by drilling two vertical wells into the coal seam at a suitable distance apart. The wells are linked by channels in the coal seam which are formed by one of several possible methods e.g. pneumatic, hydraulic or drilling methods. One well is used to inject the gasification agents, while the other is used to collect the product gases. A schematic diagram is given in Figure 2.15 and Table 2.20 shows examples of underground gasification sites and organizations involved.

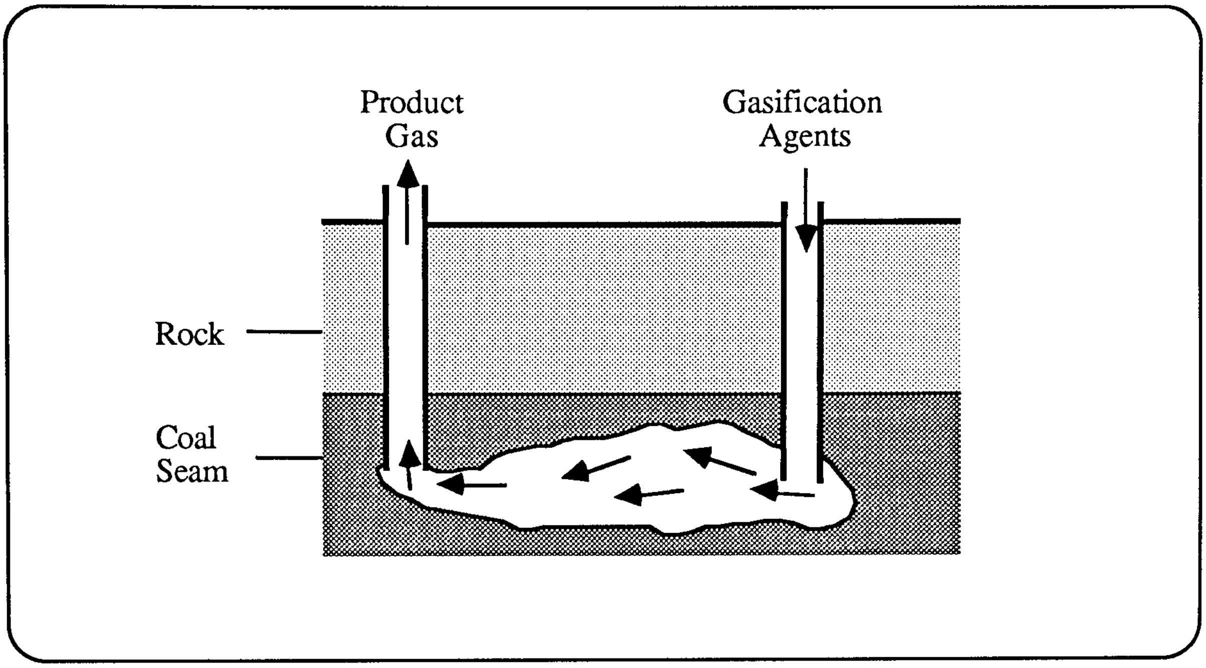

Figure 2.15 Diagrammatic Representation of Underground Gasification.

Table 2.20 Examples of Underground Coal Gasification Sites

Organization	Location	Coal gasified (In one test)	Duration (days)
IDGS	Belgium		
GEGS	France		
NCB, IDGS, GEGS	United Kingdom		
Law. Liver. Nat. Lab.	Washington	2 000 tonnes	30
Law. Liver. Nat. Lab.	Wyoming	3 251 tonnes	47
GULF	Wyoming	8 560 tonnes	66
ARCO	Wyoming	3 600 tonnes	60
Basic Resources Inc.	Texas		36
Texas A&M	Texas		2
US Department of Energy	W.Virginia	234 tonnes	12
GULF	Kentucky		
US Bureau of Mines	Alabama	236 tonnes	
US Department of Energy	Wyoming	3 414 tonnes	39

2.8. Gasification by Nuclear Process Heat

In these processes the heat for the coal gasification is supplied by high temperature nuclear process heat, via high pressure steam, rather than by the partial oxidation of the coal. Table 2.21 gives examples of processes utilizing nuclear process heat. The use of nuclear process heat has been considered for coal gasification because very high carbon conversion efficiencies approaching 100% are theoretically possible compared to about

50% for an autothermal process. This is possible as in autothermal processes whatever the technology used not enough energy is available to convert all of the carbon to CO and maintain high levels of H_2, in gasification by nuclear process heat the energy required to produce the hydrogen (by the endothermic reaction of steam on carbon) is supplied by the nuclear source.

Table 2.21 Examples of Processes Utilizing Nuclear Process Heat.

Process	Reactant gases	Gasifier type	Location
Bergbau Forshung	Hydrogen	Fluidised bed	W. Germany
Rheinische Braunkohlenwerke AG	Steam	Fluidised bed	W.Germany
Stone & Webster	Hydrogen	Fluidised bed	USA

2.9. Feed Requirements Of The Gasification Processes

The feed requirements of the various gasification processes vary in several different respects, these are:

- Size;
- Reactivity;
- Physical properties:
    - Caking and swelling properties;
    - Ash content;
    - Ash melting & softening point;
    - Moisture content;.

The above mentioned properties are generally those which form part of most grading and ranking systems for coals. However there is no ranking system which can be applied to coals for all gasifiers, therefore it is necessary to recognize the importance of physically testing coals in particular gasifiers to determine their suitability, although this may be inferred from similar coals already tested.

The price that coal can demand on the open market is related to its usefulness for particular purposes eg coke making. Gasifiers that can utilize efficiently a wide range of feedstocks are desirable for their ability to gasify coals that are comparatively cheap on an energy basis.

2.9.1. Required Feed Size

Gasifier feed size requirements vary from relatively large lumps of up to 50 mm for fixed bed gasifiers down to dust sized particles of below 70µm for entrained flow gasifiers. Fluidised bed gasifiers operate with feed coal sizes generally between these two extremes at approximately 6-10 mm sized particles.

2.9.2. Water Content

For the purposes of this report the water content of coals and lignites can be classified into two types. These are surface moisture and inherent moisture. Surface moisture which can be assumed to be all moisture contained on the surface of the coal and this includes that contained entrapped within the physical structure of the coal within capillaries. Inherent moisture is water that is chemically combined with the coal as water of gelation and hydration, and water associated with the decomposition of organic compounds. In order for coal to be successfully transported pneumatically it is normal for the coal to be dried to a few percent above the inherent moisture coal content. The inherent moisture coal content is generally greater for coals of lower ranks, values of inherent moisture content are not however readily available for different coals, but typical values are 2-3 for bituminous coals and 8-10 for lignites, these may however vary widely.

Drying of coal to a point above the inherent moisture content is a comparatively simple matter of exposing the coal to a hot dry gas, the energy being required is approximately 1500 BTU/lb after allowing for heat losses. The heat can be supplied by steam or from fuel gas. Drying of the coal to below the inherent moisture content requires a higher energy input per kg of moisture due to the energy required to break chemical bonds within the coal, and may lead to fire hazards due to the increased residence times and hence higher particle temperatures reached within the coal drier.

The required moisture content of these feeds is generally a function of the practicalities of handling the feed coal. For fixed bed gasifiers the coal is fed to the gasifier with run of the mine moisture content coal.

With fluidised bed gasifiers the moisture content of the feed coal may be lowered to prevent agglomeration of the coal in the feed mechanism or storage hoppers, a typical value of moisture content after drying being around 8-10% wt. The actual amount of drying required depending on the particular characteristics of the coal.

In the case of the dry fed entrained flow gasifiers the coal dust may be dried to a few percent moisture content to prevent agglomeration of the coal particles in the transport gas. For slurry fed gasifiers, the coal is pulverized and mixed with water to form a transportable slurry of coal in water. Generally a slurry is used which is loaded with as high a concentration of coal as possible, typically 65%, at slurry concentrations in excess of this the viscosity becomes large enough to adversely affect the pumpability of the slurry[83].

2.9.3. Reactivity

The reactivity of the feed coal is important in determining the suitability of the coal for certain gasifiers for example the High Temperature Winkler, which is limited to lignites and reactive coals[84]. It can also affect the specific throughput of the gasifiers. The coal reactivity is dependent on the chemical and physical structure of the coal and is in general (although not necessarily) lower for coals with a high inertinite content. The coal reactivity is however difficult to predict and estimates of gasifier throughput for coals of different reactivities must be obtained from experimental data.

2.9.4. Caking and Swelling

The caking and swelling properties of the coal determine its suitability for use in fixed bed gasifiers (e.g. Dry Ash Lurgi), caking coals causing problems by choking the bed. Fixed bed gasifiers which incorporate methods of breaking up the bed such as the stirrer in the British Gas Corporation/Lurgi gasifier are capable of handling caking coals and for this gasifier it is even considered an advantage, as more fines can be gasified with caking coals than with non-caking coals[85].

Entrained flow and modern fluidised bed gasifiers (excluding the High Temperature Winkler) are capable of handling caking coals

2.9.5. Ash Content and Properties

In fixed and fluidised bed gasifiers, the softening and melting points of the ash may determine the suitability of the coal for the gasifier as non slagging gasifiers must be able to operate below the softening point of the ash (eg Dry Ash Lurgi). Slagging gasifiers operate at above the melting point of the ash (eg BG/Lurgi). The temperature at which the gasifier can operate can affect the specific throughput of the coal and hence oxygen and steam requirements.

The ash content is a parameter which affects the heat balance of the gasifier, with greater ash contents in the feed leading to higher oxygen requirements due to the increased loss of enthalpy in the exit slag or ash stream. As the ash content of feed coals can vary widely this can have an effect on the gasifier heat balance and gasifying agent requirements.

A summary of feed requirements for each gasifier is given in Table 2.22

2.9.6. Classification of Coal

Most coal classification systems in use classify the coal according to its grade for a particular purpose, an example of this is the 'international classification'[86] which is strongly orientated towards coke making. Coal gasification can be strongly influenced by coal rank and therefore for the purposes of this project the type of coal classification adopted is the ASTM (American Society for Testing and Material) classification by coal rank [87]. This system is based upon fixed carbon level and heating value, see Table 2.23.

Table 2.23 ASTM Classification of Coals by Rank

Class	Group	Fixed Carbon % (daf)	Volatile Matter % (daf)	Calorific Value (kcal/kg) (daf)	Other Requirements
I. Anthracite					
	1. Metaanthracite	≥98	≤2		Non-agglomerating.
	2. Anthracite	92-98	2-8		
	3. Semianthracite	86-92	8-14		
II. Bituminous					
	1. Low Volatile	78-86	14-22		Commonly-agglomerating
	2. Medium Volatile	69-78	22-31		
	3. High Volatile A	<69	>31	≥7 840	Agglomerating
	4. High Volatile B			7 280-7 840	
	5. High Volatile C			6 440-7 280	
III. Sub-bituminous					
	1. Sub-bituminous A			5 880-6 440	Non-agglomerating
	2. Sub-bituminous B			5 320-5 880	
	3. Sub-bituminous C			4 648-5 320	
IV. Lignite					
	1. Lignite A			3 528-4 648	
	2. Lignite B			<3 528	

Table 2.22 Summary of Gasifier Feed Requirements

Process Type	Lurgi Fixed	BG/L Fixed	K-T Entrained	PRENFLO Entrained	Shell Entrained	Texaco Entrained	Dow Entrained	HTW Fluidised	U-Gas Fluidised	KRW Fluidised
Feed size range (mm)	6-50	6-50	<0.1*	<0.1*	<0.1*	<0.1*	<0.1*	<8	<6.5	<6
Maximum fines content (mm)	≈10% <6 mm	10-30%** <6 mm	N.A.	N.A.	N.A.	N.A.	N.A.	60%<1mm	10%<70μm	-
Maximum moisture (wt %) in feed	30	≈30	2-10	2-10	≈2-10	45	≈50	12-18	10-20	10
Ash										
Maximum wt %	35	≈30	40	-	30	-	-	-	20	-
Minimum wt %	-	-	-	-	-	-	-	-	10	-
Soft. Point (min °C)	1000	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	800	N.A.	N.A.
Rank/Grade or other requirements	Lignite to anthracite (non-caking)	Lignite to anthracite	All	All	All	Not lignites	Lignites & sub-bit coals	Lignite, reactive coals	All	All
Caking index (Gray King)	A-D	A-G7								
Swelling index		0-7								

*	(70%<75μm)
**	Depends on caking properties
N.A.	Not aplicable

It is possible to gasify the entire range of coal ranks from anthracites through bituminous, (strongly and weakly caking) to lignites. However not all processes can accept all ranks of coal, and process. Anthracite is unsuitable for gasification in Europe due to its relatively high price and relative scarcity to other coals. Although gasifiers exist in other parts of the world which are fed with anthracite e.g China.

Hard coal is available within the EEC both from member countries and from imports. Imported coal to the EEC is available at considerably lower cost than coal produced by member countries [88,89]. In the case of imported coal the plants will be sited near to suitable deep water ports or possible sites for ports. Lignite is not imported into the EEC in large quantities therefore only sources from within the EEC will be considered.

2.10. Selection Of Typical Feedstock Coals

In order to compare the effect of alternative feedstocks prices and qualities on the alternative process flow schemes in the model, three typical coals were selected and their properties relevant to gasification included in the model. These coals were one each of a bituminous, a sub-bituminous and lignite.

2.10.1. Bituminous Coal

Point of Ayr coal has been selected as a typical bituminous coal for inclusion in the modelling. The typical properties of this coal are given in Table 2.24 for the different grades and size ranges currently produced. The typical sale price is also given as quoted for February 1989, it should be noted however that this is not a cost of production figure and that the sale price may be subject to normal negotiations.

Table 2.24 Typical Compositions and sale prices for Point of Ayr coal

	Point of Ayr Trebles	Point of Ayr Treated Smalls	Point of Ayr Untreated & Blended	
			No 1	No.2
Size Range (mm)	100x38	32x0	32x0	32x0
Moisture Wt %	6	10.5	8.7	9.5
Volatile Matter Wt %	34.1	28.7	28	29.4
Fixed Carbon Wt %	55.7	45.8	49.6	47.1
Ash Content Wt %	4.2	15.0	13.7	14.0
Sulphur Wt %	1.4	1.9	1.47	1.5
Chlorine Wt %	0.17	0.16	0.19	0.12
Rank (B. Coal)	602	702	602	604
Swelling Index	3.5	2	4	0
Calorific Value kJ/kg (As received)	31 560	25 320	26 660	26 300
Calorific Value kJ/kg (DAF)	35 145	33 987	34 356	34 379
Sale Price At the Pithead (Feb 89)	£73.10	£51.10	£54.30	£53.50

UTIMATE ANALYSIS

Component	Carbon	Hydrogen	Oxygen	Sulphur	Nitrogen
Typical Wt %	84.1	5.2	7.9	1.6	1.2

2.10.2. Sub-Bituminous Coal

Table 2.25 gives the composition of the sub-bituminous coal used for the comparisons given in the results chapter. It represents a typical Sub-bituminous coal with high ash content and lower calorific value than the Point of Ayr coal used for the base case results as defined in section 6.1. The coal chosen was South African Sub-bituminous, which although not a European feedstock, represents typical low quality ('steam coal') coal which may be imported into Europe.

Table 2.25 Typical Compositions for Subbituminous Coal

UTIMATE ANALYSIS

Component	Carbon	Hydrogen	Oxygen	Sulphur	Nitrogen
Typical Wt %	78.8	4.3	13.6	2.0	1.3

PROXIMATE ANALYSIS

Moisture	Volatile Matter Wt %	Fixed Carbon Wt %	Ash Content Wt %	Calorific Value kJ/kg
12.4	29.8	39.5	18.2	30.51

2.10.3. Lignite

Table 2.26 gives the composition of the Lignite used for the comparisons of results given in Chapter 6. It represents a typical composition for Rhenish Lignite, which may vary considerably from particular samples. This feed was chosen for the comparisons as it has a high ash content, high moisture content and low calorific value.

Table 2.26 Typical Compositions for Rhenish Lignite

UTIMATE ANALYSIS

Component	Carbon	Hydrogen	Oxygen	Sulphur	Nitrogen
Typical Wt %	68.0	5.0	25.2	0.8	1.0

PROXIMATE ANALYSIS

Moisture	Volatile Matter Wt %	Fixed Carbon Wt %	Ash Content Wt %	Calorific Value kJ/kg
55.0	19.3	22.2	3.5	25 600

CHAPTER 3
SYNTHESIS GAS LIQUEFACTION PROCESSES

3.1 Introduction

After gasification of the feed coal and subsequent gas clean-up the gas must be converted to a suitable fuel, depending upon the market requirements. Several synthesis gas conversion processes exist and which produce a range of liquid fuels. These may be hydrocarbon based which represent the bulk of fuels in use at the present time or alcohols which although in use as fuel at the present time in several countries (eg Brazil, Cuba) represent fuels which may be considered less conventional and for which demand in the future may increase.

This chapter aims to give an overall impression of the alternative synthesis gas conversion processes available and the products that are obtainable from these processes. Detailed process descriptions are contained in Appendix A. Therefore in this chapter the discussion will be limited to overall process descriptions and the products obtained.

3.2 Fischer-Tropsch

All of the processes considered utilize the Fischer-Tropsch process as a least part of the route to producing liquid fuels from synthesis gas. The Fischer-Tropsch process catalytically converts synthesis gas (CO and H_2) into a variety of hydrocarbon, alcohol, ketone and organic acid products. A range of Fischer-Tropsch catalysts have been used including iron, cobalt, ruthenium and thorium dioxide each catalyst producing its own product spectrum, which may also depend upon the operating temperature and pressure. In the particular cases of methanol and methane almost 100% selectivity may be achieved but for higher molecular weight compounds the Fischer Tropsch process always produces a distribution of products.

3.2.1 SASOL

The Fischer -Tropsch process as used at SASOL produces motor fuels, liquefied petroleum gas, petrochemicals and petrochemical feedstocks. There are currently two reactor types in use, the Lurgi/Ruhrchemie developed Arge fixed bed reactor and the Kellogg developed Synthol fluidised bed reactor. These two reactor types produce a different product distribution from each other and operate under different conditions of temperature pressure and feed composition. The Arge and the Synthol reactors were utilized at SASOL 1 whereas the Synthol reactor only was utilized at SASOL's 2 and 3.

These are compared in Table 3.1. The range of reactions may be summarized as follows:-

At an H_2:CO ratio of 2.0	$n\,CO + 2n\,H_2 = (-CH_2-)n + n\,H_2O$
At an H_2:CO ratio of 0.5	$2n\,CO + n\,H_2 = (-CH_2-)n + n\,CO_2$
These are linked by the shift reaction	$CO + H_2O = H_2 + CO_2$

Table 3.1 Comparison of Fischer-Tropsch Fixed Bed and Fluidised Bed Operating Conditions and Product Distributions [90].

Conditions	**Fixed bed**	**Fluidised bed**
Temperature	220-255 °C	330 °C
Pressure	25 bar	23 bar
$CO + H_2$ Conversion	65%	85%
H_2/CO ratio in feed	1.7	2.8

Product composition, vol %

Conditions	**Fixed bed**	**Fluidised bed**
LPG (C_3 - C_4)	5.6	7.6
Gasoline (C_5 - C_{11})	33.4	72.4
Middle oils (Diesel, Furnace)	16.5	3.4
Waxy oil	10.3	3.0
Medium wax m.p. 59 °C	11.8	-
Hard wax m.p. 96°C	18.0	-
Alcohols, Ketones	4.3	12.6
Organic Acids	trace	1.0
TOTAL	100.0	100.0

In reality the reactions involved may be considerably more complex and are known to involve CO_2 in the reaction mechanism[91]. However the above reactions effectively summarize the overall situation. Although the Fischer -Tropsch process has been used commercially for a number of years in South Africa, the reactors and catalyst used produce a range of products which have disadvantages for straight liquid fuel production. These are a relatively high conversion of feed to methane and higher hydrocarbon gases and the production of waxy oils, alcohols, ketones and organic acids.

3.2.2 Shell Middle Distillate Synthesis Process (SMDS)

The Shell Middle Distillate Process has been tested on the laboratory and pilot plant stages and Shell are planning to bring the plant on stream in the early 1990's[92]. The process gives a product that consists of kerosine, gasoil and naphtha in two stages: the syngas is converted to heavy paraffin which is then converted to lighter products by hydro-isomerization and hydrocracking. By converting the syngas to heavy products, the production of fuel gas (C_1 & C_2 gases) is minimized, increasing the overall conversion to liquids. The products from the process are predominantly paraffinic. The information used to model the process is contained in Appendix A.

3.3 Methanol synthesis

Methanol can be produced from synthesis gas over a copper catalyst at a temperature of about 250 °C and a pressure of 50 to 100 bar. ICI was the first to introduce this process, in 1966, which improved upon earlier high pressure processes[93]. A number of similar processes have now become available[94]. The process has the advantage over other Fischer-Tropsch processes as only a single product is effectively produced (trace amounts of higher alcohols are produced). The methanol may be used as a fuel directly or converted to hydrocarbon fuels in further processes. The reactions may be represented as follows:

$$CO + 2H_2 = CH_3OH$$
$$CO_2 + 3H_2 = CH_3OH + H_2O$$

The information used to model the process is included in Appendix A where a more detailed description of the process is included.

3.4 Fuel Alcohol

Catalysts and processes have been developed by several companies for producing mixtures of alcohols, normally up to C_6 alcohols. The main constituent of the mixture is usually methanol with progressively decreasing amounts of the other alcohols as the molecular weight increases. The information used to model the process is included in Appendix A where a more detailed description of the process is included.

3.5 Mobil MTG and MOGD Processes

The methanol to gasoline (MTG) developed by Mobil is based on the ZSM-5 class of zeolitic catalysts and uses a methanol feedstock to produce a high yield of gasoline with low yields of methane, ethane and a very low coke yield [95]. The overall reactions may be represented by the simplified equation,

$$n\,CH_3OH = (CH_2)_n + n\,H_2O$$

The process has an overall conversion efficiency of up to 95%. Table 3.2 gives a comparison of products for two reactor types.

Table 3.2 Distribution of Hydrocarbon products from MTG Process [96]

Product Yield (wt% of methanol charged)	**Fixed bed**	**Fluid bed**
Gasoline	85.0	88.0
LPG	13.6	6.4
Fuel gas	1.4	5.6
TOTAL	100.0	100.0

The MOGD process uses a Mobil commercial zeolite catalyst to convert methanol to gasoline and diesel via olefins. Total methanol conversion to gasoline and diesel is 95%, and by altering the reaction conditions the product composition may be varied from 100% gasoline to 90% diesel / 10% gasoline[97]. The process has an overall conversion efficiency of up to 90%. The MOGD process is however more capital intensive than the MTG process. A comparison of products for fixed and fluidised bed reactors is given in Table 3.3. The information used to model the processes is included in Appendix A where a more detailed description of the process is included.

3.6 Product Characteristics

The end product of any process considered for this project must be a liquid that is readily assimilated into the conventional liquid fuel market, and for which a market value may readily be ascribed. The following products have been identified as meeting these criteria, and are included in the modelling work:-

- Gasoline;
- Diesel;
- Fuel oil;
- Methanol;
- Fuel alcohol (C_1-C_6 alcohols).

3.6.1 Gasoline

The products from the SASOL type Fischer-Tropsch plants effectively produce a partly refined crude oil which must be further refined and upgraded before the Gasoline may be considered suitable for marketing. The gasoline produced form the MTG and MOGD processes is blended gasoline fully compatible with current market requirements and has an RON of 93 and 94 respectively.

3.6.2 Diesel

Diesel can be produced directly from synthesis gas via Fischer-Tropsch or via methanol with the Mobil MOGD process. The products from the MOGD and the SMDS processes are fully compatible with conventional Diesel market requirements.

3.6.3 Methanol

Plants are in commercial operation to produce methanol from coal derived synthesis gas, such as in South Africa where the ICI methanol process is used to convert synthesis gas from a coal fed Koppers-Totzek gasifier[98]. Methanol is usually used as a gasoline extender in blends of up to 5% methanol for engines with no modification or of blends of up to 15% methanol for modified engines[99]. It may also be used as a neat fuel in modified diesel engines, and work has been carried out to use dissociated methanol in a conventional spark ignition engine[100].

3.6.4 Fuel alcohol

Fuel alcohol can be manufactured in a modified methanol process. It is composed of a blend of C_1-C_6 alcohols and has the advantage of being more miscible with gasoline than methanol and therefore more useful as a gasoline extender[101]. A 7 000 barrel per day demonstration plant is being operated in Japan by the Idemitsu Kosan company with a selectivity of 99% for C_1-C_6 alcohol conversion from synthesis gas[102]. Several companies have developed and patented processes[103] including IFP which is the process modeled in this thesis and for which a process description is contained in Appendix A.

3.6.5 Fuel oil

Fuel oil is a by-product of the commercial Fischer-Tropsch processes in commercial operation at SASOL (South Africa). For the processes included in this thesis the only possible source of fuel oil is from the pyrolysis tars produced from fixed bed gasifiers. As these would be recycled back to the gasifier or used on site as fuel, they would not be required to meet market specifications, they would be regarded as low to medium sulphur fuel oil as most of the sulphur exits the gasifier as hydrogen sulphide in the gas product stream.

Figure 3.1 shows the Gas Conversion Processes Discussed and the Range of Products.

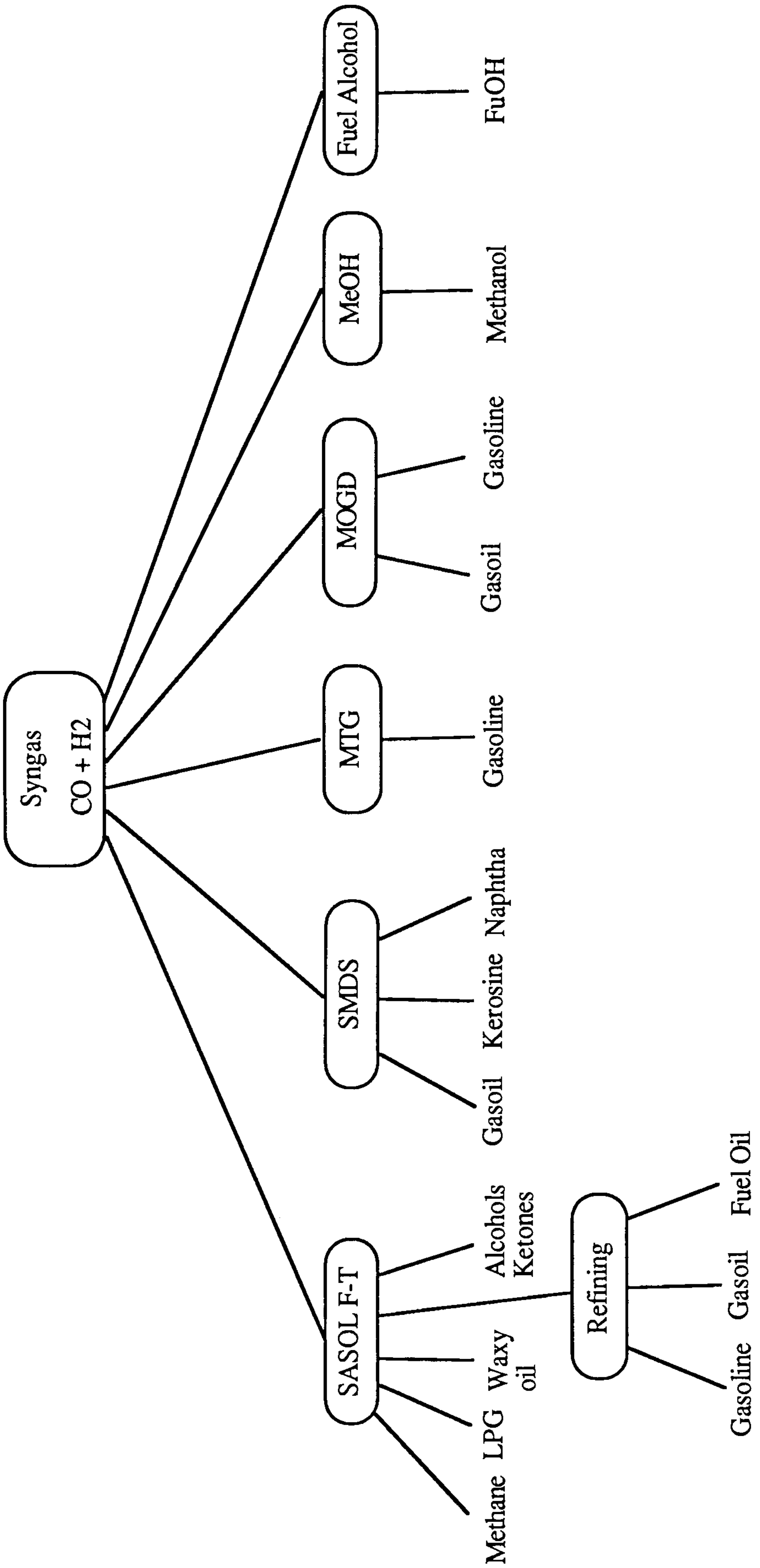

Figure 3.1 Gas Conversion Processes and Products

CHAPTER 4
THE COMPUTER MODEL

4.1. Introduction

The computer model was designed to have the ability to combine a series of step models which model individual sections of a coal conversion process and to produce a complete mass and energy balance for the complete process and to perform the economic calculations required.

4.2. The Model Structure

The computer model, which originally began development as part of a technoeconomic study of biomass conversion technologies[104], was modified to allow the program to be used for the modelling of indirect coal conversion processes. The model is divided into a number of separate parts, the executive program, data input and output sub-programs and the process step sub programs. Figure 4.1 shows the structure of the program.

The main executive program handles the selection of the process, input and output of data, economic calculations and the passing of information between the relevant step models. The step models perform the modelling of the individual process steps, such as gasification or methanol synthesis. Each step model contains all the relevant process information for that step, the step model calls the required subroutines to calculate the mass and energy balance in the correct sequences. In the gasifier models, for example, the step model calls the correct gasifier mass and energy balance calculation subroutines, and any other subroutines which may be required, such as to calculate the water quenching of the gas. After completion of the mass and energy balances and capital cost estimation, the executive section of the program summates all the information and calls the routines which calculate the operating and production costs and provides output to the user in the form of a summary on the screen and as text files on disk.

4.2.1. The Object Orientated Model

The programming language used for the modelling is object oriented Pascal on both IBM and Apple Macintosh computers. An object oriented language is one in which the code is set up as a series of objects which contain functions and procedures (known as methods) which describe how the object behaves when information known as messages are sent to the object. An object may inherit methods and variables from a parent object or objects[105], objects that have the same parent object or objects are said to be of the same class. Similarly an object which inherits methods and variables from an object of another class is in a subclass of the parent objects class.

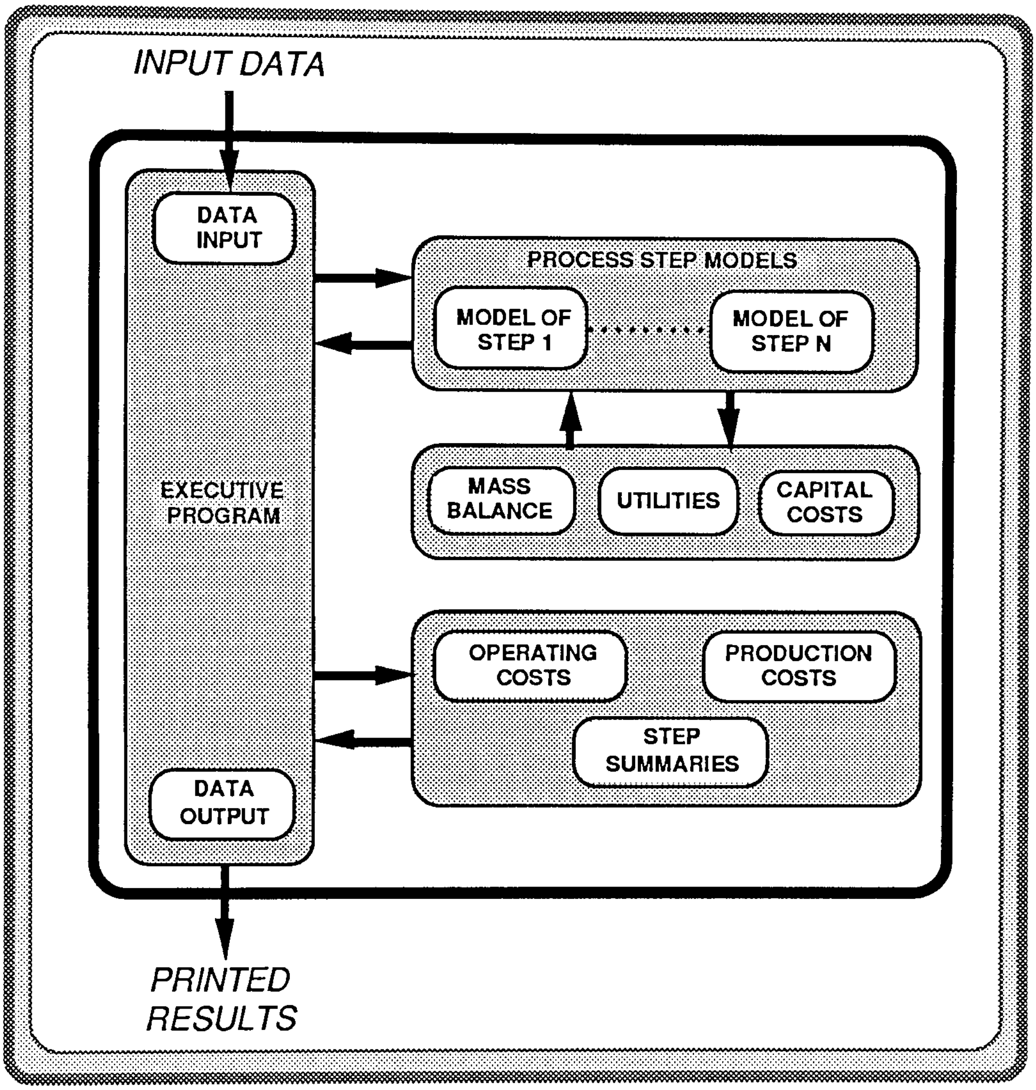

Figure 4.1 Representation of the Computer Model

Object oriented languages were originally developed for modelling real world phenomena where individual items are described as an object and the way the object behaves is described by the functions and procedures contained within that object[106]. For example the behaviour of an object, called Gasifier, is described by the methods contained within the object which perform the mass and energy balance, characteristics of the object are also inherited from other ancestor objects, such as T.GASFUNCS, which contains information describing the behaviour of the gases present in the gasifier.

Using an object oriented language improves the ease with which models of pieces of process plant or sections of process plant may be constructed as separate pieces of code and used by different sections of the overall program without duplicating the source code. Figure 4.2 shows an example of the code structure for two gasifier models. The gasifier objects, which are members of the same class called T.STEPS both send information to the class T.GASIFMODELS, which contains the basic gasifier routines. The correct gasifier routines are selected according to the information sent to the object T.GASIFMODELS, the object performs the gasifier calculation routines and passes the results back to the object (Step 202 etc) which called it. The object T.GASIFMODELS, as part of the calculation sequences contained within it, calls the object T.GASFUNCS which contains the basic routines which calculate the gas properties. The relevant calculation is performed and the results are available to T.GASIFMODELS. The Gasifier Steps 306 and 302 also call the method called Quench, which performs the function of quenching the product gas and calculating parameters such as gas temperature after quenching and the take up of water into the gas. The object T.STEP 302 first calls object T.GASIFMODELS and when Quench is not located there it automatically looks in the the Ancestor Class T.GASFUNCS, finds the method and performs the task required.

This programming structure has the advantage that each gasifier can use the same basic routines to perform similar functions without either duplicating the source code for each time it is required in the program, or making every subroutine global which is wasteful of computer memory and computing time. This structure also means that routines which perform a similar function can be located in the same file, simplifying program code structure and development. Changes are also easily incorporated by modifying the methods contained within an object or adding new methods to those already present. The independent nature of objects also has the advantage for program development, that the internal structure of the object is not visible to any other object or the main program, only the correct information has to be supplied to the object, this means that object can be developed independently of the main program and simply added to it when required.

The overall aim of using an object oriented approach was to minimize the amount of source code required, enable modifications to existing models to be made efficiently with no effect on other models, to increase the ease of which new models could be added to the program, and to increase the flexibility of the entire program.

The implementation of this approach led to the following construction for the model shown in Figure 4.3, with each object containing routines that were similar in function or a particular section of plant to be modeled and showing the inheritance paths of the objects, that is the classes and subclasses of the objects. For example all the routines necessary to simulate a gasifier are contained in two objects which can be called from the applicable gasifier model (which is also an object) and which contains only the necessary data and required procedures to be used from the relevant object containing the gasifier modelling methods. Table 4.1 gives a description of the objects used and their main function in the program:-

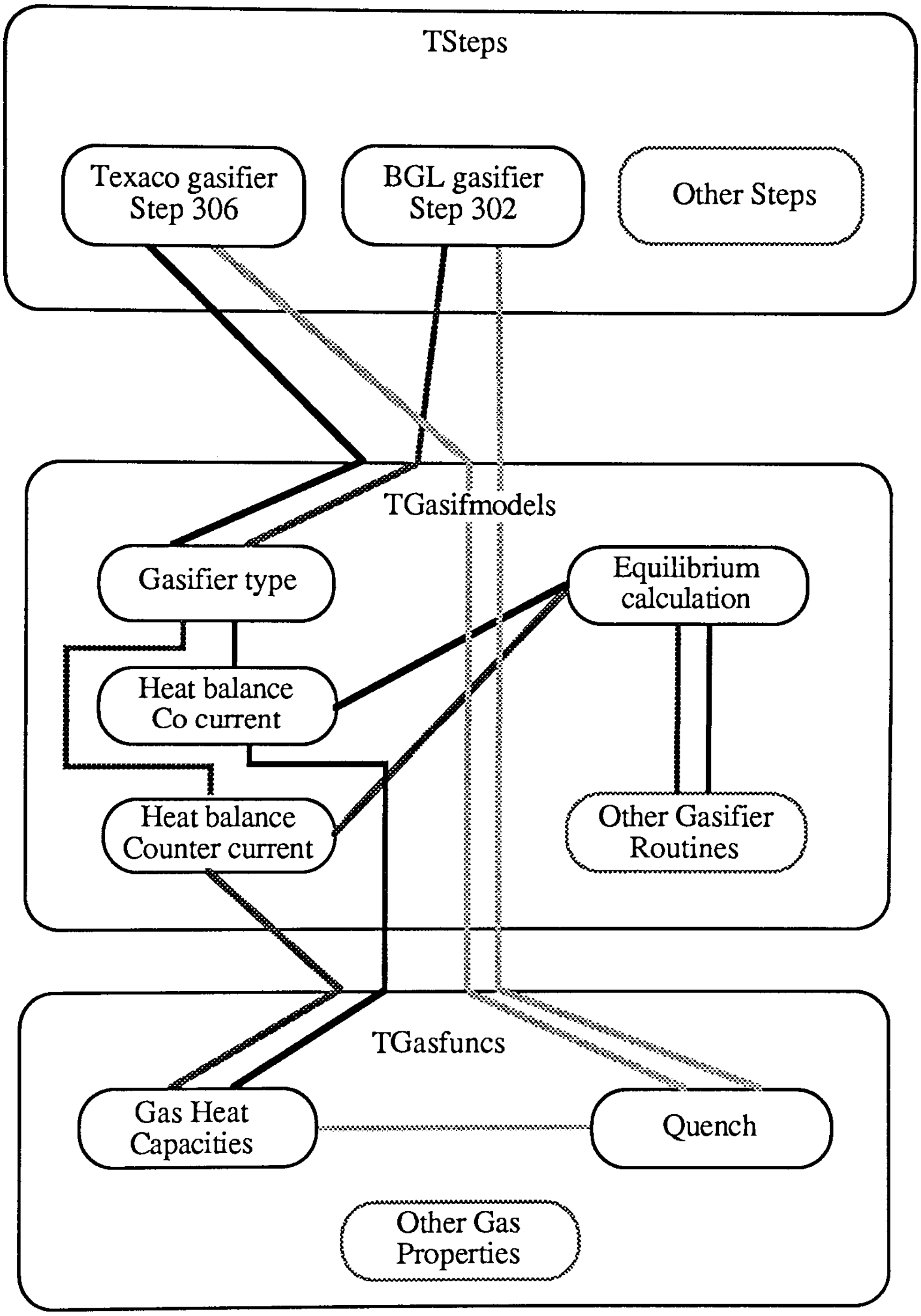

Figure 4.2 Example of Program Structure

Table 4.1 Program Objects Used

Object	Description
BASE OBJECT	Contains necessary definitions for object Pascal to operate
GLOBALS	Contains the declaration of the constants and variable which are required by all sections of the program
BASICFUNCTIONS	Contains the basic mathematical operations methods eg raising X to the power Y
MAINPROCEDURES	Contains the main methods used by the program for financial calculations and data handling etc
RW	Contains all the main methods for inputting and outputting data to the screen and to the data files
STEPFUNCS	Contains the methods for dealing with handling of data between step models and for checking data compatibility
STEPS 101-666	Individual objects for each step
CALLSTEPS	Contains necessary methods for calling the steps in the correct sequences
GASFUNCS	Contains the methods to calculate basic gas properties such as heat capacity and higher heating value, used mainly by the gasifier models
GASIFMODELS balances	Contains the methods used by the gasifier step models to calculate the output gas composition and the utility of the gasifiers
CAPCOSTS	Contains the methods used to calculate the capital cost and utility balances of the synthesis gas conditioning steps ie CO_2 removal
GASPROCS 1,2,3 conversion	Contains the methods used by the synthesis gas models to calculate the mass balances from raw synthesis gas to the liquid product
SYNTHESIS UNITS relate	Contains the methods as in T.GASPROCS but which to specific synthesis gas conversion technologies eg methanol, fuel alcohol or SMDS;
MAINOBJECT	Contains the code necessary to run the program in the correct order by calling the correct object methods in the correct sequences;
MAINPROG	Contains the main program heading and calls the main object.

4.3. Multiple Stream Sizes

Multiple streams for both gasifiers and methanol synthesis process are taken as being of equal sizes. For example a plant designed for 5000 te/day of methanol would have two 2500 methanol synthesis streams. This is because although theoretically there is a slight capital cost saving in having one stream of 3000 te/day and one 2000 te/day for example, in practice the benefits of two identical streams such as reduced design effort, identical maintenance considerations and experience gained in building the first stream being applicable to subsequent streams would potentially reduce the cost of multiple identical streams considerably. This considered so important that in South Africa Sasol III was an identical copy of Sasol II to the point that the site for SASOL III was first landscaped to be identical to SASOL II before construction began.

This general principle applies to all the gasifier and synthesis process combinations due to the use of multiple streams at throughputs of more than 5 000 te/day of feed.

4.4. Feed Preparation Step Modelling

Four distinct feed preparation steps have been modeled to cover the range of physical feed preparation required (as discussed in section 2.8) for the range of gasifiers which are being included in the project. These have been modeled as distinct steps with minor variations in feed specifications being handled by the relevant feed preparation step (as explained below), where necessary. The steps have been defined as in Table 4.2:-

Table 4.2 Feed Preparation Steps

Step Name	Typical Step Product Size	Typical Step Product Moisture Content
Fixed bed feed preparation	6 to 50 mm	As received
Fluidised bed feed preparation	3 to 8 mm	10 wt %
Entrained flow feed preparation (Dry)	70 % <0.01 mm	2 wt %
Entrained flow feed preparation (Slurry)	70 % <0.01 mm	35 to 50 wt %

The coal preparation steps contain several simplifying assumptions which are as follows:

1 The power requirements of coal crushing and pulverizing are assumed not to vary with the type of coal being fed but only with the flowrate on a moisture free basis. This a simplification of the real situation where power required is dependent on the physical properties of the coal and ash. The real power requirement must be determined by experimentation and is therefore beyond the scope of the project. As can be seen from the sensitivity studies in section 7.2 the power used has a comparatively insignificant effect on overall system performance, therefore the effect of this assumption is negligible.

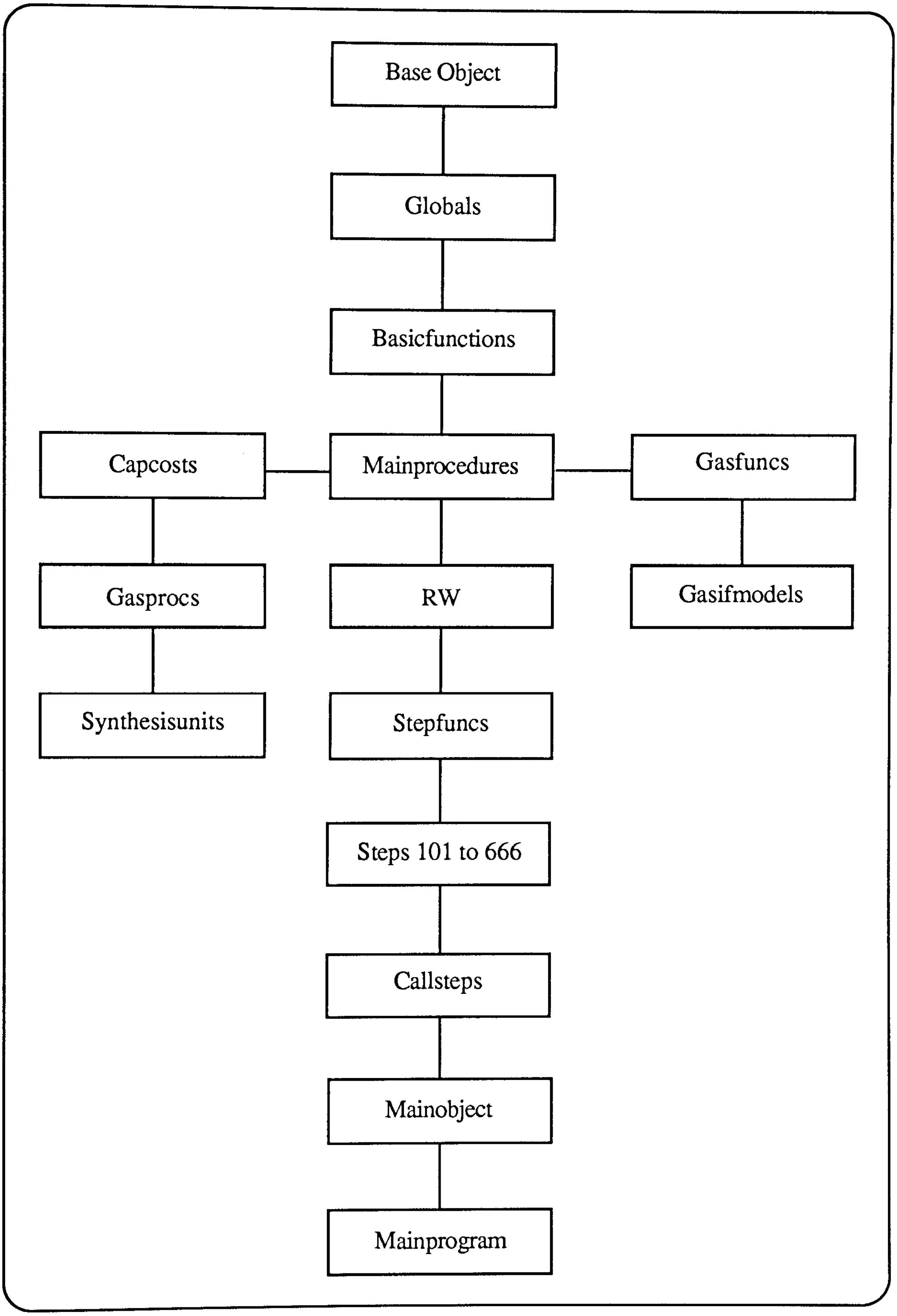

Figure 4.3 **Inheritance Paths for The Objects Contained Within the Program**

2 Coal is assumed to be delivered either as run of mine coal which will require size reduction to below 50 mm in what is here defined as a primary crushing step, or delivered as pre-crushed coal below 50 mm in size, as for example would be obtained by washed or imported coals. The results presented in Chapter 7 are based on the use of pre-crushed coal for which the cost of crushing is included in the cost of the coal.

3 Size distributions must be normally assumed for the feed coal to enable excess fines levels to be calculated for the fixed bed feed preparation steps. Excess fines can be utilized for example either to generate utilities, or processed and fed into the gasifier as briquettes. In reality the size distributions of as-received coal can vary depending on a wide range of factors which include:

- Physical, properties of the coal or lignite;
- Method of coal mining;
- Method of coal handling and transport.

Therefore the coal will be assumed to be delivered sized, with fines reduced to below 15 %. Power requirements and capital costs are estimated on this basis. Many different flow schemes are possible for coal preparation depending on for example method of coal drying, type of grinding/crushing equipment method of coal reception etc, those given here are intended to give a common basis for comparing the different processes and are typical of schemes proposed for coal preparation for gasification[107]. To give a common basis for comparisons of the feed preparation steps the heat required for drying the coal is obtained from steam in both the fluidised and dry entrained coal preparation steps, rather than from different sources such as natural gas which would make comparisons less reliable and also inefficient.

4.4.1. Feed Preparation Step Specifications

The feed preparation steps have been divided into the following sections:

1 Reception storage and reclaiming of coal;
2 Fixed bed feed preparation;
3 Fluidised bed feed preparation;
4 Entrained flow feed preparation (slurry fed);
5 Entrained flow feed preparation (dry fed).

The coal is first received at the site either by train or barge and sent to storage. It is then prepared for the type of gasifier for which it is intended. For fixed bed gasification it is screened to remove excess fines and oversized coal, which may be recycled and crushed. For fluidised bed gasification it is crushed to below a maximum size of about 1 cm and dried to a specified moisture level depending on coal type. For the entrained gasifiers the coal is pulverized and either dried for the dry fed gasifiers or slurried in water for the slurry fed gasifiers. The steps are shown in Figure 4.4.

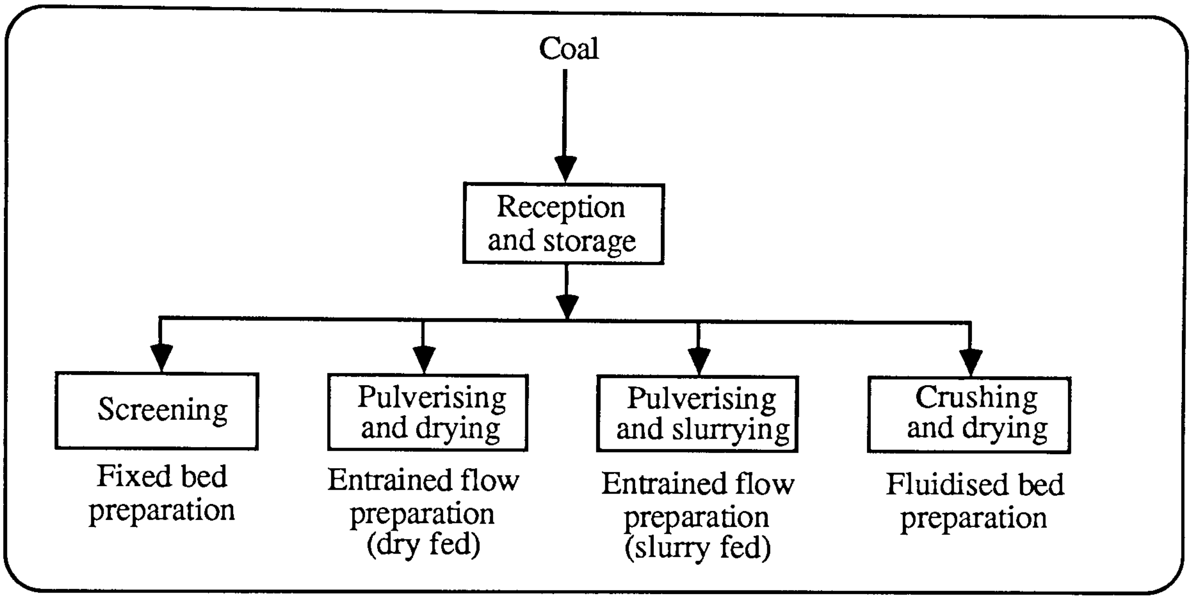

Figure 4.4 Feed Preparation Steps

4.4.1.1. Reception, Storage and Reclaiming of Coal, Step 101

A flow diagram for this step is given in Figures 4.5 and 4.6. Coal or lignite is received at the plant site by train and placed in an unloading hopper for temporary storage. The coal is withdrawn using vibrating feeders and placed on a receiving conveyor as shown in Figure 4.5. The transport rate is measured by a belt scale. Metallic fragments are removed by a magnetic separator to prevent damage to downstream equipment. From here it is conveyed to a double boom stacker which stacks the coal into two live storage piles which are covered by a roof for weather protection, normal live storage is assumed to be 7 days. Space is also provided for a dead pile of up to 60 days storage. A portion of the coal is supplied for sampling of the feed quality to a sampling system.

The coal is reclaimed from storage by a bucket wheel reclaimer which can be moved between the live storage piles. The coal is then conveyed to a surge bin before conveyance to the feed preparation steps.

4.4.1.2. Fixed bed preparation, Step 211

A flow diagram for this step is given in Figure 4.7. Coal from step 101C (reception storage and reclaiming), if run of mine coal, is conveyed to hammer mill where it is reduced to below 50 mm. From the hammer mill it is sent to a vibrating screen where the coal is screened, excess fines are removed and sent to a fines storage bin for further processing or utility use. The excess fines may be briquetted, agglomerated or pulverized and slurried for return to a gasifier such as the BGL gasifier. Oversized coal is recycled for further crushing, sized coal is sent to a coal storage bin for use in gasification steps. This represents the case where coal is received as run of mine coal. In many situations the production of excess feed fines, which may be created by the crushing, screening and handling of the coal and which could not be utilized on site, would encourage the use of pre-sized coal being delivered to the conversion site, reducing the fines content problem. If pre-sized coal is utilized as is assumed in this report the step performs screening and conveying of the coal to the gasifier from the storage pile.

4.4.1.3. Fluidised bed preparation, Step 221

A flow diagram for this step is given in Figures 4.8 and 4.9. Coal from the previous step (Reception, storage and reclaiming) is conveyed to the primary crushers to reduce the particle size to below 50 mm (if required). From here it is conveyed to a surge bin and hence to a hammer mill. From here the coal is conveyed to a coal dryer where hot nitrogen, heated by steam, is blown over the coal to dry it to the required moisture level.correct gasification process requirements (see section 2.8).

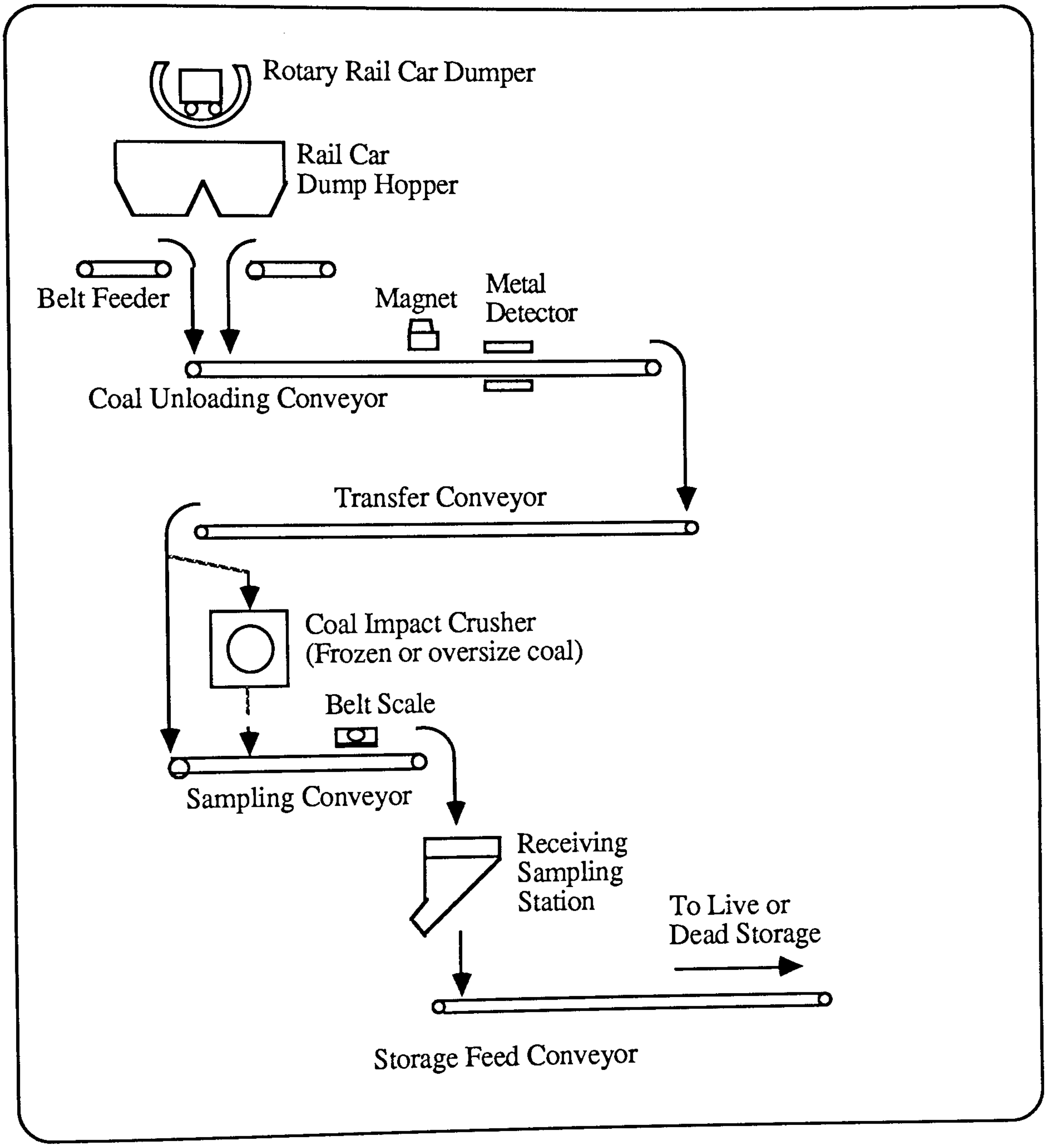

Figure 4.5 Coal Reception

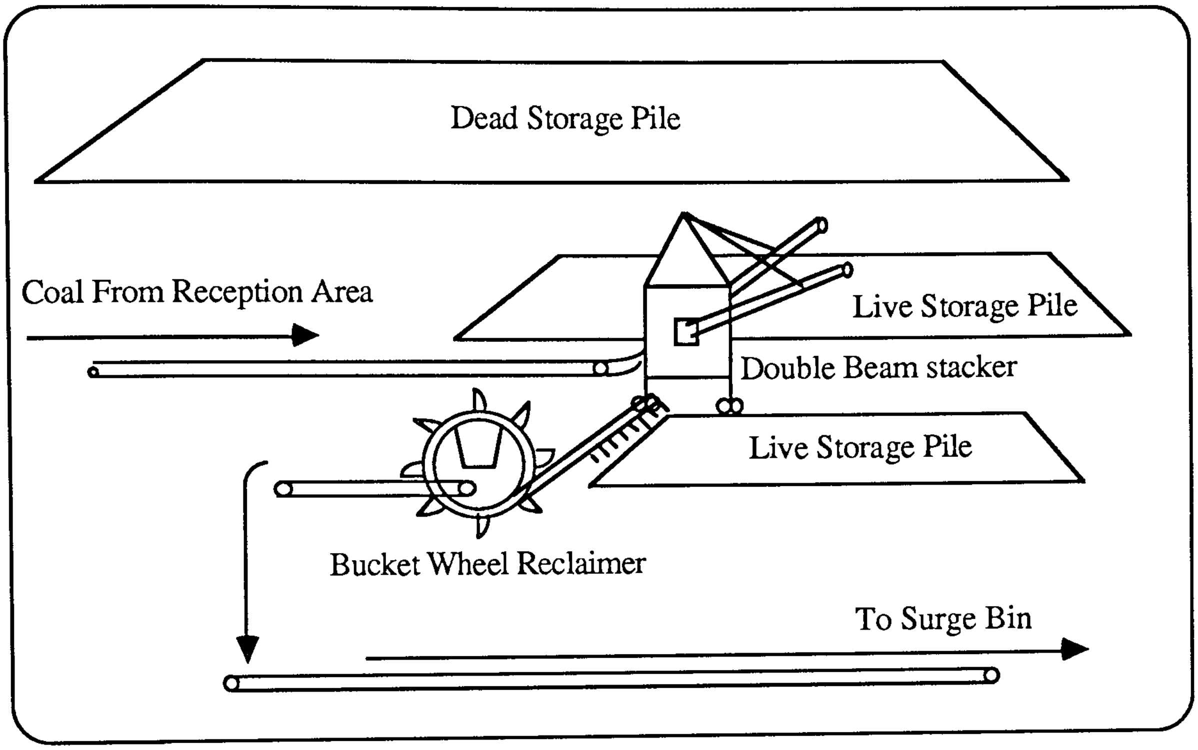

Figure 4.6 Coal Storage and Reclamation

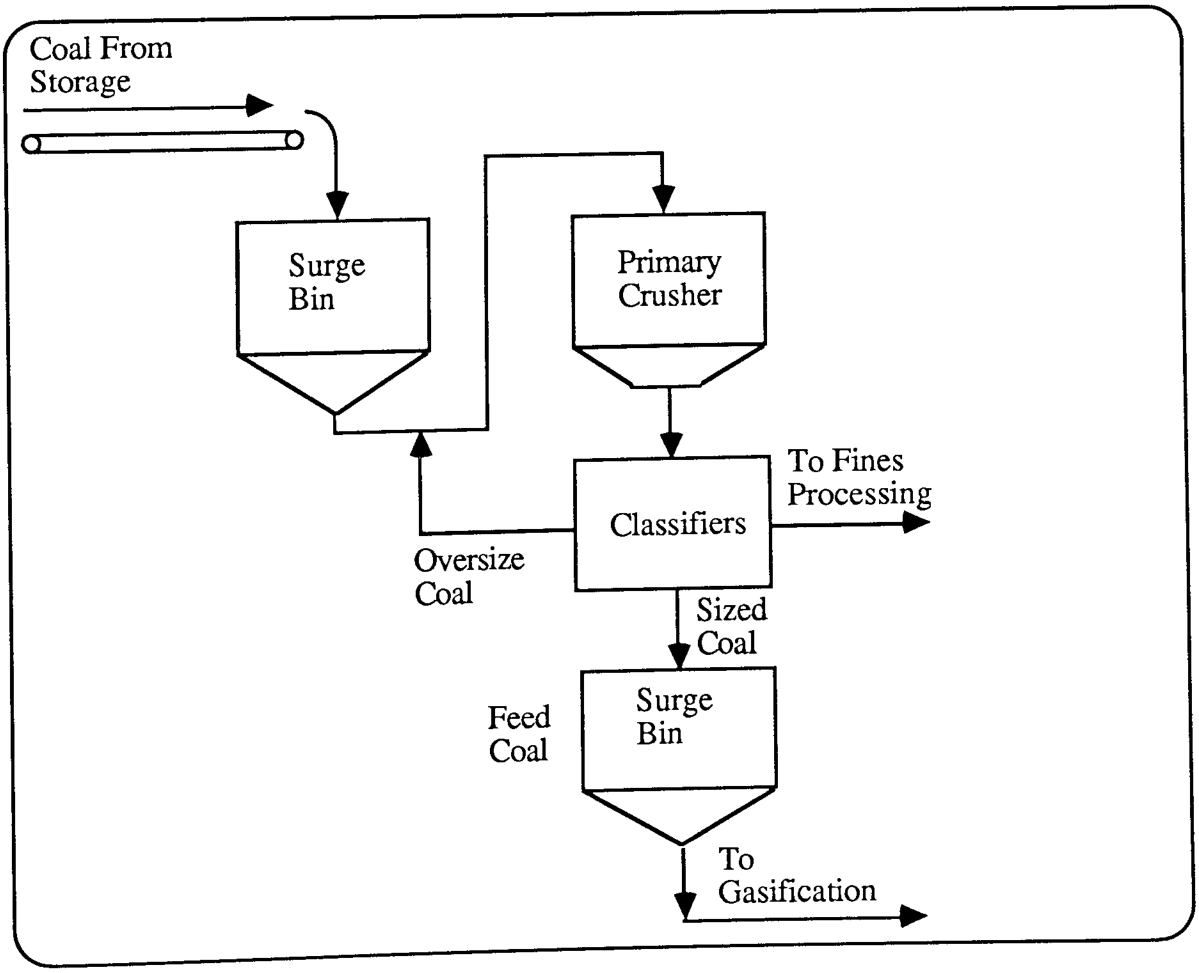

Figure 4.7 Fixed Bed Feed Preparation

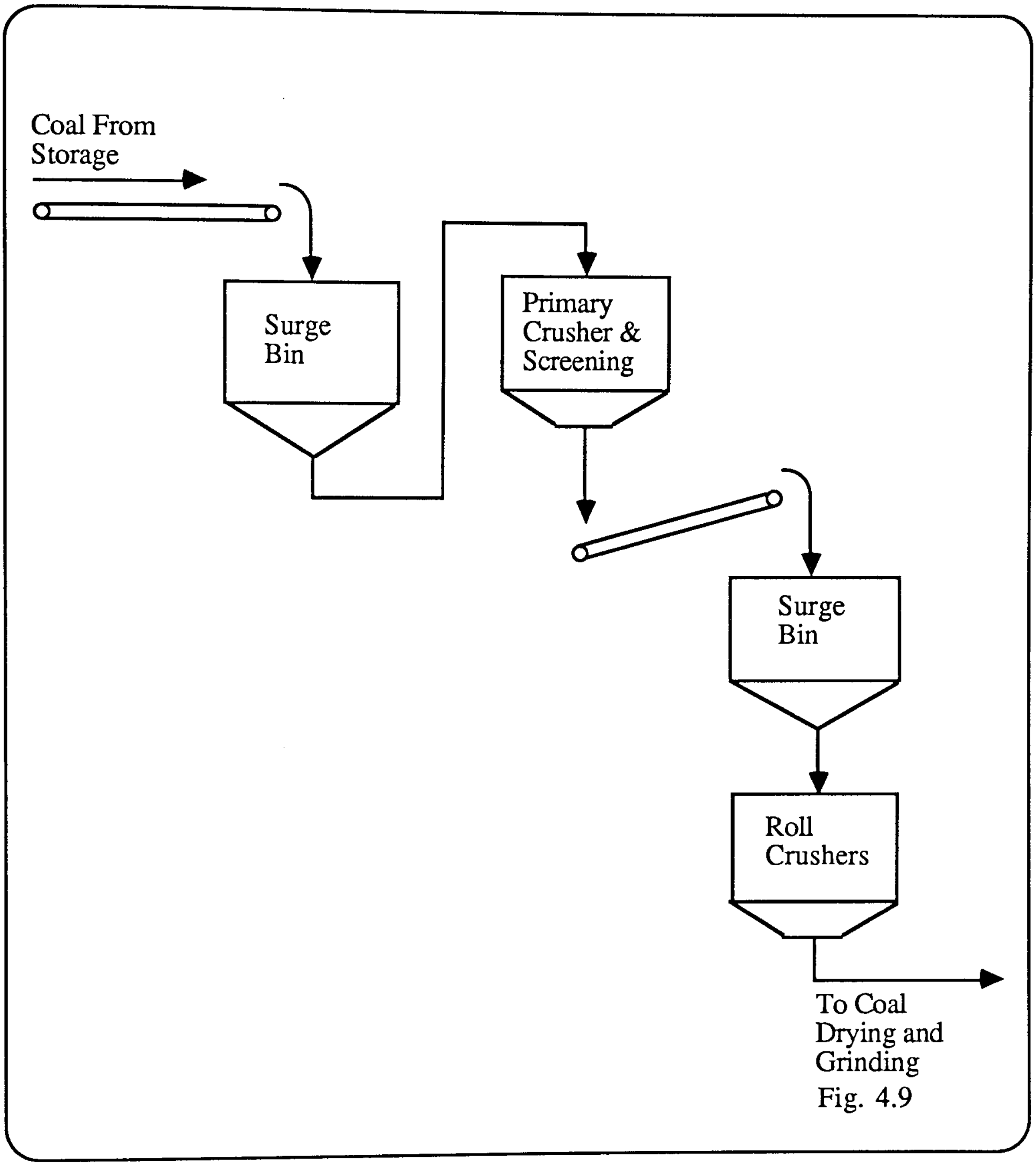

Figure 4.8 Fluidised Bed Feed Preparation, Part A

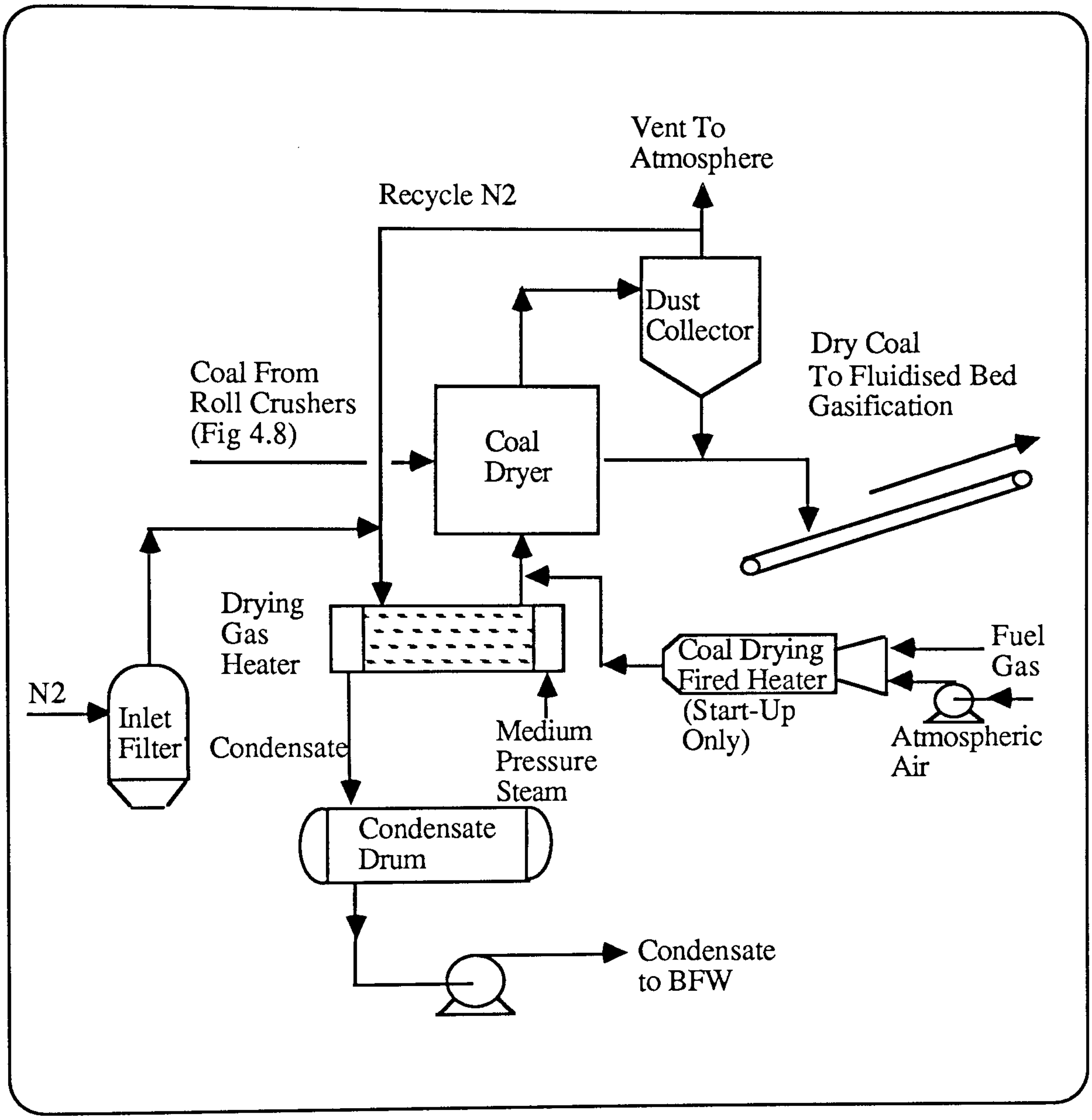

Figure 4.9 Fluidised Bed Feed Preparation; Part B Coal Drying

4.4.1.4. Entrained Flow Feed Preparation (Slurry fed), Step 231

A flow diagram for this step is given in Figure 4.10. Coal from the previous step (Reception storage and reclaiming, 101) is conveyed to a surge bin, from here it is passed to the primary crusher which reduces the particle size to below 6 mm, in preparation for grinding.

Coal below 6 mm is conveyed to the pulverisers where the coal is simultaneously pulverized to dust size (<70μm) and mixed with recycled process water to form a coal/water slurry. The slurry is pumped to a buffer storage tank ready for utilization in the following gasification step[108].

4.4.1.5. Entrained Flow Feed Preparation (Dry fed), Step 241

A flow diagram for this step is given in Figure 4.11 Coal from the previous step (Reception storage and reclaiming) is conveyed to a surge bin, from here it is passed to the primary crusher which reduces the particle size to below 6 mm.

Coal below 6 mm is conveyed via a surge bin to the roller mills where it is pulverized and simultaneously dried by blowing with hot nitrogen, which also serves to remove the pulverized coal from the mill. The entrained pulverized coal is carried to the bag filters where it is removed from the transport gas and sent to buffer storage before transport by recycled synthesis gas to the gasification stages[109,110]. The coal moisture content must be reduced to prevent mechanical handling problems associated with the coal dust sticking together. The moisture is therefore normally reduced to the point where only the intrinsic moisture remains and the surface moisture is removed. This is normally around 2 % for bituminous coals and 4-10 % for lower rank coals and lignites.

4.4.2. Analysis of Preparation Capital Cost Data

The data used in the preparation of the capital cost estimates was obtained from variety of sources. As coal storage and reclaiming is used extensively in the coal industry and particularly in the power industry, where large stocks of coal are standard practice, the step has a well defined capital cost associated with it and cost estimates are obtainable from several sources. Bechtel undertook a conceptual study of coal preparation and gasification in 1980[111] and divided the feed preparation into four distinct steps for capital cost estimation. At the date of publication, the cost of coal storage was estimated from Bechtel's experience in the area between 10 to 20 $ / te of coal stored, depending on total storage capacity. The main sources of coal storage capital cost data collated where similar to sources of information on coal preparation for gasification as discussed later. Information sources for coal storage capital costs are too numerous to discuss in detail.

As the main incentive for coal gasification development during the 1980's was the development of integrated gasification combined cycle plants, the largest single source of recent data for coal preparation capital cost estimates was publications from bodies engaged in economic studies of power and gas generation from coal. These effectively consisted of the Electric Power Research Institute (EPRI) and the Institute of Gas Technology (IGT) both of whom have sponsored development of gasification processes and have undertaken several evaluations of gasification technologies for power and gas production. The data taken from the publications is given in Appendix D with the relevant references to particular publications.

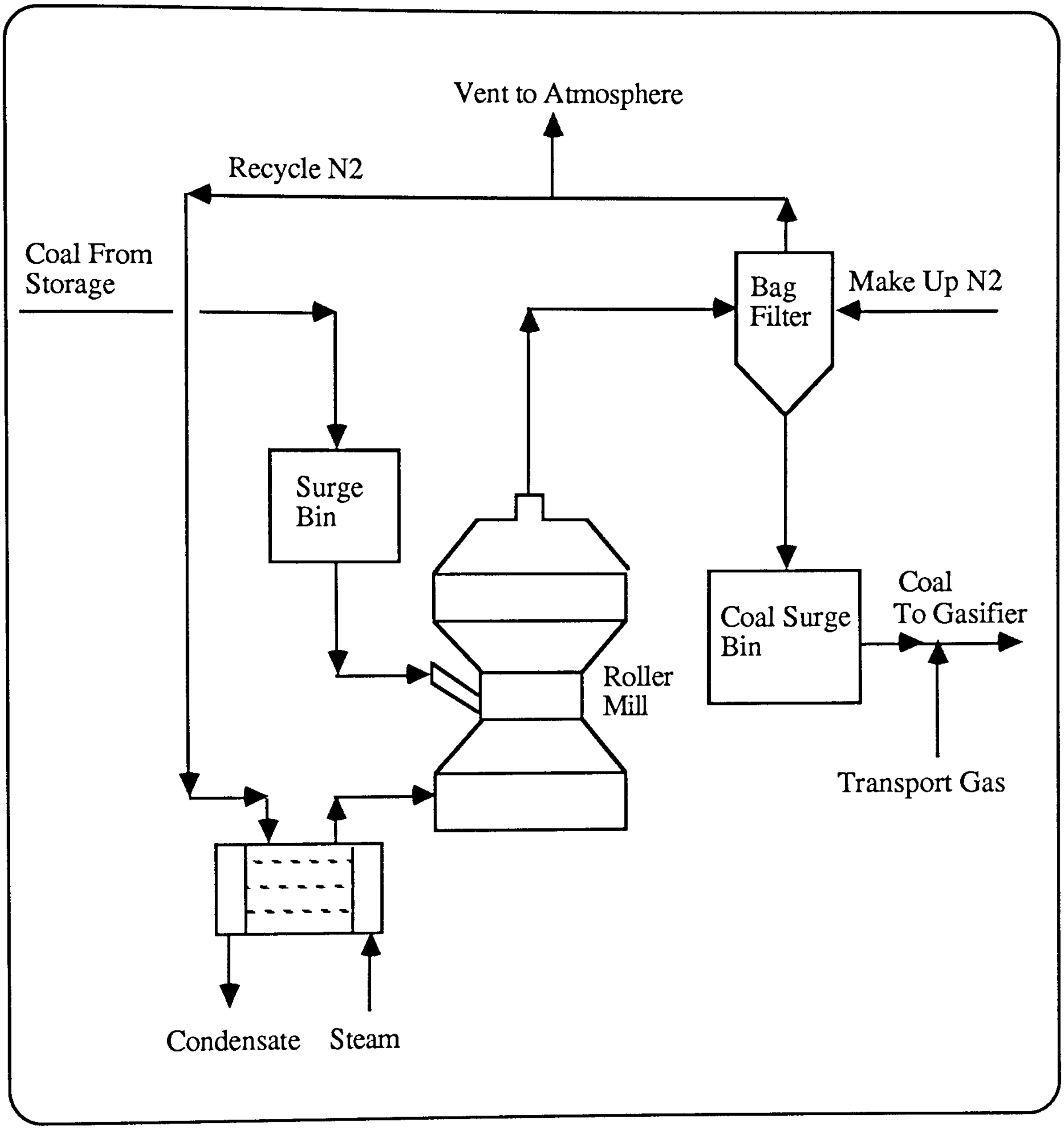

Figure 4.10 Entrained Flow Feed Preparation (Dry Feed)

In many cases the coal preparation step is comparatively simple and consists of simply coal screening (such as for fixed bed gasifiers). For the more sophisticated coal preparation steps such as coal pulverizing with either drying or slurrying the capital cost estimates are based on original estimates by the

Capital cost data for the coal preparation steps was analysed after conversion to a common basis of mid £ 1988 . This has shown for the data collated that for the purposes of this project the capital costs may be divided into the four categories previously discussed this can be seen from Figure 4.12 The figure suggests that there is no detectable economy of scale for the data points used in the analysis. The graph also shows the difference in capital cost for the four different cases under consideration,

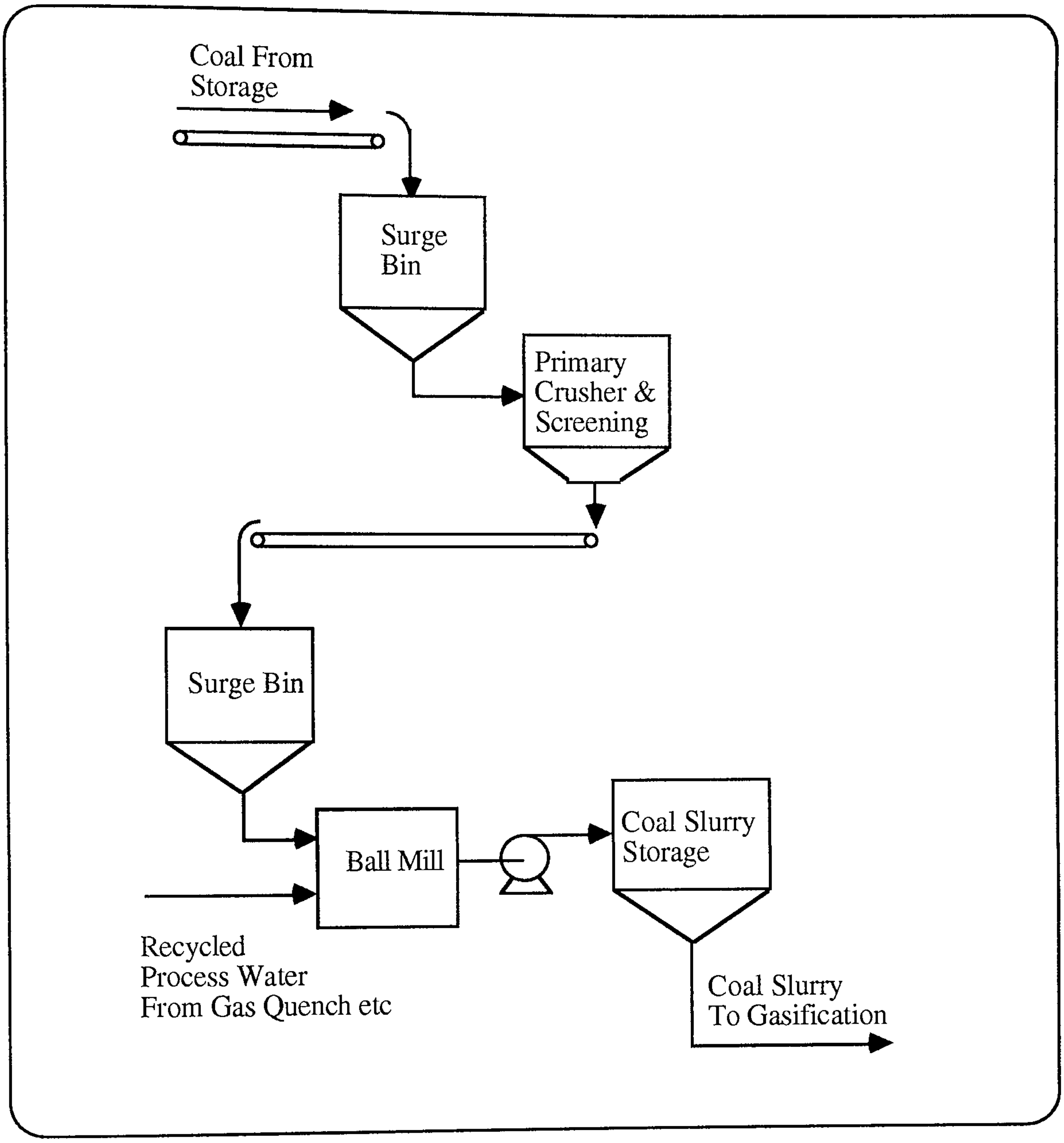

Figure 4.11 Entrained Flow Feed Preparation (Slurry Feed)

which is due to the difference in the complexity of the preparation step required and resulting differences in equipment for the steps. The raw data is given in Appendix D

After analysis of the data available after 1980 and contained within the publications discussed later for coal preparation, a value of 24.5 $ / te of coal was used within the model. There appears from the data to be no detectable economy of scale for the ranges of throughput used within the model ie above 1000 te/day of dry ash free coal.

The results show that the capital costs for the entrained feed preparation steps are higher than for the fixed and fluidised feed preparation steps. This is reasonable considering the degree of processing and the more complicated equipment required for the entrained feed preparation steps.

For the purposes of capital cost estimation it was found that there was no distinguishable cost difference between dry and slurried pulverized coal preparation. Therefore a single cost estimation correlation was used for both cases.

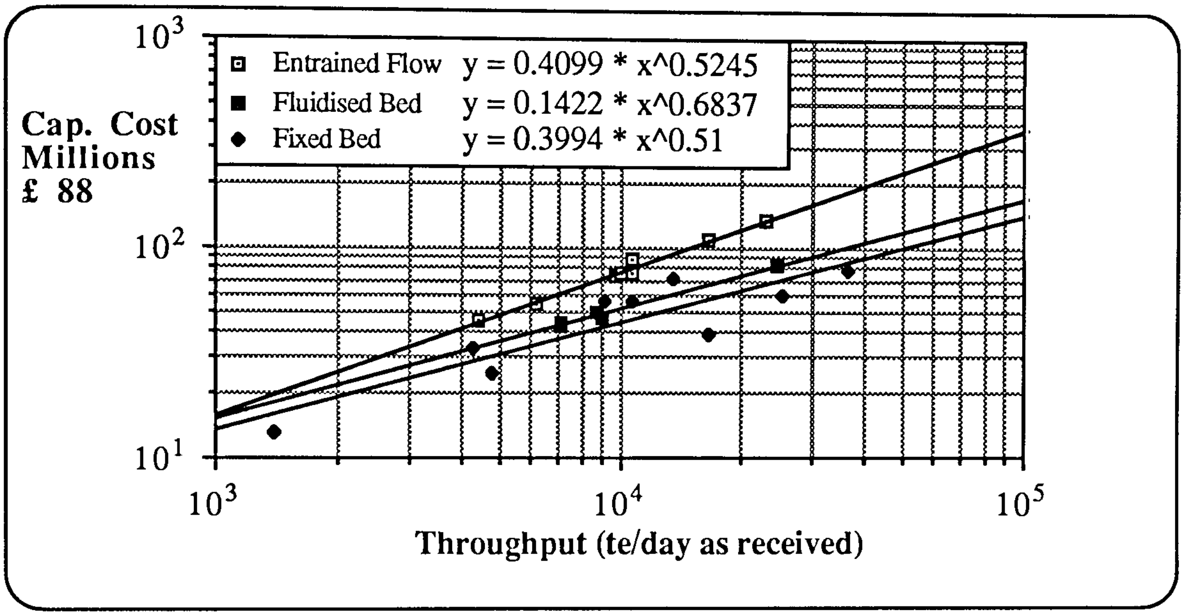

Figure 4.12 Feed Preparation Capital Costs (Including Storage & Handling)

CHAPTER 5
GASIFICATION STEP MODELLING

5.1 Aim

For many of the gasifiers included in the modelling published gas compositions and yields are available for several coal feedstocks and in many cases the gasifiers have been tested on similar coals (eg Illinois No.6). This is not, however, true for all the gasifiers. For ease of comparison of the different gasification processes and to provide greater flexibility of the models with respect to feedstock choice it would be advantageous to enable the gasifier models to respond to changes in feedstock. This would have the following advantages, provided that the feedstock is compatible with the gasifier:

- All the gasifiers can be compared with the same feedstock;
- Feedstocks other than for which data is available can be included in the model.

The gasifier process modelling section of the program has as its main aim the ability to predict gasifier product gas compositions, flowrates and utility usages of steam and oxygen for a wide range of feedstocks from bituminous coal to lignites. This will enable the gasifiers to be compared with the same feedstock and with feedstocks which are available in Europe.

No attempt has been made to model the kinetics of the processes occurring within the gasifiers. The main advantage of modelling the kinetics of the reactions is that the throughputs of the gasifiers may be estimated from first principles, accurate temperature profiles may be predicted throughout the gasifier and dynamic models may be created. There is little advantage for predicting output gas compositions or utility requirements, furthermore, kinetic models require large amounts of development time for each gasifier configuration and the solution of the resulting differential equations is mathematically complex and require large amounts of computer time to solve. For these reasons, kinetics based models were considered unattractive for a steady state model to be included as part of a much larger program.

The models should be kept as simple as possible without unnecessary loss of accuracy and should be able to account for changes in:

- Coal analysis, with respect to C, H, O, N and S content;
- Ash content;
- Moisture content;
- Higher Heating Value.

The criterion for the gasifier model acceptability will be the ability to model experimental data to within acceptable levels of tolerance. Data for one feedstock can always be reproduced by a computer model by adjusting internal parameters to fit the results to the experimental case, therefore model acceptability was tested by matching the predicted gas composition for one feedstock such as Illinois No 6, for which many of the gasifiers have been tested on, and then comparing the model prediction for a completely different type of feedstock such as lignite, with no changes to the model. If the model predictions were accurate over a very wide range of coal rank, such as bituminous coal to lignite then the model was considered acceptable. An accurate prediction is considered to be better than 5 % for the oxygen requirement and gas compositions.

Many coal gasification models exist for the gasifiers included in the modelling but these are either unavailable or far too complicated for inclusion into the program. Models are also not available for all of the gasifiers included in the program and the approach taken was to develop a model which could be adapted to any gasifier by the use of suitable parameters, this reduced development time for the gasifier models and reduced the size of the program code.

The different types of gasifier require different conceptual approaches to modelling and for the final program the gasifier models were built out of a small number of sections of computer code which are called in the necessary order and with the required parameters to model the gasifiers.

5.2 Modification of the Biomass Gasification Computer Model

The basic subroutines for the modelling of the gasification processes were originally developed by Double[112] for the modelling of fluidised bed biomass gasification. The original model performs two functions:- it calculates the equilibrium composition of the gas from the exit temperature of the gasifier and composition of the feed and utility usages using the water gas shift equilibrium reaction and adds the pyrolysis products, when present, to the equilibrium gas composition. The routines which perform the energy balance over the gasifier and the equilibrium calculation were modified and used as the basis of the coal gasification models as described below.

5.2.1 Modification of the Equilibrium Calculation Subroutines

The routines developed by Double for modelling biomass gasifiers were found to be unsuitable for coal gasification modelling without modification. This was due to the inability of the model to give acceptable predictions over wide ranges of feed coal rank.

The main modifications made to the equilibrium composition calculation routines were as described in the following sections.

a) Allowance for Varying Coal Ash Content

The original equilibrium calculation procedures made no allowance for the presence of ash in the feedstock. This was due to the low ash content of wood, which could therefore be neglected, which was the fuel used by the gasifiers for which the model was developed. With coal, however, the ash content may be appreciable (>20 %)[113] and varies considerably depending on a wide range of factors which include coal rank, method of mining, the use of coal washing techniques and can vary from seam to seam and from different positions within the same seam. The effect of not allowing for the existence of ash in the coal and of the different ash contents between different feedstocks has a significant effect on the heat balance in the gasifier models. As the ash effectively leaves the gasifier reaction zone at elevated temperatures (300°C to over 1500°C, depending on the gasification process) the enthalpy contained in the ash may be significant. If this is not allowed for, the heat balance is not correct and the predicted gasifier utility requirements and output gas compositions are not reliable. As the models contain parameters which are not known accurately from published data such as reaction temperature and heat loss from the gasifier, these allow adjustment of the predicted gas composition to reflect published data. Hence errors were only noticeable when the same gasifier was modeled using different feedstocks. After adjusting the model to one feedstock the prediction for the second feedstock was significantly improved by including the ash content in the enthalpy balance.

b) Alteration of Model Enthalpy Balance Calculation

The enthalpy balance calculations over the gasifier were originally performed by Double using an averaged heat capacity over the expected temperature range and for a typical gas composition. This was believed to be inadequate for modelling coal gasifiers as there is a wide temperature range for the exit gas from different gasifiers for which an averaged heat capacity value is therefore inadequate. Furthermore the gas composition from the coal gasifiers varies widely, and the heat capacities of the constituent gases varied enough that it was assumed to be more accurate to consider the enthalpy of each gas individually. For these reasons the enthalpy of the gases was calculated using the integrated form of the heat capacity equations, for all the enthalpy calculations used in the models, with zero °C was taken as the datum point. The heat capacity equations used were as follows[114]:

H_2	$Cp = 27.143 + 9.273E\text{-}3 * T - 1.38E\text{-}5 * T^2 + 7.645E\text{-}9 * T^3$
CO	$Cp = 30.869 - 1.285E\text{-}2 * T + 2.789E\text{-}5 * T^2 - 1.271E\text{-}8 * T^3$
CO_2	$Cp = 19.795 + 7.343E\text{-}2 * T - 5.601E\text{-}5 * T^2 + 1.715E\text{-}8 * T^3$
H_2S	$Cp = 31.941 + 1.436E\text{-}3 * T - 2.432E\text{-}5 * T^2 - 1.176E\text{-}9 * T^3$
N_2	$Cp = 31.150 - 1.356E\text{-}2 * T + 2.679E\text{-}5 * T^2 - 1.168E\text{-}8 * T^3$
H_2O	$Cp = 32.243 + 1.923E\text{-}3 * T + 1.055E\text{-}5 * T^2 - 3.596E\text{-}9 * T^3$

Where Cp is J / Mol / K and T is °K.

The inclusion of the above two modifications produced significant improvements in the equilibrium calculation as shown in Table 5.1 for the Texaco gasifier. The accuracy of the predictions improved for alternative feedstocks and the parameters used to adjust the model to real gasifiers became more realistic, for example the heat loss from the gasifier for the Dow model changed from -1.7 % from the original model to 1 % with the modified model. Normal heat loss from a gasifier is usually less than 3 %, (this includes heat used to generate jacket steam, if applicable). A negative value of heat loss is nonsensical in reality, as it implies that heat energy is created in the gasifier.

Table 5.1

Comparison of Unmodified and Modified Equilibrium Calculation.

	Equilibrium temp.	Gas outlet temperature	Heat loss
Original Model	1175	1316	-3 %
Modified Model	1175	1316	0.3 %
Published Conditions	-	1316	< 3 %

5.2.2 Calculation of Combustion Zone Temperature

In order to model many of the gasifiers more accurately it was found necessary to construct routines to calculate the temperature in the combustion zone of the gasifiers. As explained below, it was found that two separate routines were required, one to model co-current processes and one to model counter-current processes. This was due to the following differences in the calculations required, for co-current gasifiers, (for example the entrained flow gasifiers), the maximum temperature is simply the adiabatic temperature rise of the solid and gaseous materials present when all of the oxidizing agent has been utilized. The carbon is assumed to be oxidized to 50 % carbon dioxide and 50 % CO. This assumption is unlikely to be valid, as the distribution of products between CO and CO_2 is unknown. However, the effect of the ratio of CO / CO_2 in the combustion gas on the temperature of the combustion zone, is of the order of 150 °C difference from zero CO content to 100 % CO content[115]. If the gasifier has a combustion zone temperature of 2000 °C then the maximum error is 7.5 %, hence the maximum error by assuming a 1:1 ratio of CO and CO_2 is 3.75 %. Furthermore, the actual maximum temperature in the gasifier is not known from experimental data and must be calculated form the inputs and outputs to the gasifier, also the product distribution between CO and CO_2 is not known, therefore the maximum temperature is calculated for one feedstock, the required maximum temperature is set for all feedstocks at the same level and hence the steam required to maintain the temperature below the maximum may be estimated. The error introduced by assuming 100 % CO_2 production is then reduced considerably in the final result.

For countercurrent gasifiers the calculation is more complicated by the opposing directions of flow of the coal and the gasification agents. The maximum temperature is therefore calculated by assuming:

- The ash exits the gasifier at the input temperature of the oxygen and steam for non-slagging gasifiers, and at the maximum temperature for slagging gasifiers;
- All of the oxygen is utilized before the gasification reactions begin;
- The product of combustion is assumed to be 100 % CO_2 as for particles greater than 0.1 cm in diameter, as used in fixed bed gasifiers the only product is CO_2[116];
- The gases are assumed to be at thermodynamic equilibrium according to the water gas shift reaction.

5.2.3 Calculation Of Water Quench

The raw hot gas form the gasifiers can be cooled by two basic methods which are indirect by using a heat exchanger and using the surplus heat to generate high or low pressure steam, or by direct quenching of the gas with water which produces a cooled and saturated synthesis gas. When the synthesis gas requires CO shifting the gas must contain adequate water to enable the water gas shift reaction to convert the correct amount of water and carbon monoxide to hydrogen and carbon dioxide. Therefore it is beneficial to quench the gases directly rather than use the energy to raise steam externally and then inject steam into the shift reactor feed gases. Therefore a routine was developed to calculate the temperature and composition of the gases exiting a water quench system from a known feed temperature and composition. The calculation sequence was as shown in Figure 5.1

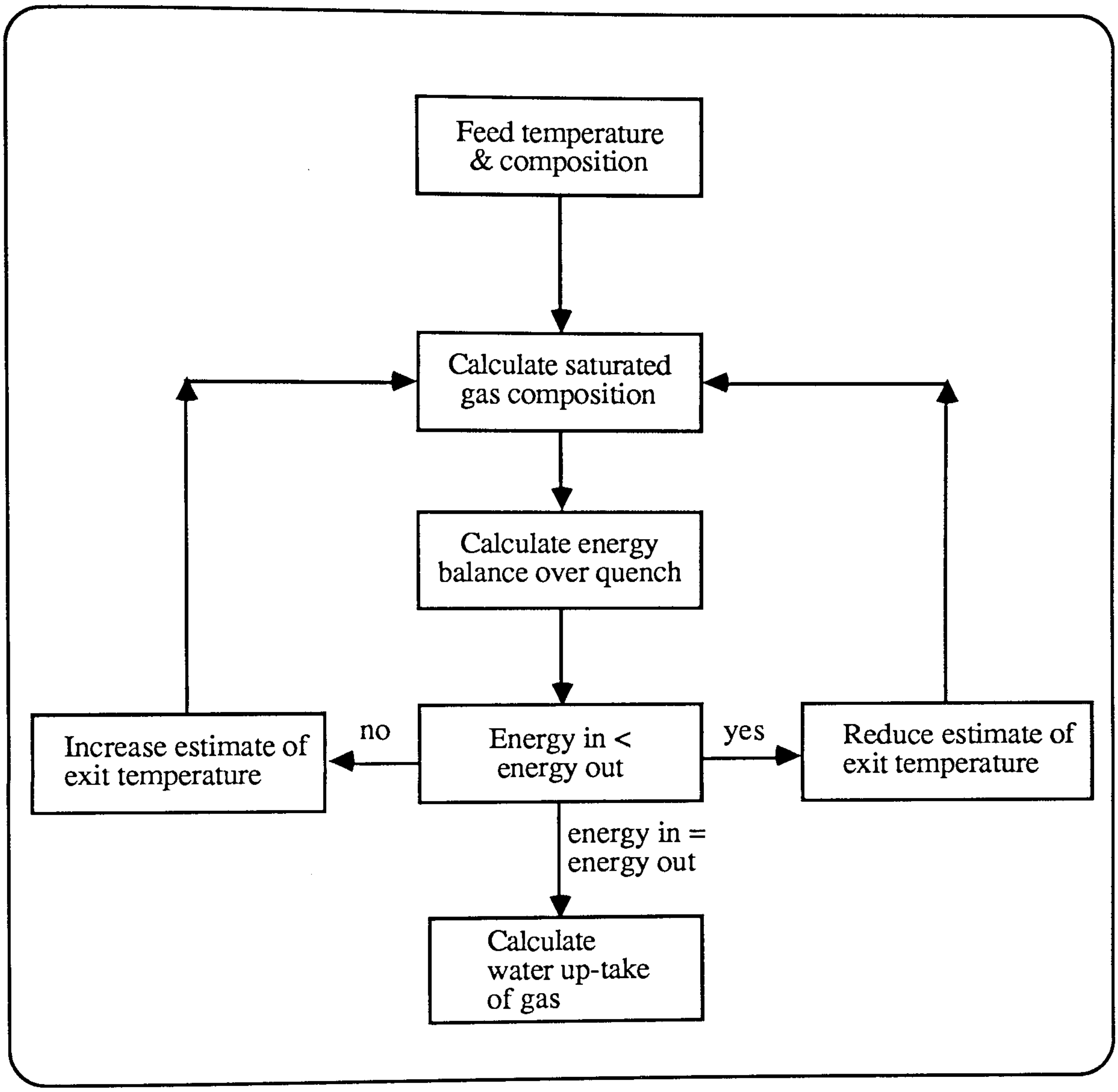

Figure 5.1 Quench System Calculation Procedure

5.3 Entrained Flow Gasifiers

In general these gasifiers operate at relatively high temperatures and hot spots of over 2 000 °C may occur locally as in the PRENFLO gasifier[117]. The relatively high temperatures ensure that higher hydrocarbons and tars are decomposed and do not appear in the product gas. Methane is only produced in small quantities (generally <1% vol), or is not present. Chemical equilibrium can, therefore, be assumed to be the dominating factor in the gas composition. These gasifiers, were, therefore be modeled on this basis. The water gas shift reaction is the dominating reaction:

$$CO + H_2O <=> H_2 + CO_2 \quad \Delta H \text{ -41.2 kJ/Mol}$$

5.3.1 Modelling Approach

The entrained flow gasifiers have been modeled on an equilibrium basis. The approach adopted is to perform mass and energy balances over the gasifier section to calculate the gasifying agent requirements and then to adjust the final gas composition using the water gas shift reaction equation. As the water gas shift reaction is independent of pressure only the temperature of the reaction is necessary to predict the equilibrium constant. The reaction temperature is not constant over the entire gasification region and therefore in the calculation procedure an 'effective temperature' is used for equilibrium calculation and is calculated from experimental data. A separate variable, the exit gas temperature, is also required for the energy balance calculation and this is obtained directly from reported operational or experimental data. Figure 5.2 shows a diagrammatic representation of the equilibrium gasifier model.

For the slurry fed gasifiers the equilibrium and exit temperature are sufficient to fix all of the parameters required to calculate the gas composition and oxygen requirement as the water content in the feed is input by the program user. For the dry fed gasifiers an additional parameter is needed to enable the steam requirement, if needed, to be calculated. The temperature of operation of entrained flow gasifiers is relatively high (up to 2000°C), to provide the required rate of reaction to give high carbon conversion with short residence time in the gasifier. There is, however, a temperature above which the materials of construction of the gasifier may become adversely affected, increasing maintenance costs or shortening reactor life. The maximum temperature in the gasifier is therefore set, and the steam requirement needed to keep the temperature below this value can be calculated. In cases where the calculated combustion temperature is still below the maximum temperature with no steam usage, the steam requirement is set to zero, this may occur if the feed contains a large enough amount of moisture.

5.3.2 Testing of Entrained Gasifier Model

The entrained gasifier model has been tested on several of the entrained gasifiers, the results shown in Table 5.2 below are for two coal types used in the Dow gasifier for which gas compositions have been published and Table 5.3 shows a comparison for the Shell gasifier. As a result of the mass and energy balances performed by the model, it will predict oxygen and steam requirements for the gasifier. The suitability of alternate coals for each gasifier cannot, however, be determined from this model and must be determined separately from the physical and chemical properties of the coal, this information is included in the modelling program with the basic properties of the feedstocks.

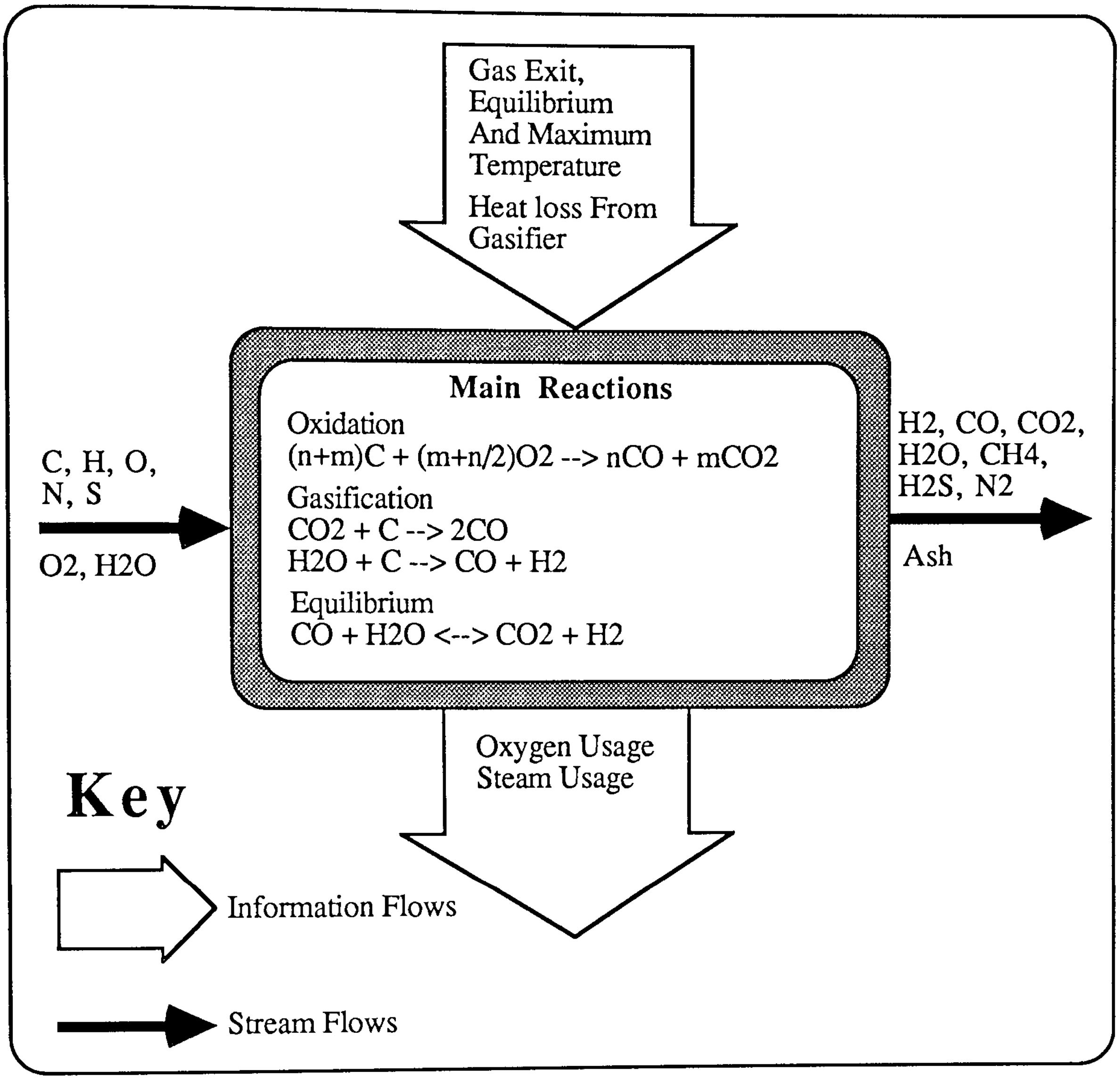

Figure 5.2 Diagrammatic Representation of Equilibrium Gasifier Model

Table 5.2 Example of Model Results Compared to Published Values for Dow Gasifier[118]

Feedstock	H_2	CO	CO_2	CH_4	H_2S/ COS	N_2	HHV MJ/Nm^3
West. Sub-bit.							
Published value	41.35	38.46	18.46	0.11	0.14	1.48	10.19
(Model prediction)	40.48	39.49	19.43	0.05	0.15	0.40	10.19
N. Dak. Lig.							
Published value	38.92	33.74	25.26	0.04	0.22	1.82	9.26
(Model prediction)	39.26	33.92	25.91	0.05	0.41	0.45	9.35

Table 5.3

Comparison of Published & Predicted Gas Flows, mol %, for the Shell Gasifier

Feedstock	H_2	CO	CO_2	CH_4	H_2S/ COS	N_2	O_2 Usage*	Steam Usage*
Illinois No.6								
Published value	31.1	62.2	1.67	0.06	1.28	3.69	889	32
Model prediction	32.0	64.2	1.67	0.06	1.47	0.50	889.6	32
Texas Lignite								
Published value	28.1	59.1	6.2	0	0.5	6.1	873	0
Model prediction	30.2	62.5	6.2	0.06	0.5	0.5	863	0

* te/te daf coal

The published values for the two gasifiers were obtained form information used for assessments of Integrated Gasification Combined Cycle (IGCC) power plants. The oxygen purity used as feed to the gasifiers in these studies is lower than that required for chemical production. This is due to the build up of inert gases in chemical plant recycle systems which does not affect IGCC plants where no major recycles of the synthesis (or fuel) gas occurs. There is a small effect on the heat balance of the gasifiers of changing the nitrogen content of the gas, but for the above comparison it is negligible.

5.4 Fluidised Bed Gasifiers

These gasifiers in general produce more methane than entrained gasifiers due to the lower temperature of operation. Tars and other hydrocarbons may be produced by fluidised bed gasifiers due to the products of pyrolysis of the volatile matter of the coal, however, for the gasifiers included in the modelling tars and hydrocarbons above methane are not produced. One of the distinguishing characteristics of modern fluidised bed gasifiers is the inclusion of special design features to minimize the formation of these compounds. The approach to modelling, outlined above, of using an equilibrium model was adopted for these gasifiers as a combined equilibrium and pyrolysis model (see section 4.3.5). The methane content of the outlet gas was calculated separately by comparison of feedstocks gasified experimentally or commercially with those selected for modelling. Theoretical methods exist for estimating methane levels based on equilibrium and kinetic mechanisms but these in general require experimentally determined variables (eg the carbon "activity" [119]) and are considered beyond the aims of this model.

5.5 Fixed Bed Gasifiers

These gasifiers are comparatively difficult to model in comparison to the entrained and fluidised bed gasifiers included in the program. The product gas contains large amounts of non-equilibrium and pyrolysis products, for example tars and higher hydrocarbons from the thermal decomposition of the volatile matter in the coal.

5.5.1 Modelling of Fixed Bed Gasifiers

The approach taken to modelling these gasifiers is based on that developed by Kosky and Floess[120]. The volatile matter in the coal is assumed to be decomposed to give gas and liquid products. The product gas from the gasifier is thus assumed to be composed of gases formed from the oxidation and gasification of the coal and which have undergone the usual equilibrium reactions. The gas also includes gases which are released from the thermal decomposition of the volatile matter in the coal and which do not undergo any further equilibrium reactions. The product gas also contains a number of non gaseous (at room temperature) components from the decomposition of the volatile matter. These include tars, oils, and phenols. A diagrammatic representation of this approach to modelling the fixed bed gasifiers is given in Figure 5.3. The tars and other liquid products need to be removed from the gas stream and recycled or otherwise disposed of. For the purposes of this model the gas/oil liquor from the gasifier will be assumed to be sent to a tar and oil separator and from there the tars recycled back to the gasifier to be injected through the tuyeres and gasified. The phenolic liquor is sent to a phenolsolvan extraction plant where they are recovered as crude phenols and can be assigned a by-product value, the oils can be used as fuel and assigned a value equal to that of heavy fuel oil on an energy basis.

The parameters which need to be determined for realistic simulation of the gasifier are the product gas composition, the oxygen requirement and the steam requirement. In this model the steam requirement is that required to moderate the temperature of the combusting coal in the combustion zone of the gasifier. In the case of the Dry Ash Lurgi gasifier this requires large amounts of steam to prevent the ash from being heated above the ash softening point, otherwise the gasifier becomes inoperable due to sintering of the ash and blocking of the gasifier. The gasifying agent requirement is estimated by calculating the amount of gasifying agent in total (steam + oxygen) to give a gas exit temperature above the dew point of the tars and oils, approximately 650 °C. The steam requirement is calculated by adjusting the steam oxygen ratio until the temperature in the combustion zone is below that of the ash softening point. This is done as an iterative procedure until both temperature conditions are satisfied by a unique steam / oxygen ratio.

The temperature in the combustion zone of the gasifier is calculated approximately by assuming that all of the oxygen is consumed before any gasification reactions occur and that the oxygen is converted to 100 % CO_2 as discussed in section 4.3.3.

In the case of the slagging Lurgi gasifier the criteria are slightly different in that the maximum temperature is required to be well above the melting point of the ash. This has the effect of considerably reducing the amount of steam required to moderate the temperature, which has significant effects on gas quality and thermal efficiency. The calculation sequence is, however, essentially the same but with higher temperatures specified for the combustion zone. The calculation sequence for calculating the utility requirements of oxygen and steam is shown in Figure 5.4.

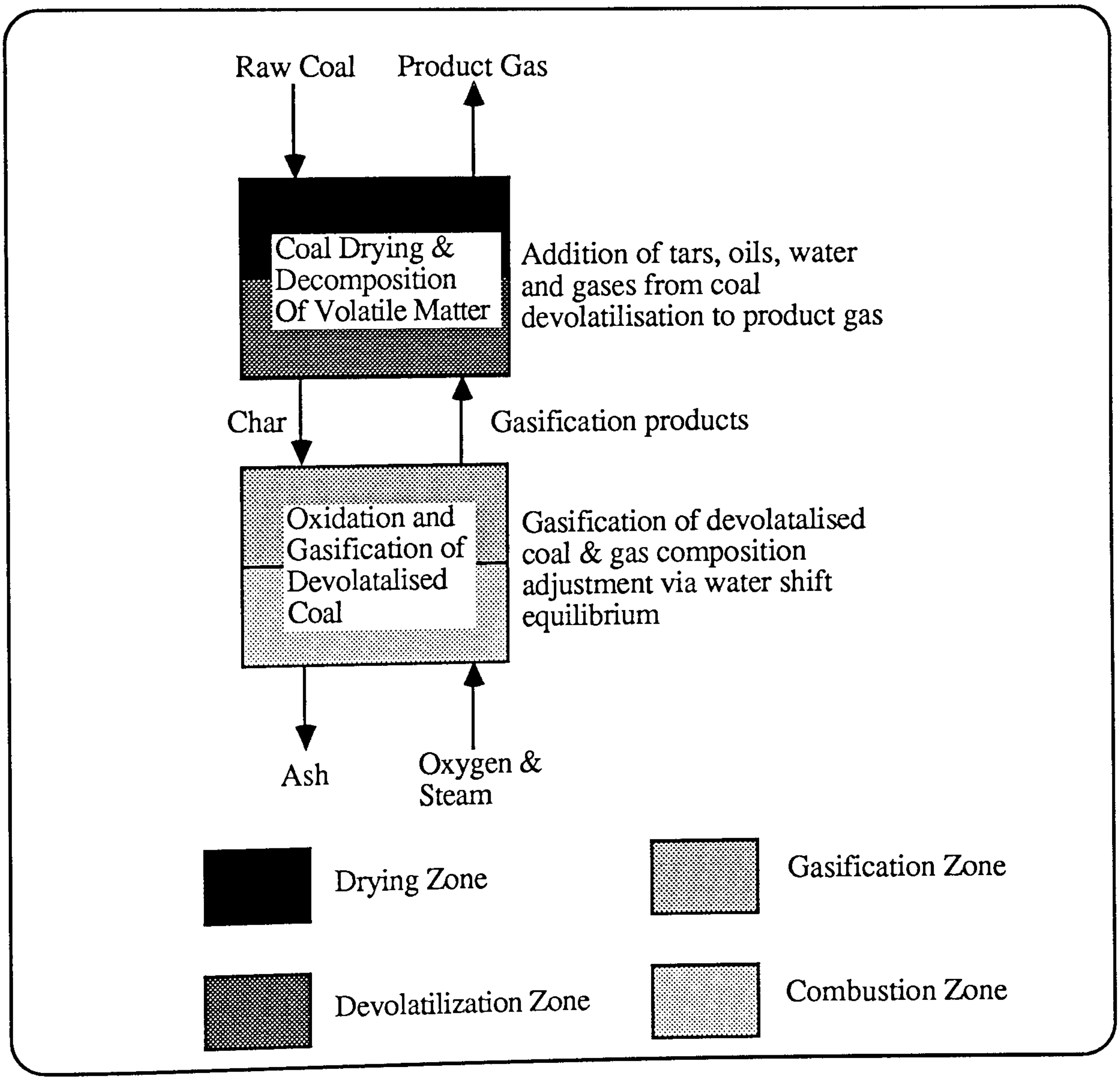

Figure 5.3 Fixed Bed Model Diagram[121]

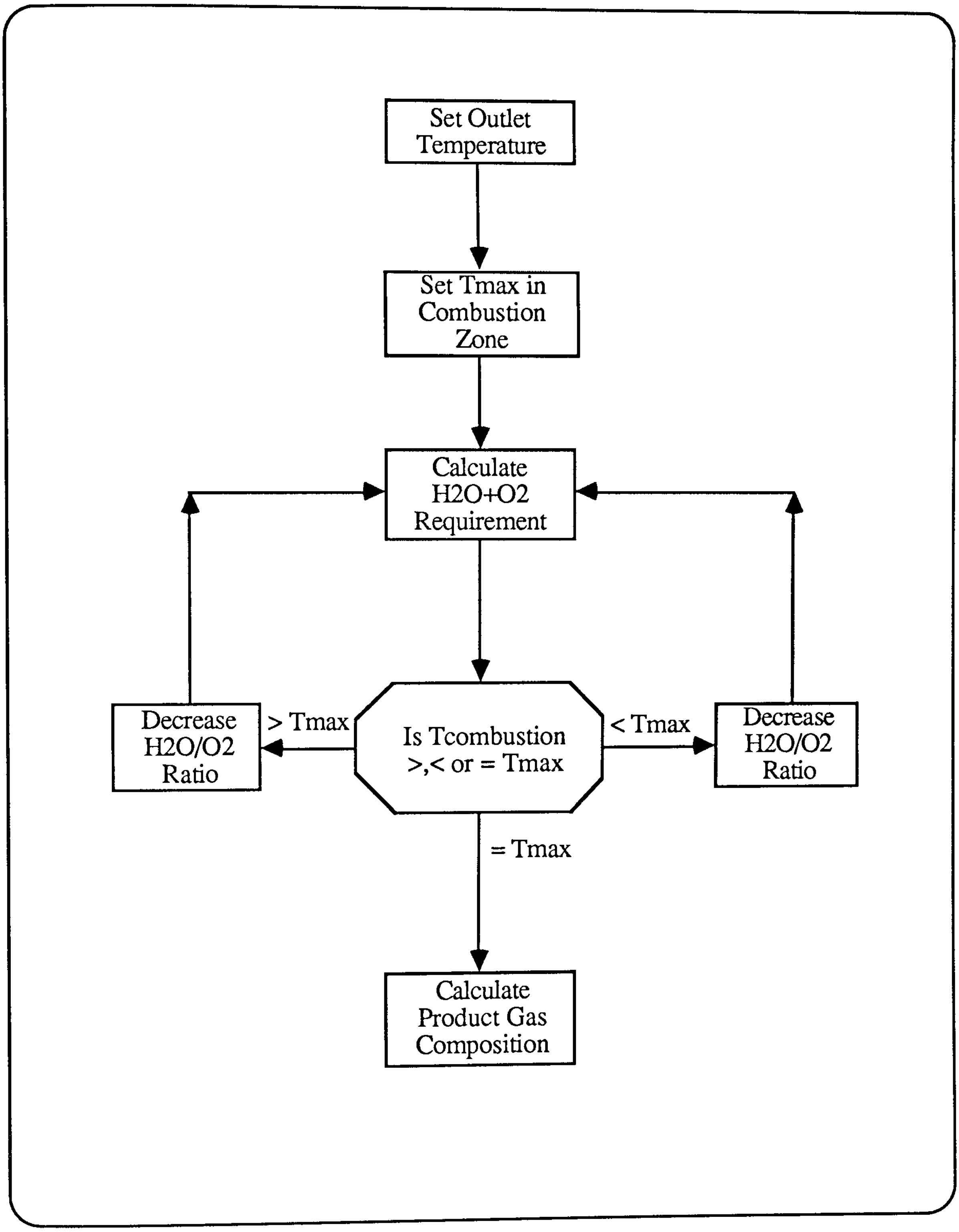

Figure 5.4 Fixed Bed Model Calculation Sequence

5.6 Flexible Gasification Model

In order to facilitate access to the internal parameters used within the gasification step models, a gasification step was developed to allow the program user to alter the gasification process parameters interactively from the keyboard. The step model will allow the user access to the following calculation types and gasification parameters. The aims of the step are to:

- Enable the step to be able to model to a good degree of accuracy a wide variety of gasification processes;
- Enable the user to alter parameters and examine the effects on gas quality for particular gasifiers such as Texaco, KRW, BG / L or Shell.

The step is incorporated into the model similarly as the specific gasifier gasification steps and it can be accessed after any of the coal preparation steps. The step enables the program user to modify any of the process parameters described above, and to view the resultant gas composition from the gasifier, on the screen, before completing the run through to a final product or again re-modifying the gasification process parameters.

5.6.1 Calculation Type

Four calculation types have been implemented within this gasifier step to enable alternative combinations of process parameters to be altered as desired and to enable as many gasifiers as possible to be modeled. The four calculation types are :

1 - Iterate for gasification agent requirement,
(fixed oxygen / steam ratio and outlet temperature);

2 - Iterate for gas exit temperature,
(fixed oxygen / steam and carbon ratio);

3 - Iterate for steam usage,
(fixed oxygen / carbon ratio and gas exit temperature);

4 - Iterate for gasification agents,
(fixed gas exit temperature and outlet gas composition ie H_2, CO, CO_2 or H_2O).

The alternative calculation types do not allow all of the parameters to be altered independently and the menu driven input procedure alters automatically according to the choice of calculation specified. The step enables the following gasification parameters to be altered:

- Reaction Temperature

This parameter alters the equilibrium position of the water gas shift reaction and hence alters the gas composition accordingly. It may be taken to be the effective average temperature of the gas equivalent to the average value of the water gas shift constant of the gas in the gasifier ie the average value of the shift constant in the gasifier need not be equal to the value of the shift constant at the average temperature, due to the non-linear relationship of the shift constant with temperature.

- Gas Exit Temperature

This affects the heat balance of the gasifier and hence the gasification agent requirements and the product gas composition. It is not necessarily equal to the average temperature of the gases within the gasifier, as many gasifiers cool the gases before they leave the gasifier.

- Percentage of Feedstock Energy Lost To Environment Via Gasifier Walls etc

The heat lost through the walls of the gasifier accounts for a very small percentage (≈ 1 %) of the total energy throughput of the gasifier and thus has a small effect on product gas composition. An artificial value for this parameter may be used to compensate for inaccuracies in the calculation of the overall heat balance. These errors may for example appear due to pressure effects on the chemical component enthalpy equations.

- Gas Methane Content

The methane content, which may be appreciable in fixed or fluidised bed gasifiers, is difficult to predict without testing the feedstock, or obtaining detailed information on the catalytic effectiveness of the particular coal on methane formation under gasification conditions. Therefore, this variable is entered as a best estimate of its magnitude. It can be altered easily to examine the sensitivity effect.

- Higher Hydrocarbons Content

C_2 and C_3 hydrocarbons are produced from the pyrolysis of the feed coal. The quantity of these compounds present in the product gas is difficult to predict theoretically. Therefore, as in the case of methane, the value must be entered as a best estimate of the likely content in the product gas.

- Tar Production

This option allows the user to specify whether the gasifier being modeled produces large amounts of tars. The tars are assumed to come from the decomposition of the volatile matter in the coal. Choosing this option automatically selects the following option (pyrolysis gas production).

- Pyrolysis Gas Production (automatically chosen with tar production)

If this option is specified the model assumes that a percentage of the volatile matter contained in the coal is converted to pyrolysis gases. The user then selects the percentage of this pyrolysis gas which by-passes through the gasifier to be seen in the product gas. It assumes that equal proportions of all gases pass the reactor and do not undergo equilibrium reactions.

- Molar Steam / Oxygen ratio

This parameter sets the molar oxygen to steam ratio in the gasifying agent that is fed to the gasifier.

- Molar Oxygen / Carbon ratio

This can be used to specify the ratio of oxygen used to gasify the coal to the amount of carbon in the feed coal on a molar basis.

- Carbon Conversion Efficiency

The carbon conversion efficiency is set by the user to the correct value for the particular gasifier / coal combination being used. It can be varied easily to observe the effect on the overall process.

- Water Quench System

The water quench system option instructs the model to include a water quench in the raw gas stream. It then calculates the amount of water used in the quench which is added to the synthesis gas and the exit temperature of the gas leaving the quench system.

- Gasifier Operating Pressure

The gasifier operating pressure must be specified by the program user. The variable is used in the calculation of the enthalpy balances over the gasifier, in the calculation of the mass and energy balances over the quench system and in the proceeding step models after the gasification step.

5.7 Analysis of Gasification Capital Cost Data

Usable data on capital costs was difficult to obtain and many of the cost estimates are based on published values and hence may be unreliable. However most of the reported capital costs are similar for the same size gasifier regardless of gasifier type, as shown in Figure 5.5. Differences in gasifier economics are therefore more dependent on operational costs and gas quality than on capital cost.

The capital costs estimates used are given in Appendix D. Many capital cost estimates of gasifiers were published in the 1970's with the increase in interest in gasification for liquid fuels production such as the papers contained in Synthetic Fuels Processing[122]. However these capital cost estimates are for the mid 1970's and for gasifiers no longer of commercial interest. The most recent interest in coal gasification has been for Integrated Coal Gasification Combined Cycle power plant use and also for generating substitute natural gas. For these reasons many of the capital cost estimates have been obtained form publications by the Electric Power Research Institute (EPRI) or form the Gas Research Institute (IGT), both of these organizations being involved in the sponsoring of gasifier development and in performing economic analyses several gasifiers for various purposes.

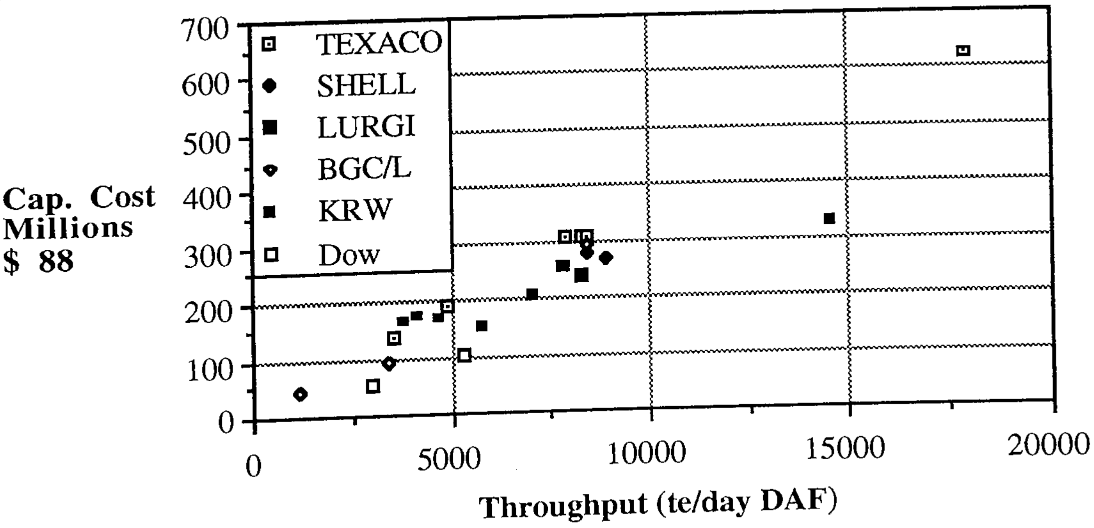

Figure 5.5 Gasifier Capital Costs

The gasifier models cannot predict power requirement from first principles and depend on published data for these values. However the power requirement is quite small in comparison to other utility requirement costs such as oxygen and steam, and these are predicted from the mass and energy balance over the gasifier.

The largest limitations of the gasifier models are, therefore, the accuracy of the mass and energy balance calculations and the inability of the models to check the applicability of the feedstock for the gasifier from first principles. This information has to be input by the program user if alternative feedstocks are input into the data files. Capital cost data for several coal gasification steps were converted to a common mid 1988 UK £ basis for inclusion in the model.

CHAPTER 6
SYNGAS CONVERSION MODELS

6.1 Introduction

After the gas has been produced by the gasification step it first has to be conditioned to provide a gas suitable for use in the particular gas conversion step and impurities such as excess CO_2 and sulphur dioxide must be removed. It is the purpose of this chapter to describe the steps necessary for the conditioning of the gas and its conversion to a liquid fuel and to describe the modelling of the processes involved.

6.2 Fuel Alcohol Synthesis and Distillation

The fuel alcohol step mass balance was modeled based on data provided by John Brown Engineers and Constructors Ltd on the IFP fuel alcohol synthesis process. The step performs a mass balance from the compressed raw feed synthesis gas to a product fuel alcohol containing C_1 to C_6 alcohols. It includes the CO shift and acid gas removal steps within the mass balance. A sample mass balance is given in section 4.4.1.6 showing the main stream compositions, from the feed of raw pressurized synthesis gas, to distiled fuel alcohol. A block flow diagram is shown in Figure 6.1. The variables used in the equations and the equations used are given in Appendix C. The derivation of the equations are given in Appendix C. The step model includes the following process steps:

- CO Shift (where required);
- H_2S removal;
- CO_2 removal;
- Alcohol synthesis, which also includes a shift and CO_2 absorber;
- Steam reformer or PSA Unit in the recycle stream, where required.

It excludes raw syngas compression which is not part of the iterative solution. As the syngas feed varies in composition particularly with respect to the methane content, a number of recycle options were included to allow for optimising the choice of recycle with the feed gas. For example syngas feeds with no methane content may not require recycling of the offgas, whereas feeds with a high methane content may have the offgas, containing methane, converted to CO and H_2 by steam reforming and fed back to the alcohol unit as feed. The following options were therefore provided for handling the recycle stream from the alcohol unit:

- Zero recycle, ie no recycle loop is included;
- Recycle with no treating, ie the recycle stream is simply returned to the alcohol unit feed, a purge stream is included;
- Recycle with reformer, ie a reformer is included in the recycle stream to convert methane and other hydrocarbons to H_2, CO and CO_2;
- Recycle with PSA (pressure swing absorption) unit, ie a PSA unit is included to recover hydrogen from the recycle stream.

The key variables in running the different cases to obtain the optimum yield for the different feed gas compositions are as follows:

- Selection of recycle option;
- Varying the recycle ratio, which changes the level of inerts in the system, the amount of hydrocarbons in the reformer feed and the yield of alcohol produced.

6.2.1 Basis Of Mass Balances

The following sub-sections form the basis of the mass balances as used in the fuel alcohol steps model. The variables and array names as used in the program are shown in brackets for each parameter and these correspond to the names used in the equation descriptions and derivations given in the Appendix C.

The basis of the units which perform the CO shift, CO_2 and H_2S removal, tail gas treating, steam reforming and pressure swing absorption (for H_2 purification) are described in sections 4.4.6 to 4.4.8.

6.2.2 Alcohol Unit

a) The data given below is based on IFP published literature.

b) The catalyst used for the synthesis of the alcohols also promotes the water gas shift reaction, producing CO_2 and reducing the water content of the product. In order to simulate this the alcohol unit is assumed to contain a shift reactor section, which is located after the synthesis reactor. The shift is used to reduce the amount of water in the final alcohol product.

c) The alcohol unit contains a CO_2 removal tower, which is located in the recycle gas stream within the alcohol unit.

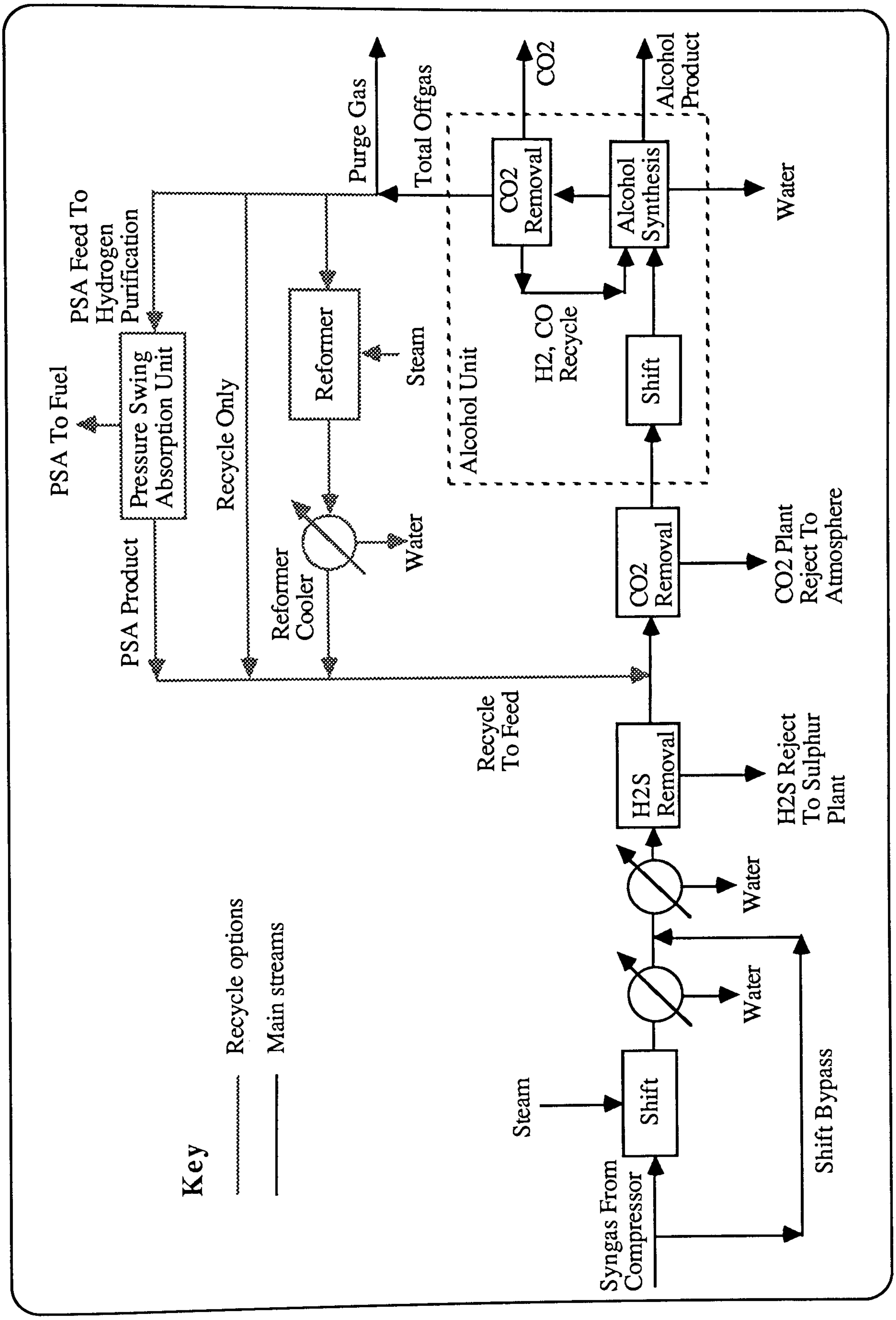

Figure 6.1 Fuel Alcohol Plant Block Flow Diagram

d) The following chemical reactions are used in the mass balances:

i) Alcohol Production

$$\begin{aligned}
CO + 2H_2 &\longrightarrow CH_3OH \\
2CO + 4H_2 &\longrightarrow C_2H_5OH + H_2O \\
3CO + 6H_2 &\longrightarrow C_3H_7OH + 2H_2O \\
4CO + 8H_2 &\longrightarrow C_4H_9OH + 3H_2O \\
5CO + 10H_2 &\longrightarrow C_5H_{11}OH + 4H_2O \\
6CO + 12H_2 &\longrightarrow C_6H_{13}OH + 5H_2O
\end{aligned}$$

ii) Hydrocarbon Production
Hydrocarbons are produced as well as the alcohols shown above, they are added to the offgas from the alcohol unit and are either purged off or recycled back to the feed depending on the choice of recycle.

$$\begin{aligned}
CO + 3H_2 &\longrightarrow CH_4 + H_2O \\
2CO + 5H_2 &\longrightarrow C_2H_6 + 2H_2O \\
3CO + 7H_2 &\longrightarrow C_3H_8 + 3H_2O \\
4CO + 9H_2 &\longrightarrow C_4H_{10} + 4H_2O \\
5CO + 11H_2 &\longrightarrow C_5H_{12} + 5H_2O
\end{aligned}$$

iii) Shift

$$CO + H_2O \longrightarrow CO_2 + H_2$$

e) Input Variables

i) Product Compositions.
The yields of alcohols and hydrocarbons are as follows in weight fractions. These are used for all cases.

	Alcohols WFA[N]	Hydrocarbons WFG[N]
C_1	0.600	0.743
C_2	0.190	0.152
C_3	0.110	0.079
C_4	0.055	0.018
C_5	0.025	0.008
C_6	0.020	-------

ii) The feed H_2 : CO molar ratio [RH], is specified as 1.5 for all cases.

iii) The mol fraction CO in feed shifted [SM], is specified as 0.28 for all cases, ie 28 mol % of the CO in the feed is shifted to CO_2. This gives about 5 wt % water in the final alcohol product.

iv) The mol fraction CO conversion to alcohols & hydrocarbons [CNV], is specified as 0.90 for all cases. It relates to the amount of CO in the feed after 28 mol % of the feed has been shifted to CO_2.

v) The mol fraction selectivity to alcohols [SAC], is specified as 0.75 for all cases. Thus 75 mol % of CO that is converted (to hydrocarbons and alcohols) produces alcohols, and 25 mol % produces hydrocarbons.

vi) The mol fraction CO_2 in offgas / recycle gas, dry basis [AA], is specified as 0.02 for all cases.

vii) The operating pressures used are as follows and were used in all cases for the calculation of the water balance only.

	Pressure Bar (abs)	Variable
Downstream feed compressor	85	PM1
HP Separator	80	PM2
SVP H_2O at 38 °C	0.06624	VP1

6.2.3 Recycle Stream

a) Three different types of recycle system can be evaluated. The type of system is selected as follows by setting the variable [RQ] from the keyboard when the program is running:

[RQ] = 0 Recycle with no processing of the stream;

[RQ] = 1 Recycle stream processes in steam reformer to convert hydrocarbons to H_2 & CO;

[RQ] = 2 Recycle stream processed in PSA Unit to recover hydrogen for recycling, or utility use.

b) The recycle ratio [RR], is the molar ratio of the recycle reformer etc, to the purge gas.

c) If hydrocarbons are present in large enough concentrations, depending on the particular feed gas composition, in the offgas, the off gas may be steam reformed and recycled back to the feed. As an excess of hydrogen is produced by steam reforming enough gas can be recycled to eliminate the shift unit. Recycling more than this amount is not beneficial as the feed gas would then contain an excess of hydrogen which can not be utilized in the alcohol unit. The recycle convergence to eliminate shift [SK], is specified as:

- 0 if convergence not required;
- 1 if convergence required.

If convergence is specified as 1, then the recycle ratio will be adjusted from that specified in the input data until the water shift is eliminated.

6.2.4 Simplified Calculation Sequence

A summary of the variables used and the associated equations is given in Appendix C and the derivation of the equations is given in Appendix C. Figures 4.19 to 4.26 show simplified calculation sequence of the mass balance for the fuel alcohol step, including gas shifting, acid gas removal and the associated recycle loops.

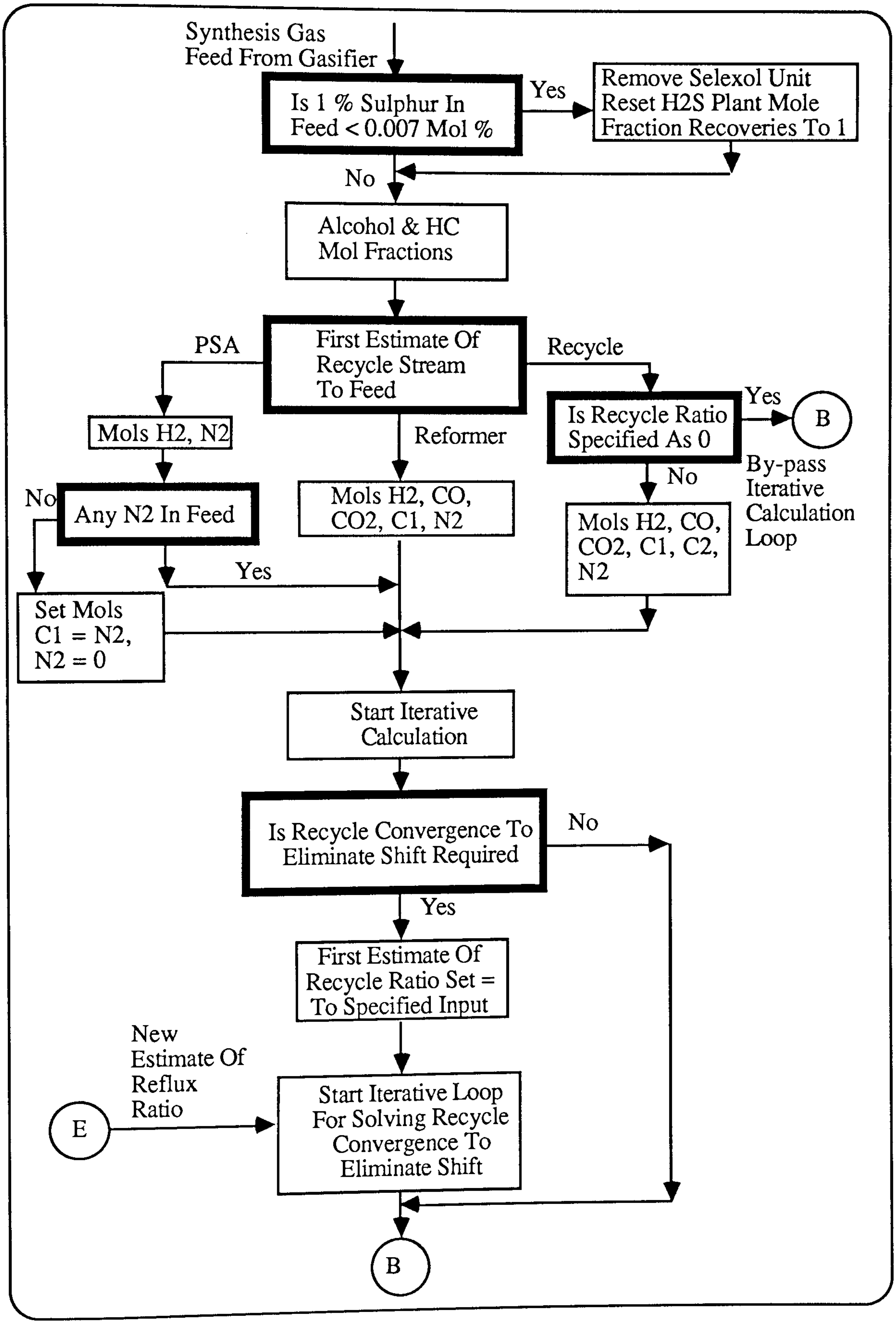

Figure 6.2 Fuel Alcohol Program Calculation Sequence, Part A

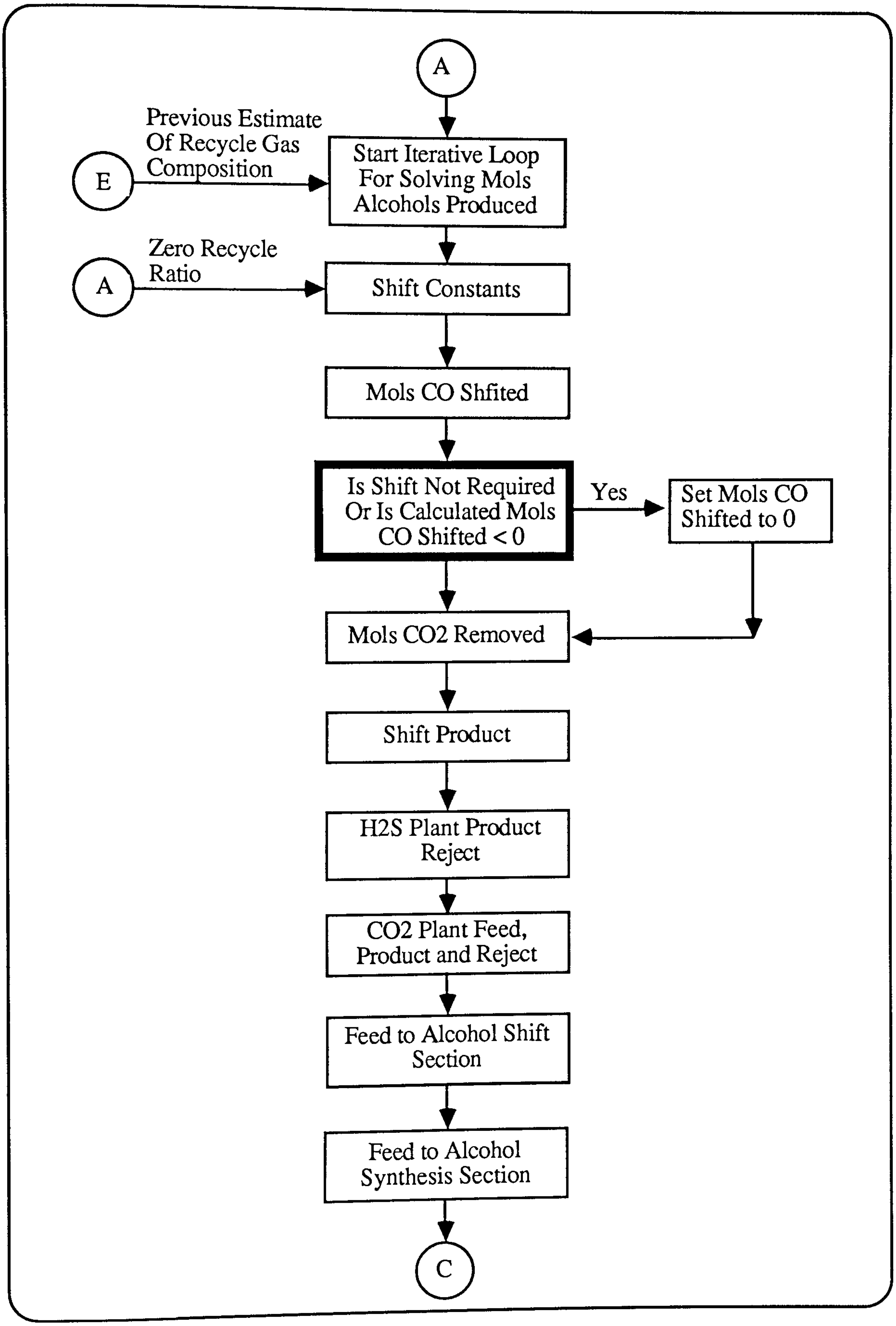

Figure 6.3 Fuel Alcohol Program Calculation Sequence, Part B

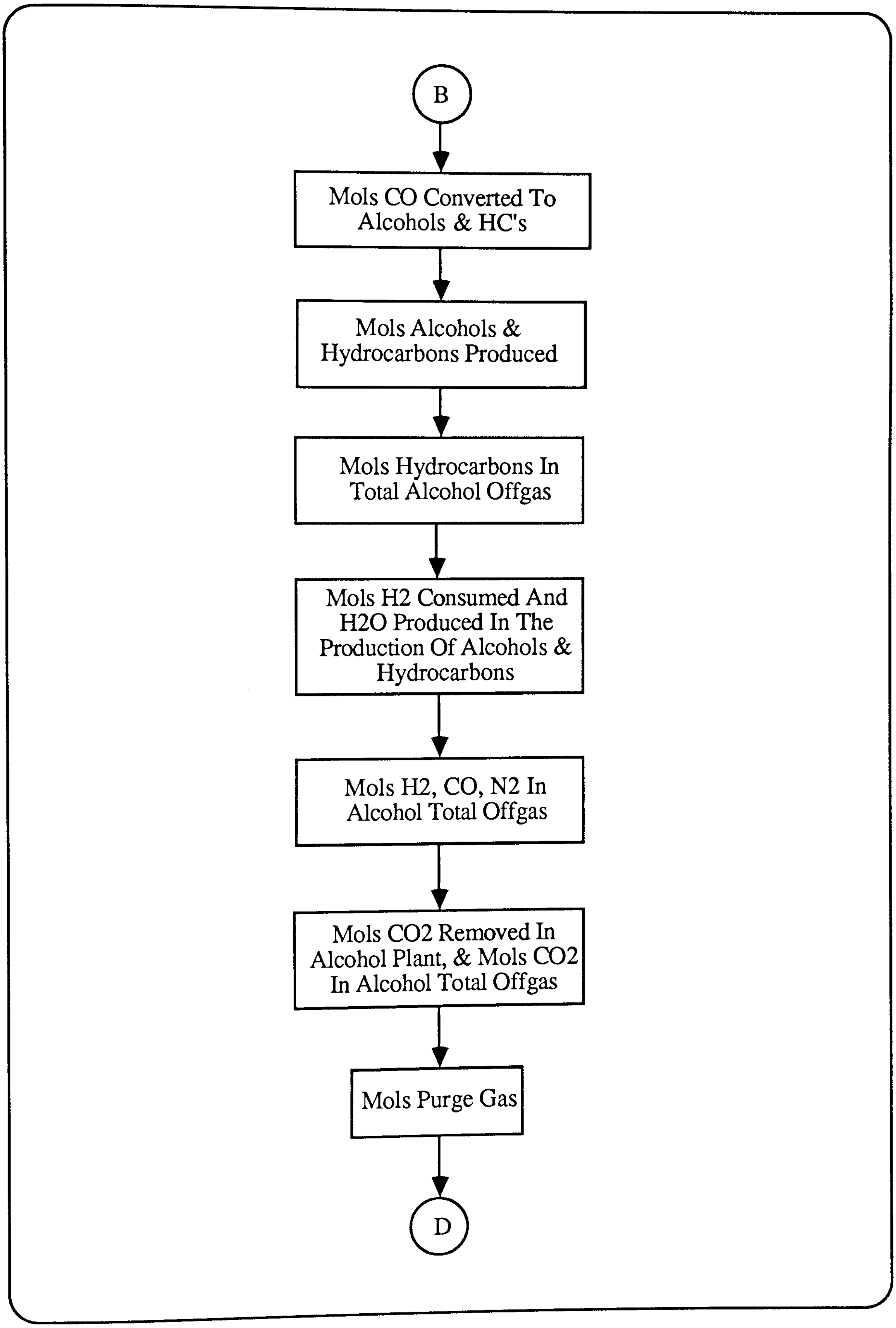

Figure 6.4 Fuel Alcohol Program Calculation Sequence, Part C

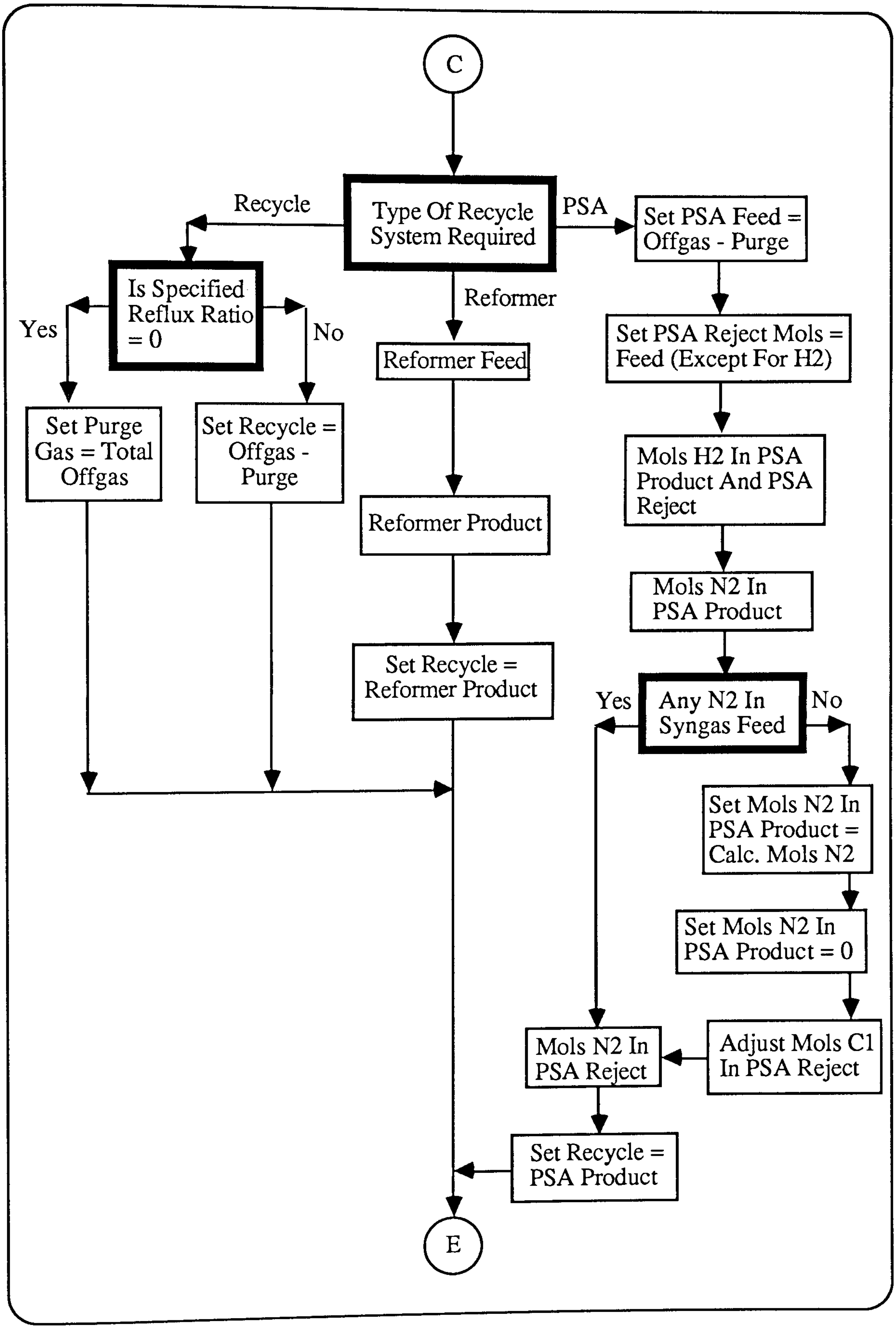

Figure 6.5 Fuel Alcohol Program Calculation Sequence, Part D

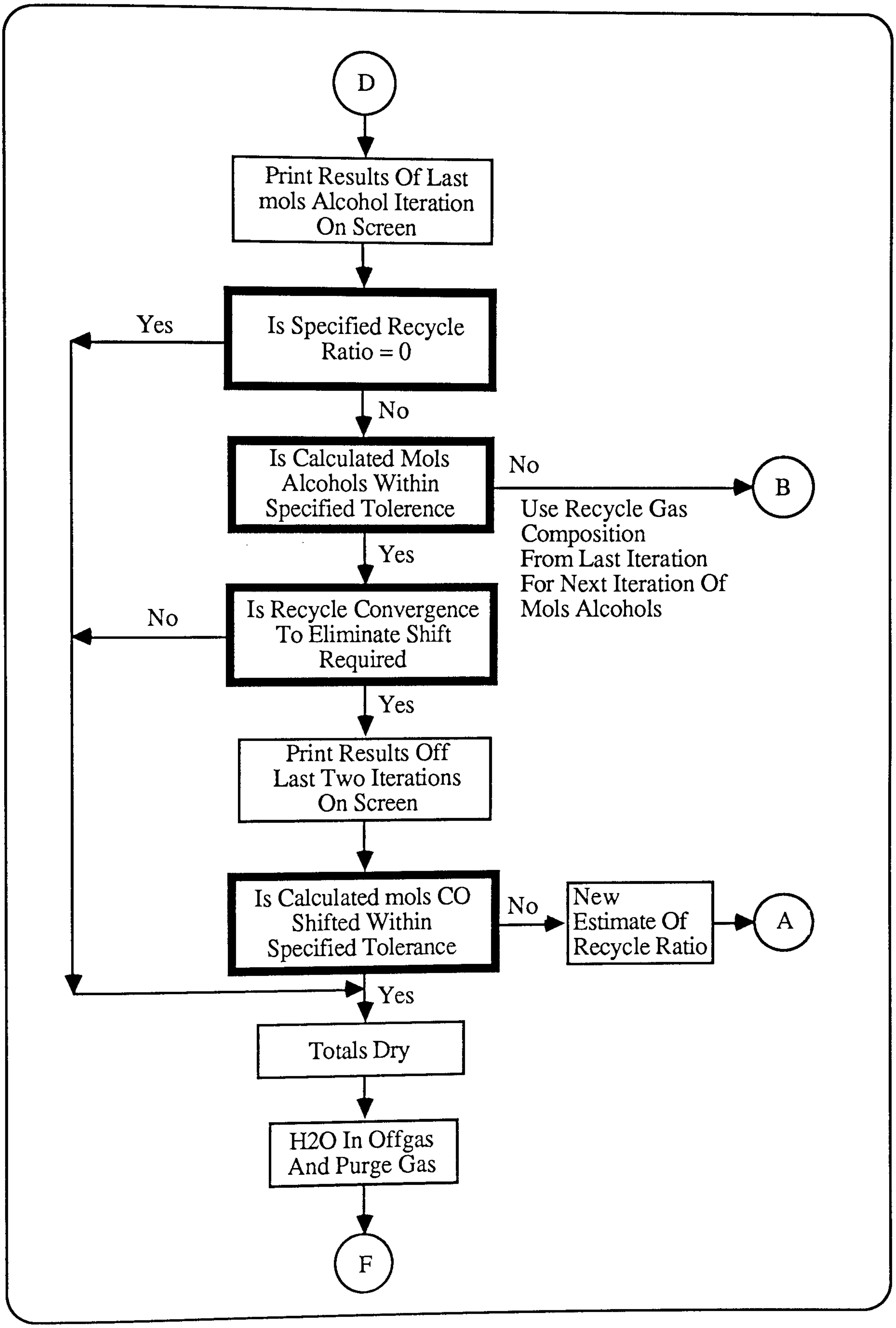

Figure 6.6 Fuel Alcohol Program Calculation Sequence, Part E

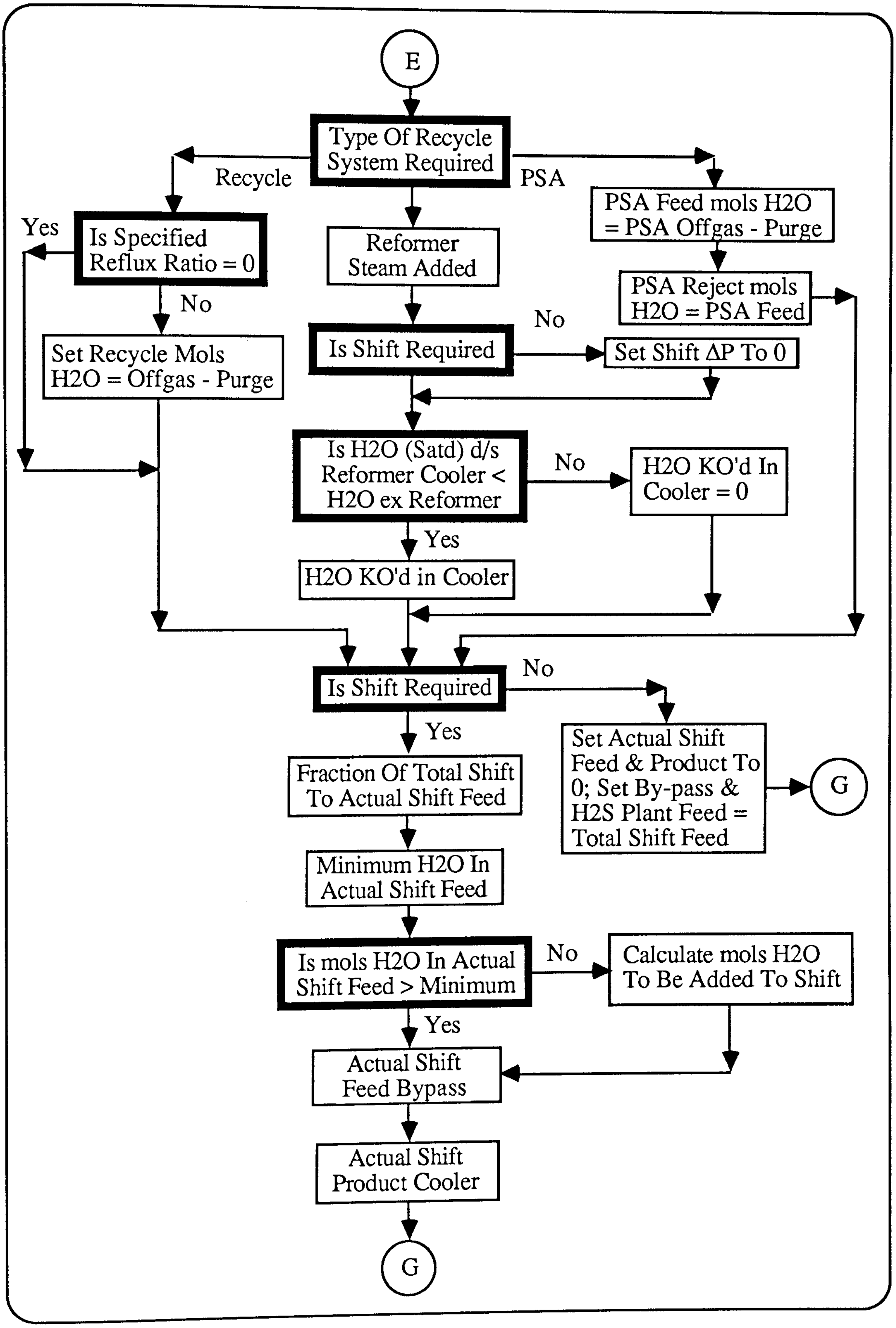

Figure 6.7 **Fuel Alcohol Program Calculation Sequence, Part F**

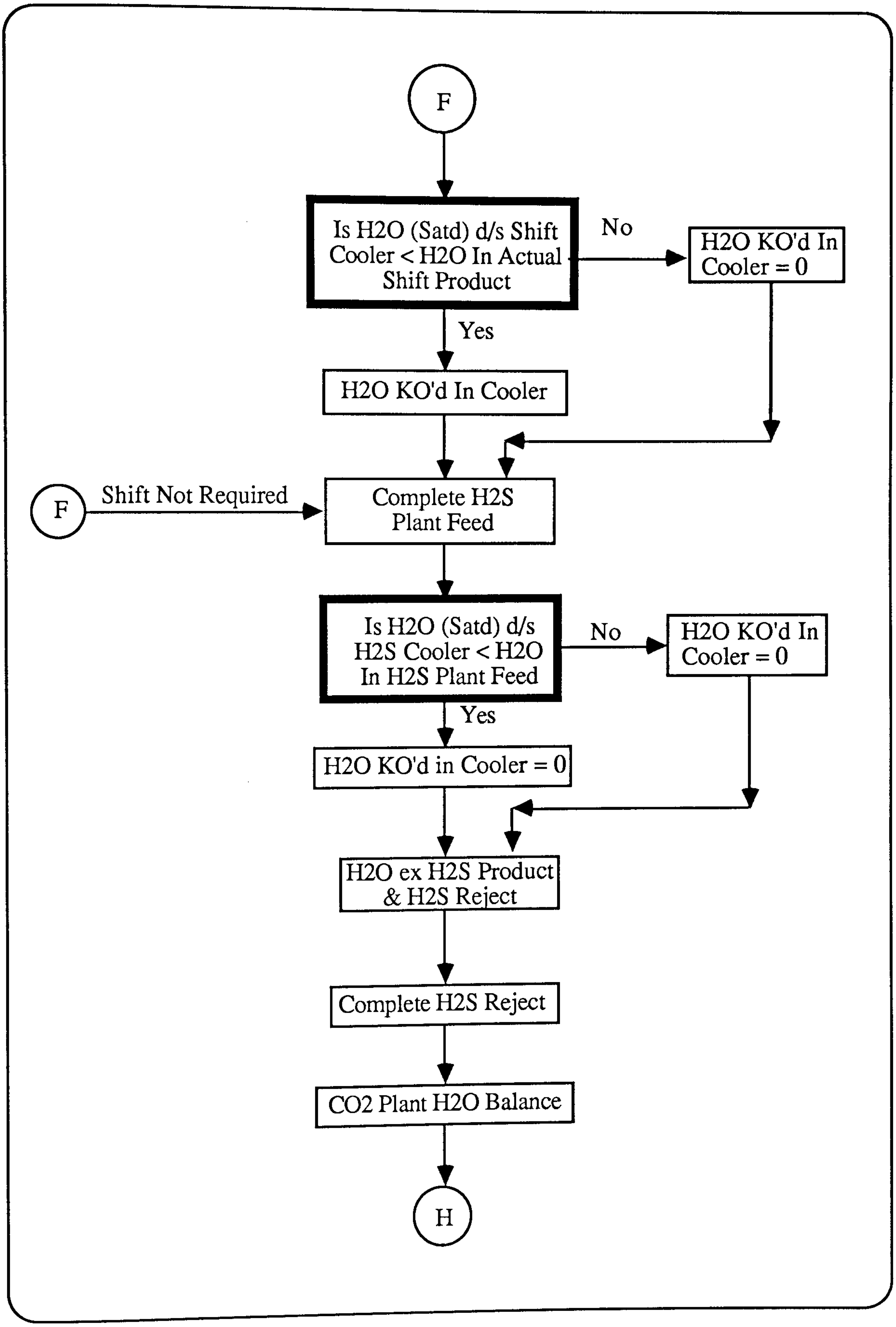

Figure 6.8 Fuel Alcohol Program Calculation Sequence, Part G

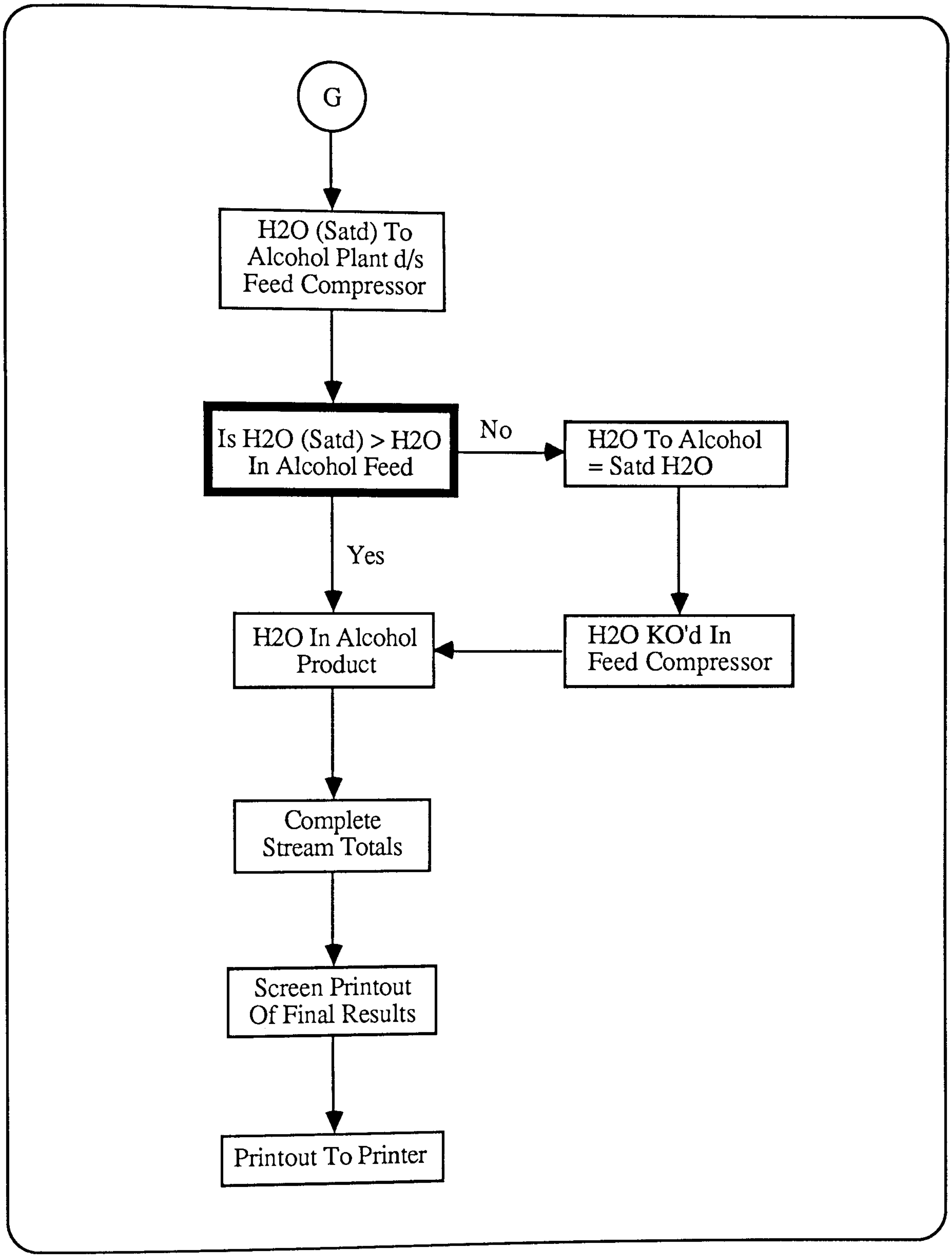

Figure 6.9 Fuel Alcohol Program Calculation Sequence, Part H

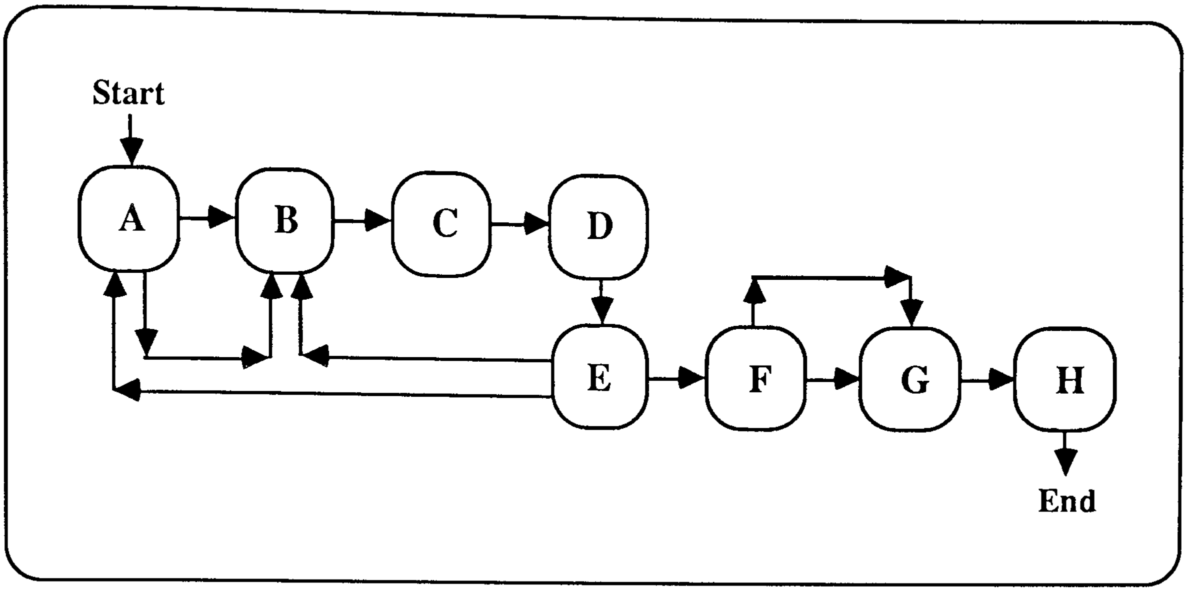

Figure 6.10 Overall Fuel Alcohol Calculation Procedure

6.2.5 Mass Balance For Fuel Alcohol Step (With Shell Gasifier)

The following is an example of the model output for the fuel alcohol step including CO shift acid gas removal and alcohol synthesis.

```
MOLS RECYCLE               0.000
MOL% N2+HC TO ALC.         0.483
MOLS N2 IN PURGE           4.249
MOL% H2 IN OFFGAS         59.915
MOL% H2O EX SHIFT          7.179
CASE:Shell Gasifier
************************************************
           SYNGAS        ACTUAL**      ACTUAL**      SHIFT
           FEED          SHIFT FEED    SHIFT PROD    BY-PASS
           -----------   -----------   -----------   -----------
H2            319.797       134.381       406.185       185.416
CO            666.837       280.210         8.406       386.627
CO2            25.698        10.799       282.602        14.900
C1              0.631         0.265         0.265         0.366
C2              0.000         0.000         0.000         0.000
N2              4.264         1.792         1.792         2.472
H2O            52.895       322.153        50.349        30.668
H2S             4.975         2.090         2.090         2.884
COS             0.000         0.000         0.000         0.000
SO2             0.000         0.000         0.000         0.000
CS2             0.000         0.000         0.000         0.000
MERCAPTAN       0.000         0.000         0.000         0.000
THIOPHENE       0.000         0.000         0.000         0.000
           -----------   -----------   -----------   -----------
TOTAL        1075.098       751.690       751.690       623.334
```

	H2S PLANT FEED	H2S PLANT REJECT	H2S PLANT PRODUCT	CO2 PLANT FEED
H2	591.601	0.769	590.832	590.832
CO	395.033	0.830	394.204	394.204
CO2	297.502	45.310	252.192	252.192
C1	0.631	0.003	0.628	0.628
C2	0.000	0.000	0.000	0.000
N2	4.264	0.008	4.257	4.257
H2O	81.018	2.040	0.922	0.922
C3	0.000	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000
C5	0.000	0.000	0.000	0.000
H2S	4.975	4.975	0.000	0.000
COS	0.000	0.000	0.000	0.000
SO2	0.000	0.000	0.000	0.000
CS2	0.000	0.000	0.000	0.000
MERCAPTAN	0.000	0.000	0.000	0.000
THIOPHENE	0.000	0.000	0.000	0.000
TOTAL	1375.024	53.934	1243.034	1243.034

	CO2 PLANT REJECT	ALCOHOL FEED	ALC.FEED D/S SHIFT	TOTAL OFFGAS
H2	0.768	590.064	700.209	136.699
CO	0.828	393.376	283.231	28.323
CO2	232.023	20.170	130.315	4.563
C1	0.003	0.625	0.625	47.037
C2	0.000	0.000	0.000	5.066
N2	0.008	4.249	4.249	4.249
H2O	0.635	0.287	-109.858	0.189
C3	0.000	0.000	0.000	1.795
C4	0.000	0.000	0.000	0.310
C5	0.000	0.000	0.000	0.111
TOTAL	234.264	1008.770	1008.770	228.343

CASE:Shell Gasifier

	PURGE GAS	REFORMER FEED	REFORMER PRODUCT
H2	136.699	0.000	0.000
CO	28.323	0.000	0.000
CO2	4.563	0.000	0.000
C1	47.037	0.000	0.000
C2	5.066	0.000	0.000
N2	4.249	0.000	0.000
H2O	0.189	0.000	0.000
C3	1.795	0.000	0.000
C4	0.310	0.000	0.000
C5	0.111	0.000	0.000
TOTAL	228.343	0.000	0.000

```
                 PSA             PSA            PSA            RECYCLE
                 FEED            PRODUCT        TO FUEL        TO FEED
                 -----------     -----------    -----------    -----------
H2                     0.000           0.000          0.000          0.000
CO                     0.000           0.000          0.000          0.000
CO2                    0.000           0.000          0.000          0.000
C1                     0.000           0.000          0.000          0.000
C2                     0.000           0.000          0.000          0.000
N2                     0.000           0.000          0.000          0.000
H2O                    0.000           0.000          0.000          0.000
C3                     0.000           0.000          0.000          0.000
C4                     0.000           0.000          0.000          0.000
C5                     0.000           0.000          0.000          0.000
                 -----------     -----------    -----------    -----------
TOTAL                  0.000           0.000          0.000          0.000

ALC.PROD   C1OH         C2OH        C3OH        C4OH        C5OH        C6OH
--------   ----------   ----------  ----------  ----------  ----------  ----------
MOLS           94.144       20.736       9.203       3.731       1.426       0.984
H2O MOLS:=     14.637
TOTAL ALC(D):=     130.223 TOTAL ALC(W):=     144.860

                    REFORMER     SHIFT        H2S PLANT    ALCOHOL
                    -----------  -----------  -----------  -----------
H2O ADDED                 0.000      299.926
H2O REMOVED               0.000        0.000       78.055        0.000
CO SHIFTED                           271.804                   110.145
CO2 REMOVED                                                    125.752

MOL% @ UNIT FEED,DRY                               CO2 PLANT
--------------------                               ----------
N2                        0.000        0.417        0.343        0.421
C1-C5                     0.000                                  0.062
C1-C5,N2                               0.682        0.393        0.483
H2                                                              58.510
CO                                    65.235                    39.007
CO2                                                 20.303       2.000

INPUT SPECIFICATIONS
--------------------
ALCOHOL PLANT
-------------
WT.FRACTION  C1          C2          C3          C4          C5          H2S
-----------  ---------   ---------   ---------   ---------   ---------   ---------
ALCOHOLS         0.600       0.190       0.110       0.055       0.025       0.020
HC,S GAS         0.743       0.152       0.079       0.018       0.008

MOLAR H2:CO RATIO                1.500  CO SELECT.ALCOHOLS           0.750
MOL FR.CO SHIFTED                0.280  MF CO CONVERTED              0.900
MOLAR RECYCLE RATIO             15.555
PRESS.,BARA-FEED                85.000  -HP SEPARATOR               80.000
SVP H2O @ 38 C                   0.066

REFORMER & PSA
--------------
MF C1 IN PRODUCT                 0.040  MF HC TO CO                  0.600
STEAM/HC MOL RATIO               3.000  MF PSA H2 RECOVERY           0.900
MF PSA H2 PURITY                 0.995

SHIFT
-----
MF FEED CONV.                    0.970  MOLS H2O/MOL DRY GAS         0.750
SYNGAS FEED PRESS, BARA         30.000  PRESSURE DROP, BAR           1.000
TEMP C,D/S COOLER              170.000  SVP H2O @ TAMP, BARA         7.920

H2S/CO2 REMOVAL
---------------
MF CO2 IN PRODUCT (MAIN)         0.020  PRESS. DROP H2S, BAR         0.500
MF CO2 IN PRODUCT (ALC)          0.020  PRESS. DROP CO2, BAR         0.500
```

6.2.6 Example Of Model Results

By varying the feedstock, the alternative internal options available in the step such as choice of recycle system were tested. By checking the mass balances manually based on the information provided for the steps and by comparing with mass balances prepared by John Brown Engineers & Constructors Ltd, the mass balance was found to work satisfactorily for the feedstocks tested.

Figure 6.11 shows the model results in terms of product mass and energy yields for a Texaco gasifier. The figure shows the variation of product yield for varying coal slurry concentrations fed to the gasifier and illustrates the ability of the model to respond to changes in feed specifications.

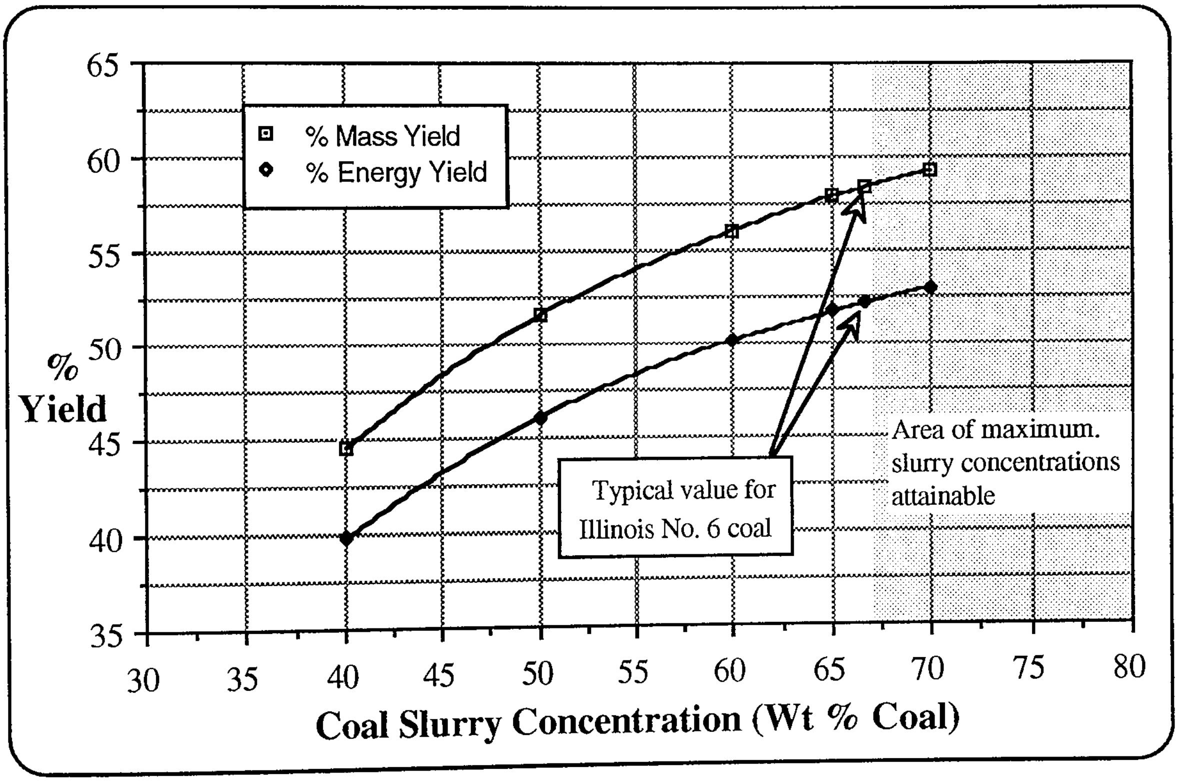

Figure 6.11 Example Model Result For Texaco Gasifier And Fuel Alcohol Product

The drop in product yield with increasing content of water in the slurry is due to more of the energy in the feed being required to evaporate the water in the gasifier. This leads to greater proportions of the energy appearing in the raw synthesis gas as sensible rather than chemical energy. The greater level of steam in the gas also changes the gas composition via the water gas shift reaction. For feeds with high slurry water content the sensible heat must be recovered and used as efficiently as possible.

A similar but less critical situation exists where gasifiers are fed with dried coal as opposed to a slurry, where product yield improves with drier feedstocks. However the expense of coal drying precludes very low moisture feeds. In these cases the coal feed moisture content is usually reduced to allow easy handling of the coal.

6.3 Methanol Synthesis And Distillation

The methanol step mass balance was modeled, based on the data provided by John Brown Engineers and Constructors Ltd and given in Appendix A. The step performs similar balances from the compressed raw feed synthesis gas to methanol as for fuel alcohol. The product can be either crude methanol containing some water and traces of other impurities, or distiled methanol, depending on the required product or the feed requirements of further processes. The variables used in the equations and the equations used are given in Appendix C. The derivation of the equations are also given in Appendix C.

6.3.1 Introduction

This step model calculates the overall molar and mass balance for the conversion of all the design feedstocks to methanol, a block flow diagram is shown in Figure 6.12. The model includes the following process steps:

- CO Shift (where required);
- H_2S removal;
- CO_2 removal;
- Methanol synthesis;
- Steam reformer or PSA Unit in the recycle stream, where required.

It excludes raw syngas compression and as discussed in section 4.4.1 for the fuel alcohol model the following recycle options are provided:

- Zero recycle, ie no recycle loop is included;
- Recycle with no treating, ie the recycle stream is simply returned to the alcohol unit feed, a purge stream is included;
- Recycle with reformer, ie a reformer is included in the recycle stream to convert methane and other hydrocarbons to H_2, CO and CO_2;
- Recycle with PSA (pressure swing absorption) unit, ie a PSA unit is included to recover hydrogen from the recycle stream.

The key variables in running the different cases are as follows:

- Selection of recycle option;
- Varying the recycle ratio, which changes the level of inerts in the system, the amount of hydrocarbons in the reformer feed and the mols of alcohol produced.

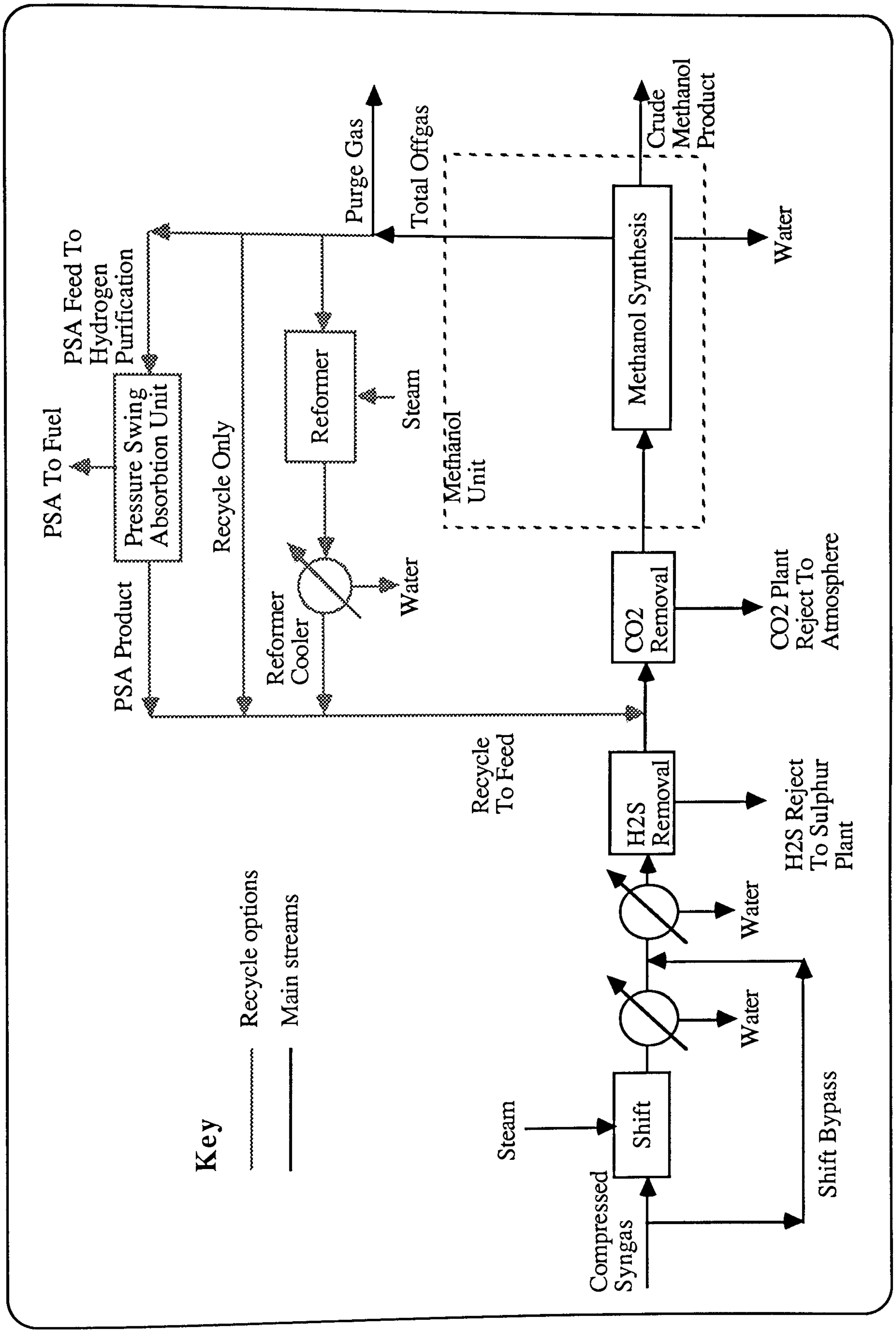

Figure 6.12 Methanol Plant Block Flow Diagram

6.3.2 Basis Of Mass Balances

The following sub-sections form the basis of the mass balances as used in the methanol step model. The variables and array names as used in the program are shown in brackets for each parameter and these correspond to the names used in the equation descriptions and derivations given in the Appendix C.

The basis of the Units which perform the CO shift, CO_2 and H_2S removal, tail gas treating, steam reforming and pressure swing absorption (for H_2 purification) are described in sections 4.4.6 to 4.4.8.

The methanol synthesis Step 431, differs from the fuel alcohol step in the actual synthesis unit only. The choice of recycle system and the basis of the models which perform the gas conditioning is identical to that for the fuel alcohol step.

6.3.3 Methanol Unit

The methanol unit converts the cleaned and conditioned synthesis gas to a crude product methanol which contains water and other impurities such as higher alcohols in small amounts. The methanol distillation unit is a separate model.

a) The data given below is based on ICI and Lurgi published literature.

b) The following chemical reactions are used in the mass balances:

i) Methanol Production

$$CO + 2H_2 \text{ --> } CH_3OH$$

e) Input Variables

i) Product compositions.

ii) The composition of the syngas produced in the gasification steps is generally adjusted in the syngas treating/conditioning units to meet the following approximate molar ratio, which is the optimum feed H_2 : CO molar ratio [RH] for methanol synthesis:

$$\frac{H2 + CO2}{CO + CO2} = 2.1$$

iv) The mole fraction CO converted to products [CNV], is specified as 0.951. The mole fraction of CO2 converted to products is specified as 49.1.

v) The mol fraction selectivity to methanol [SAC], is specified as 0.991 for all cases. Thus 99 mol % of CO that is converted produces methanol, and 0.009 mol % produces impurities.

vi) The mol fraction CO_2 in offgas / recycle gas, dry basis [AA], is specified as 0.02 for all cases.

vii) The operating pressures are following data is used in all cases and is only used for the calculations of the water balance.

	Pressure bar (abs)	Variable
Downstream feed compressor	85	PM1
High Pressure Separator	80	PM2
Saturated Vapour Pressure H_2O at 38 °C	0.06624	VP1

6.3.4 Recycle Stream.

The recycle system for the methanol synthesis step 431 is identical in basis as explained in section 4.4.1.4 for the fuel alcohol step.

6.3.5 Simplified Calculation Sequence

A summary of the variables used and the associated equations is given in Appendix C and the derivation of the equations is given in Appendix C. Figures 4.30 to 4.36 show simplified calculation sequence of the mass balance for the methanol synthesis step, including gas shifting, acid gas removal and the associated recycle loops.

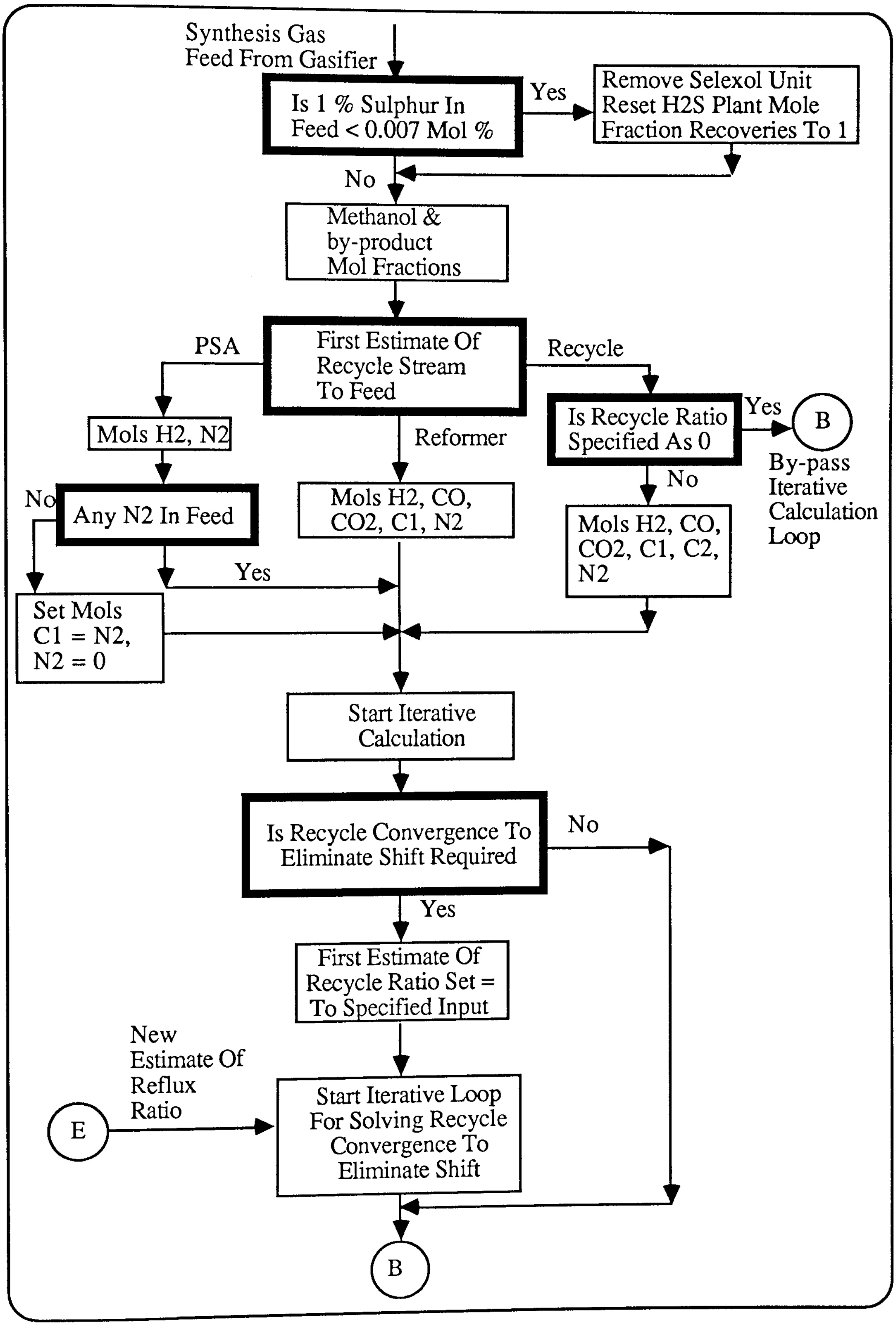

Figure 6.13 Methanol Program Calculation Sequence, Part A

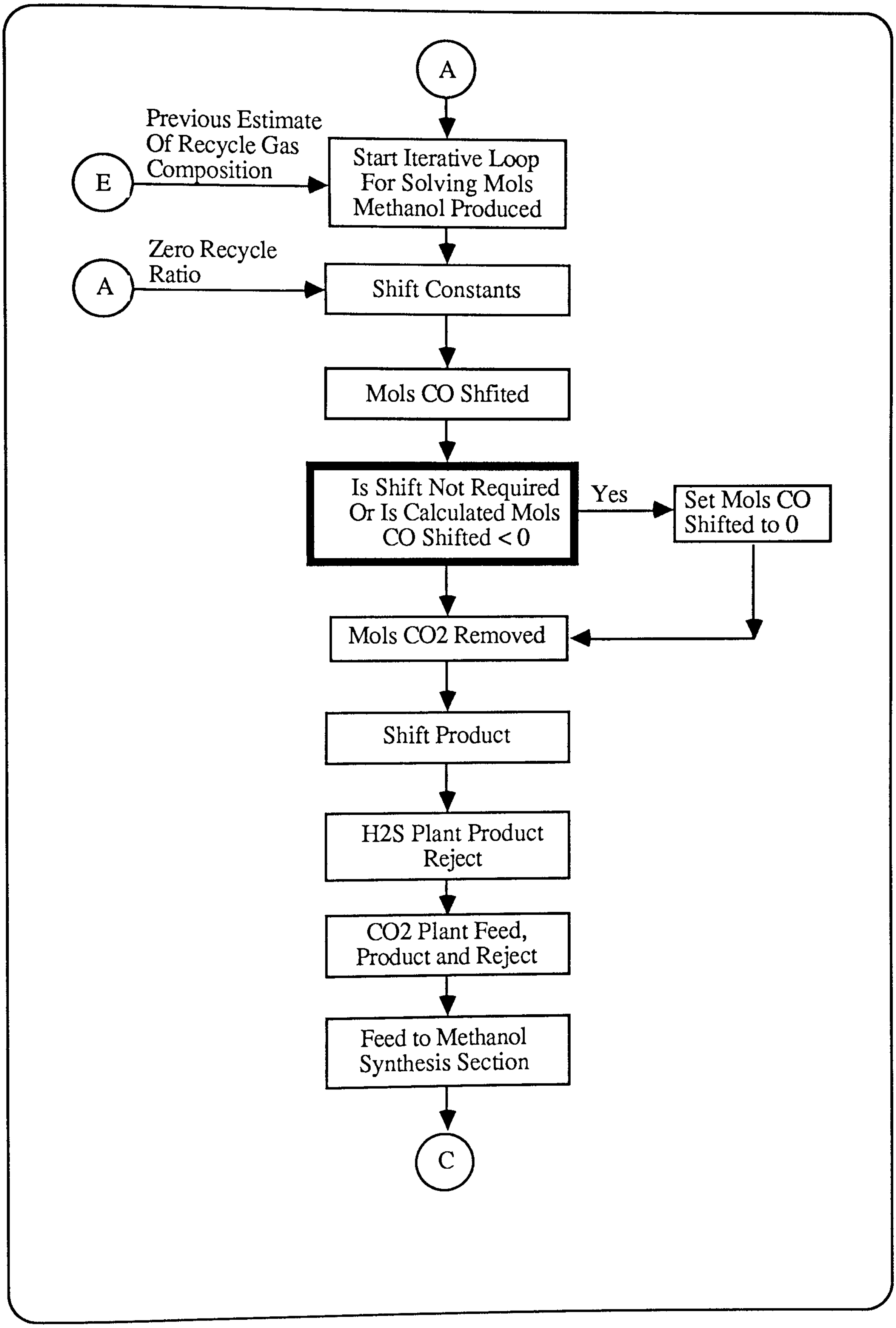

Figure 6.14 **Methanol Program Calculation Sequence, Part B**

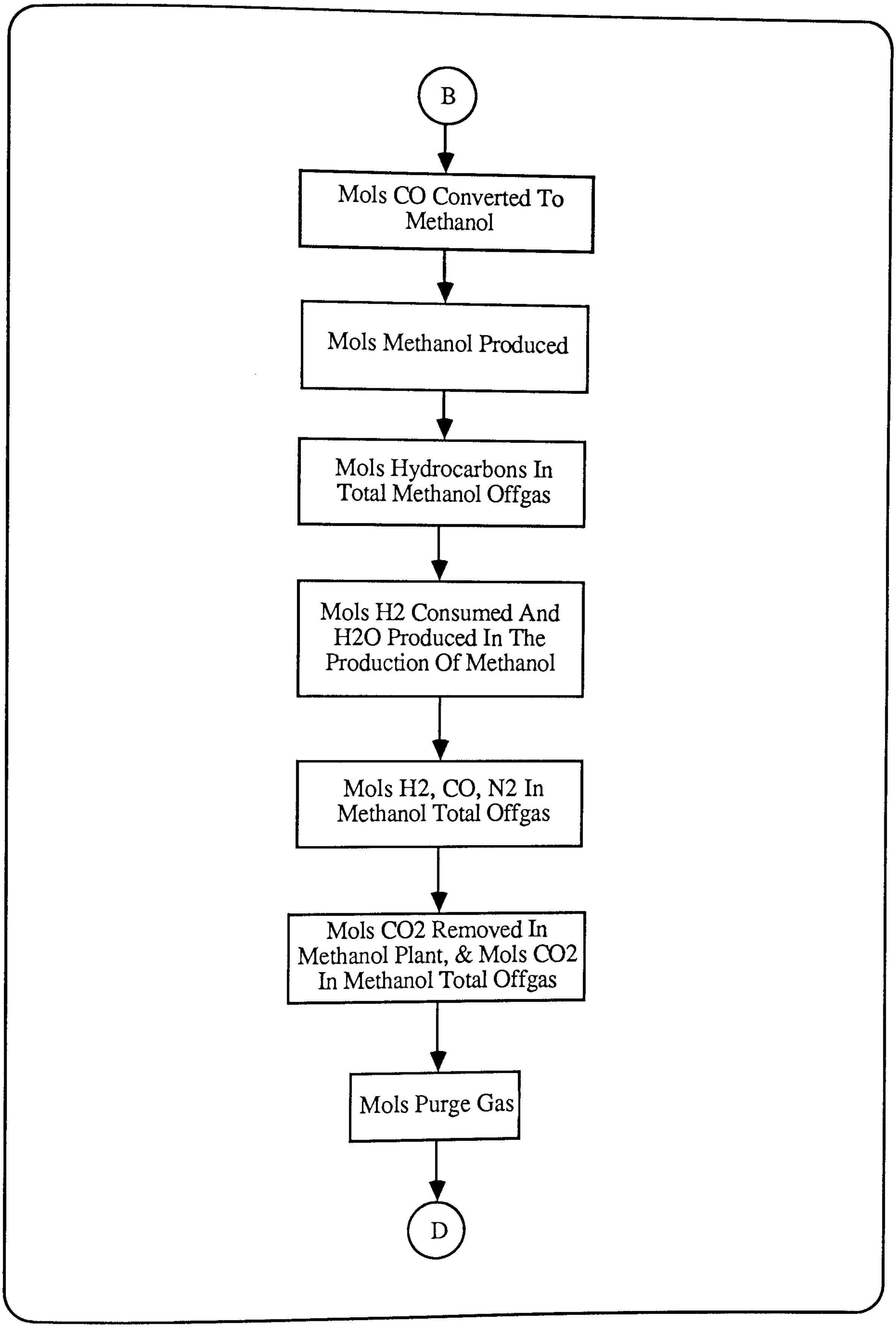

Figure 6.15 Methanol Program Calculation Sequence, Part C

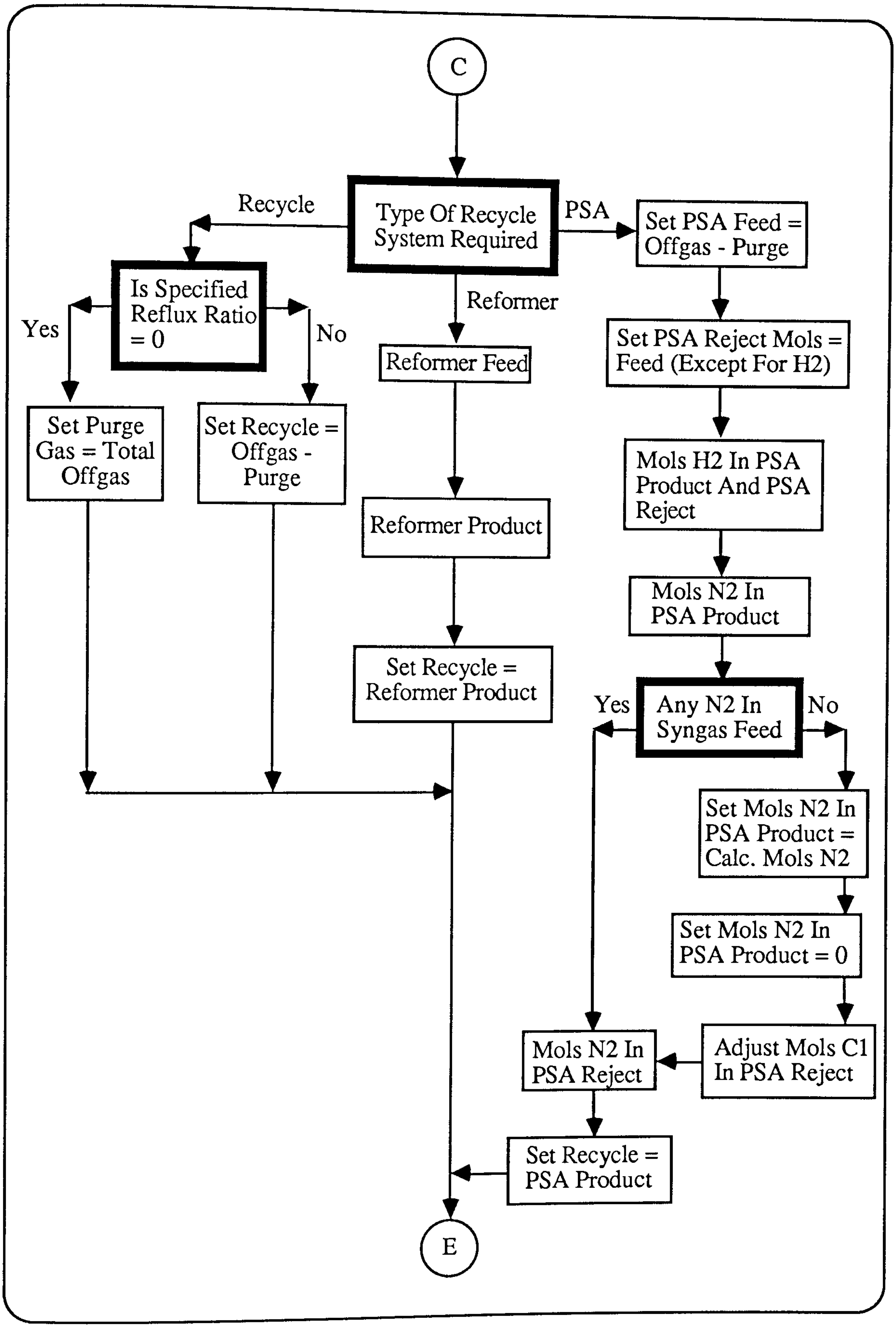

Figure 6.16 Methanol Program Calculation Sequence, Part D

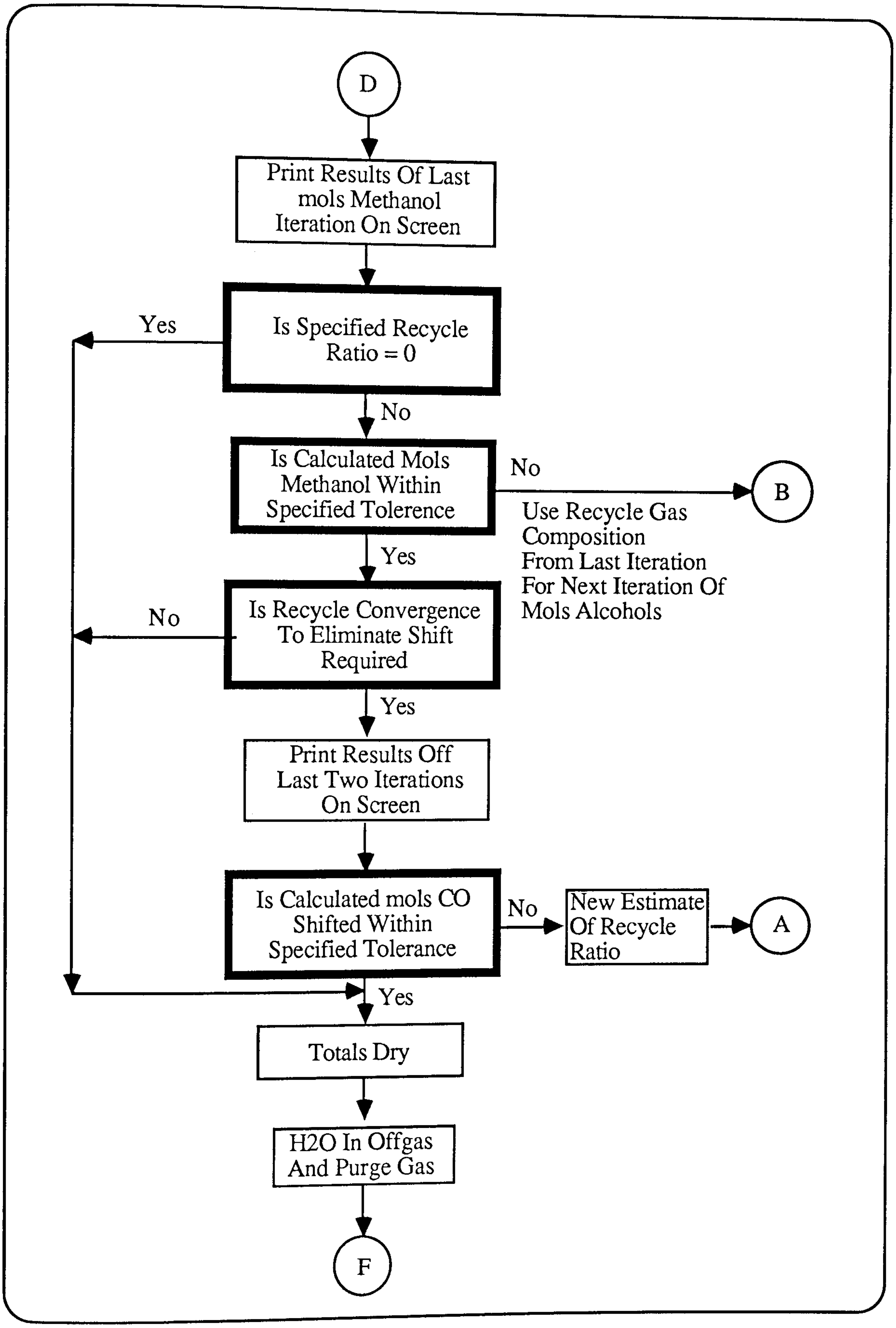

Figure 6.17 Methanol Program Calculation Sequence, Part E

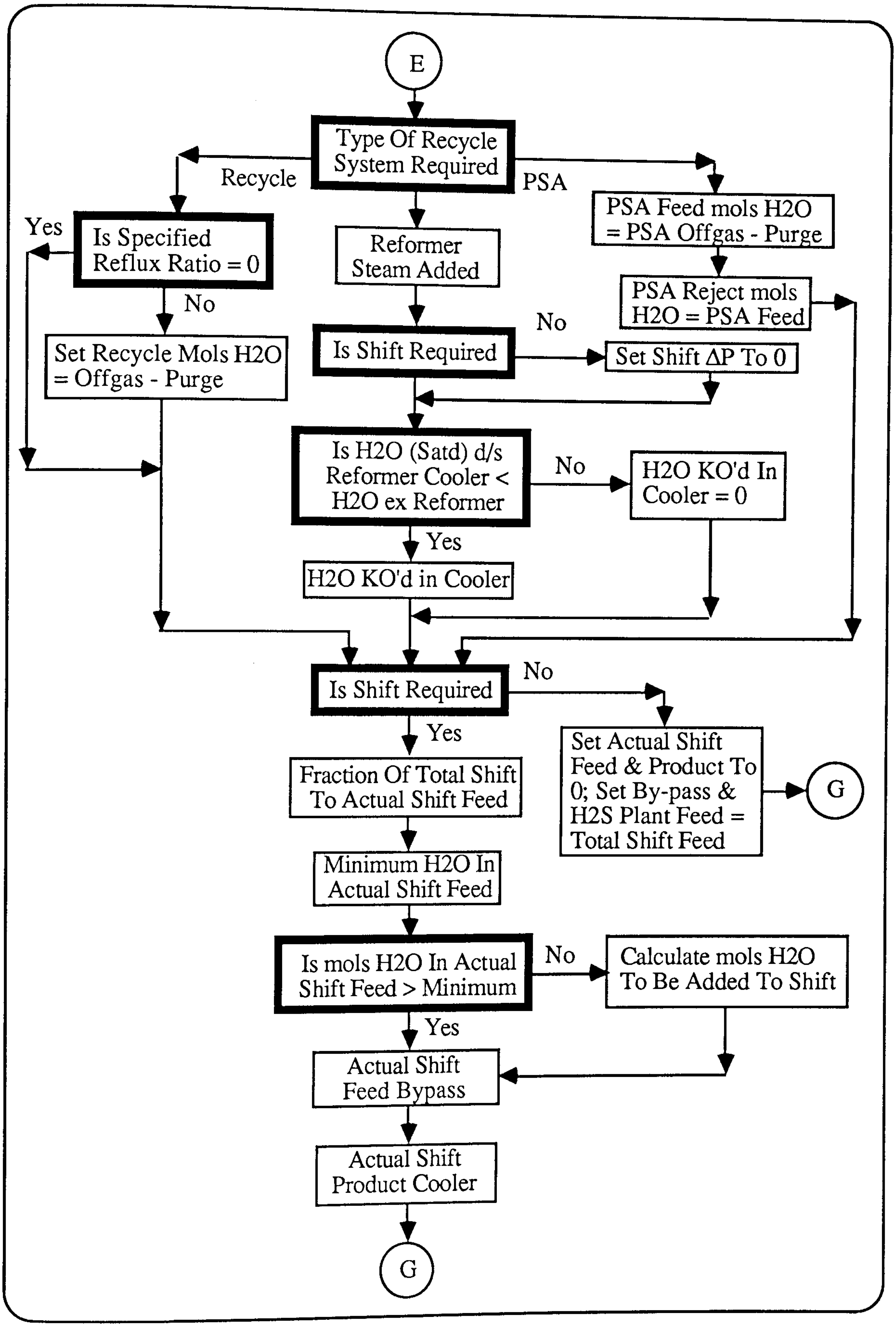

Figure 6.18 Methanol Program Calculation Sequence, Part F

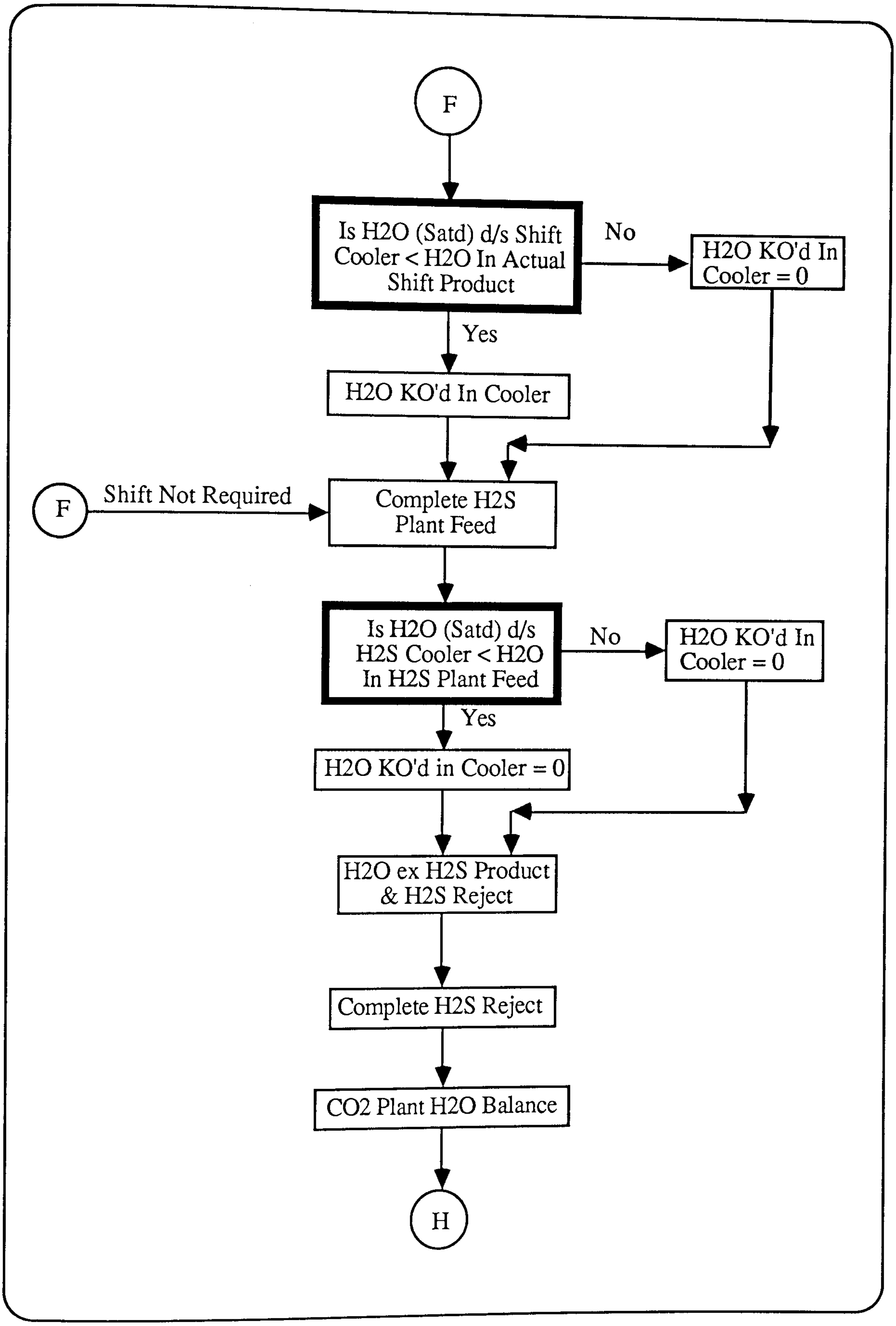

Figure 6.19 Methanol Program Calculation Sequence, Part G

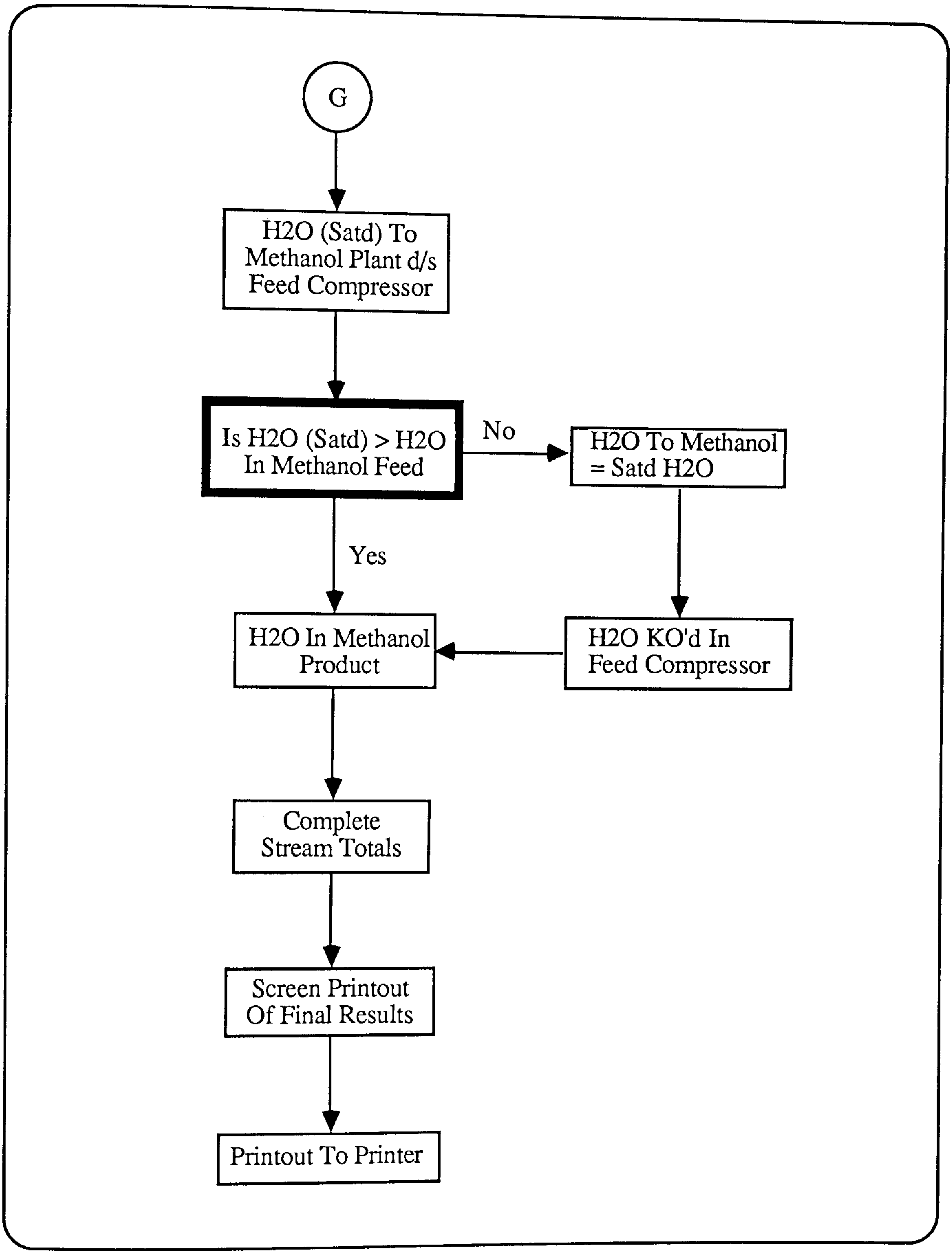

Figure 6.20 Methanol Program Calculation Sequence, Part H

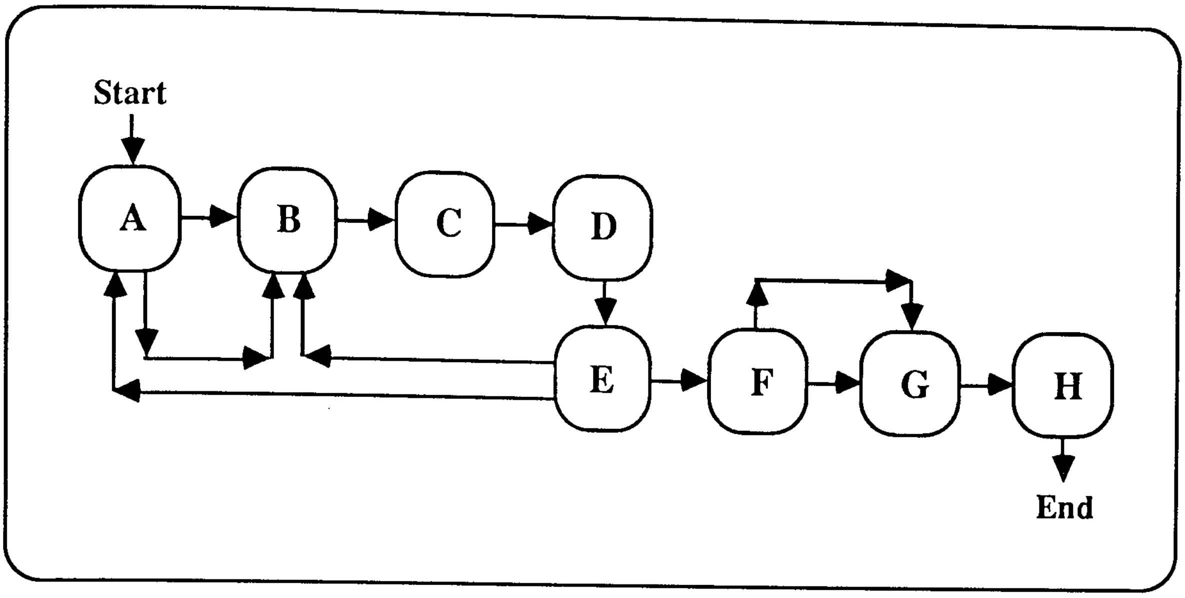

Figure 6.21 Overall Methanol Calculation Procedure

6.3.6 Mass Balance For Methanol Step (With Shell Gasifier)

The following is an example of the model output for the methanol step including CO shift acid gas removal and alcohol synthesis.

```
MOLS RECYCLE              0.000
MOL% N2+HC TO ALC.        0.483
MOLS N2 IN PURGE          4.249
MOL% H2 IN OFFGAS        61.920
MOL% H2O EX SHIFT          7.179
CASE: Shell Gasifier, Point of Ayr, Methanol Synthesis, No Recycle
************************************************
           SYNGAS         ACTUAL**      ACTUAL**      SHIFT
           FEED           SHIFT FEED    SHIFT PROD    BY-PASS
           -----------    -----------   -----------   -----------
H2             319.797       174.169       526.447       145.629
CO             666.837       363.174        10.895       303.663
CO2             25.698        13.996       366.275        11.702
C1               0.631         0.344         0.344         0.287
C2               0.000         0.000         0.000         0.000
N2               4.264         2.322         2.322         1.942
H2O             52.895       417.535        65.257        24.087
H2S              4.975         2.709         2.709         2.265
COS              0.000         0.000         0.000         0.000
SO2              0.000         0.000         0.000         0.000
CS2              0.000         0.000         0.000         0.000
MERCAPTAN        0.000         0.000         0.000         0.000
THIOPHENE        0.000         0.000         0.000         0.000
           -----------    -----------   -----------   -----------
TOTAL         1075.098       974.249       974.249       489.576
```

	H2S PLANT FEED	H2S PLANT REJECT	H2S PLANT PRODUCT	CO2 PLANT FEED
H2	672.076	0.874	671.202	671.202
CO	314.558	0.661	313.897	313.897
CO2	377.977	57.566	320.411	320.411
C1	0.631	0.003	0.628	0.628
C2	0.000	0.000	0.000	0.000
N2	4.264	0.008	4.257	4.257
H2O	89.344	2.167	0.980	0.980
C3	0.000	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000
C5	0.000	0.000	0.000	0.000
H2S	4.975	4.975	0.000	0.000
COS	0.000	0.000	0.000	0.000
SO2	0.000	0.000	0.000	0.000
CS2	0.000	0.000	0.000	0.000
MERCAPTAN	0.000	0.000	0.000	0.000
THIOPHENE	0.000	0.000	0.000	0.000
TOTAL	1463.825	66.253	1311.375	1311.375

	CO2 PLANT REJECT	METHANOL FEED	TOTAL OFFGAS	PURGE GAS
H2	0.873	670.330	42.817	42.817
CO	0.659	313.238	15.223	15.223
CO2	300.239	20.172	6.860	6.860
C1	0.003	0.625	0.000	0.000
C2	0.000	0.000	0.000	0.000
N2	0.008	4.249	4.249	4.249
H2O	0.675	0.305	0.057	0.057
C3	0.000	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000
C5	0.000	0.000	0.000	0.000
TOTAL	302.456	1008.919	69.206	69.206

	CRUDE (HP) METHANOL	CRUDE (LP) METHANOL	LP OFFGAS	TOTAL GAS TO FUEL
H2	1.280	0.089	1.191	0.000
CO	0.511	0.047	0.464	0.000
CO2	3.245	1.300	1.944	0.000
C1	0.625	0.095	0.530	0.000
C2	0.000	0.000	0.000	0.000
N2	0.275	0.000	0.000	0.000
H2O	10.316	0.000	0.000	0.000
C3	0.000	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000
C5	0.000	0.000	0.000	0.000
TOTAL	301.442	296.814	4.413	0.000

CASE: Shell Gasifier, Point of Ayr, Methanol Synthesis, No Recycle

```
               PURGE          REFORMER       REFORMER
               GAS            FEED           PRODUCT
               -----------    -----------    -----------
H2                 42.817          0.000          0.000
CO                 15.223          0.000          0.000
CO2                 6.860          0.000          0.000
C1                  0.000          0.000          0.000
C2                  0.000          0.000          0.000
N2                  4.249          0.000          0.000
H2O                 0.057          0.000          0.000
C3                  0.000          0.000          0.000
C4                  0.000          0.000          0.000
C5                  0.000          0.000          0.000
               -----------    -----------    -----------
TOTAL              69.206          0.000          0.000


               PSA            PSA            PSA            RECYCLE
               FEED           PRODUCT        TO FUEL        TO FEED
               -----------    -----------    -----------    -----------
H2                  0.000          0.000          0.000          0.000
CO                  0.000          0.000          0.000          0.000
CO2                 0.000          0.000          0.000          0.000
C1                  0.000          0.000          0.000          0.000
C2                  0.000          0.000          0.000          0.000
N2                  0.000          0.000          0.000          0.000
H2O                 0.000          0.000          0.000          0.000
C3                  0.000          0.000          0.000          0.000
C4                  0.000          0.000          0.000          0.000
C5                  0.000          0.000          0.000          0.000
               -----------    -----------    -----------    -----------
TOTAL               0.000          0.000          0.000          0.000

TOTAL ALC(D):=      295.506

%ERROR ON CLOSURES-MOLS ALCOHOL                  0.000
                  -RECYCLE RATIO                 0.000

                  REFORMER       SHIFT          H2S PLANT      ALCOHOL
                  -----------    -----------    -----------    -----------
H20 ADDED               0.000        388.727
H20 REMOVED             0.000          0.000         86.197          0.000
CO SHIFTED                           352.279                         0.000
CO2 REMOVED                                                          0.000

MOL% @ UNIT FEED,DRY                            CO2 PLANT
--------------------                            ----------
N2                      0.000          0.417          0.325          0.421
C1-C5                   0.000                                        0.062
C1-C5,N2                               0.761          0.373          0.483
H2                                                                  66.460
CO                                    65.235                        31.056
CO2                                                  24.451          2.000

CASE: Shell Gasifier, Point of Ayr, Methanol Synthesis, No Recycle
```

```
INPUT SPECIFICATIONS
--------------------
ALCOHOL PLANT
-------------
WT.FRACTION  C1           C2           C3           C4           H2S
-----------  -----------  -----------  -----------  -----------  -----------
ALCOHOLS           1.000        0.000        0.000        0.000        0.000
HC,S GAS           0.000        0.000        0.000        0.000        0.000

MOLAR H2:CO RATIO               2.100  CO SELECT.ALCOHOLS              0.992
MOL FR.CO SHIFTED               0.000  MF CO CONVERTED                 0.951
MOLAR RECYCLE RATIO            15.557
PRESS.,BARA-FEED               85.000  -HP SEPARATOR                  80.000
SVP H20 @ 38 C                  0.066

REFORMER & PSA
--------------
MF C1 IN PRODUCT                0.040  MF HC TO CO                     0.600
STEAM/HC MOL RATIO              3.000  MF PSA H2 RECOVERY              0.900
MF PSA H2 PURITY                0.995

SHIFT
-----
MF FEED CONV.                   0.970  MOLS H20/MOL DRY GAS            0.750
SYNGAS FEED PRESS, BARA        30.000  PRESSURE DROP, BAR              1.000
TEMP C,D/S COOLER             170.000  SVP H20 @ TAMP, BARA            7.920

H2S/CO2 REMOVAL
---------------
MF CO2 IN PRODUCT (MAIN)        0.020  PRESS. DROP H2S, BAR            0.500
```

6.4 Shell Middle Distillate Synthesis (SMDS)

6.4.1 Introduction

The Shell Middle Distillate Synthesis (SMDS) step mass balance was modeled based on data provided by John Brown Engineers and Constructors Ltd. The step performs a mass balance from the compressed raw feed synthesis gas to a product fuel alcohol containing C_1 to C_6 alcohols and it includes the CO shift and acid gas removal steps within the mass balance. A sample mass balance is given in section 4.4.3.6 showing the main stream compositions, from the feed of raw pressurized synthesis gas, to distiled fuel alcohol. This includes CO shift, desulphurisation and CO_2 removal. The variables used in the equations and the equations used are given in Appendix C. The derivation of the equations are given in Appendix C. This step model calculates the overall molar and mass balance for the conversion of all the design feedstocks to a mixture of kerosine, naptha and diesel. It includes the following process steps:

- CO Shift (where required);
- H_2S removal;
- CO_2 removal;

- Middle Distillate synthesis, which also includes a shift steam reformer and a PSA unit to recover hydrogen for reuse in the synthesis;
- Steam reformer or PSA Unit in the recycle stream, where required.

It excludes the following step which is not part of the iterative solution.

- Raw syngas compression.

A block flow diagram is shown in Figure 6.22. The following option is specified for handling the recycle stream from the SMDS unit:

- Recycle with reformer, ie a reformer is included in the recycle stream to convert methane and other hydrocarbons to H_2, CO and CO_2;
- Recycle with PSA (pressure swing absorption) unit, ie a PSA unit is included to recover hydrogen from the recycle stream.

The key variable in running the different cases are as follows:

- Varying the recycle ratio, which changes the level of inerts in the system, the amount of hydrocarbons in the reformer feed and the mols of product produced.

6.4.2 Basis Of Mass Balances

The following sub-sections form the basis of the mass balances as used in the SMDS step model. The variables and array names as used in the program are shown in brackets for each parameter and these correspond to the names used in the equation descriptions and derivations given in the Appendix C

The basis of the units which perform the CO shift, CO_2 and H_2S removal, tail gas treating, steam reforming and pressure swing absorption (for H_2 purification) are described in sections 4.4.6 to 4.4.8.

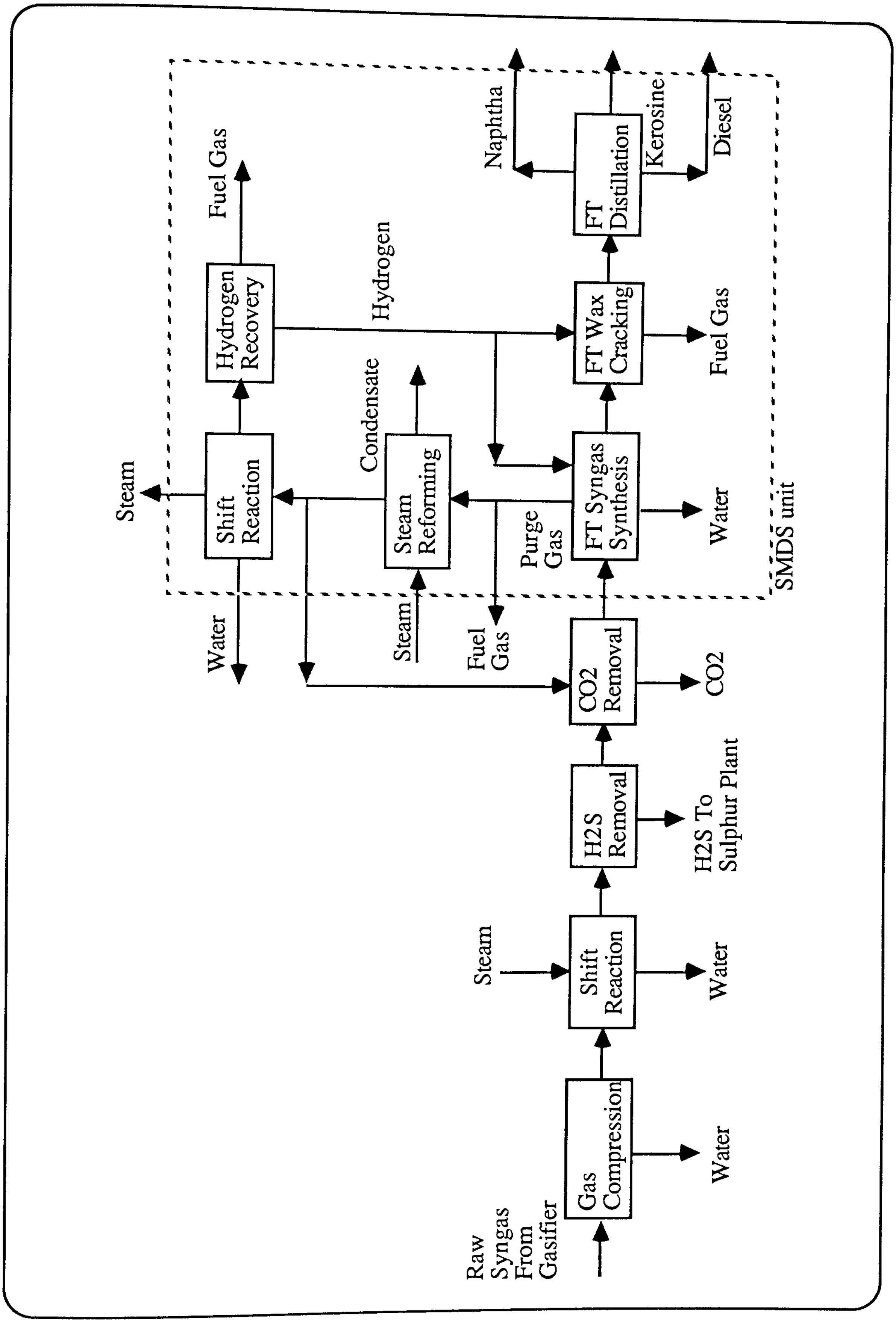

Figure 6.22 SMDS Plant Block Flow Diagram

6.4.3 SMDS Unit

a) The data given below is based on Shell published literature. The results of the model have been confirmed with Shell as giving a reasonable estimate of the process yields and product cost.

b) The SMDS is contains a heavy paraffin synthesis section, a hydrocracking unit, a steam reformer to reform hydrocarbon off gases, a CO shift unit and a PSA unit to recover hydrogen for use in the hydrocracking unit.

c) The following chemical reactions are used in the mass balances:

i) Hydrocarbon Liquids Production

$$nCO + 2nH_2 \dashrightarrow (-CH_2-)_n + nH_2O$$

ii) Hydrocarbon Gases Production

$$\begin{aligned} CO + 3H_2 &\dashrightarrow CH_4 + H_2O \\ 2CO + 5H_2 &\dashrightarrow C_2H_6 + 2H_2O \\ 3CO + 7H_2 &\dashrightarrow C_3H_8 + 3H_2O \\ 4CO + 9H_2 &\dashrightarrow C_4H_{10} + 4H_2O \\ 5CO + 11H_2 &\dashrightarrow C_5H_{12} + 5H_2O \end{aligned}$$

iii) Shift

$$CO + H_2O \dashrightarrow CO_2 + H_2$$

e) Input Variables

i) Product Compositions.

The shell SMDS process can be operated in different modes with different distributions of products being produced, the step 421 has two modes of operation and these two modes are assumed to only affect the distribution of products and not the overall conversion of gas to liquids or other operating parameters. The yields of products for the two modes are as follows in wt. fractions.

	Gas Oil Mode	Kerosine Mode
Fuel Gas	5.4	5.5
Naptha	5.9	5.2
Kerosine	9.6	18.3

ii) The feed H_2 : CO molar ratio [RH], is specified as 1.7 for all cases.

iv) The mol fraction CO conversion to products (gas and liquid) [CNV], is specified as 0.98 for all cases.

v) The mol fraction selectivity to liquids [SAC], is specified as 0.75 for all cases. Thus 75 mol % of CO that is converted (to liquids and gases) produces liquids, and 25 mol % produces hydrocarbon gases.

vi) The mol fraction CO_2 in offgas / recycle gas, dry basis [AA], is specified as 0.02 for all cases

vii) The operating pressures are as follows, the data is used in all cases and is only used for the calculation of the water balance.

	Pressure Bar (abs)	Variable
Downstream feed compressor	40	PM1
SVP H_2O at 38 °C	0.06624	VP1

6.4.4 Recycle Stream.

a) The type of recycle system is selected as follows:

As the SMDS unit produces hydrocarbon gases as a by-product the offgas from the unit contains large concentrations of hydrocarbon gases regardless of the methane content of the feed. The offgas stream is therefore steam reformed in all cases. Part of the steam reformed offgas stream is CO shifted and sent to a PSA unit to recover hydrogen for use as a feed to the hydrocracking unit in the SMDS plant. The remaining offgas stream is recycled to the CO_2 removal plant for re-feeding to the SMDS plant.

For this step the only recycle options are therefore either recycling of the excess steam reformed offgas or no recycle.

The normal configuration of units is that shown in Figure 6.23. With the large variation in gas compositions from the gasifiers included in the model, the calculation sequence was altered to be that shown in Figure 6.24. This was to allow the program to increment the cost of the unit more precisely with respect to alternative feed gas compositions as the capital cost estimate for the unit contains the cost of of the required units to provide enough steam reformed gas for the hydrogen recycle only.

To allow for recycling of part of the purge gas in the capital cost estimate, two steam reforming units are used in the model to simplify calculation of the capital cost. In a real plant only one unit would be used. The estimated total cost is then:

Cost Estimate = cost estimate (hydrogen production only) - cost of steam reforming (hydrogen production) + cost of steam reforming (hydrogen and recycle)

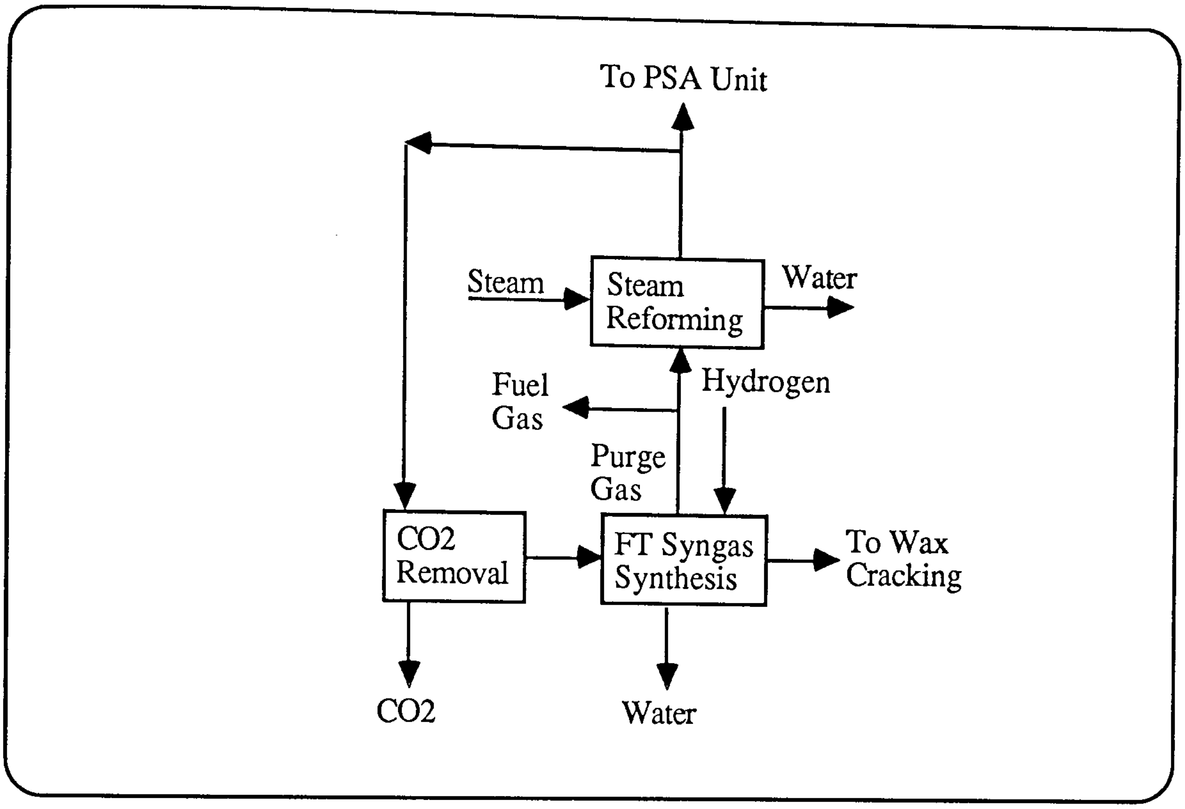

Figure 6.23 Normal Unit Configuration

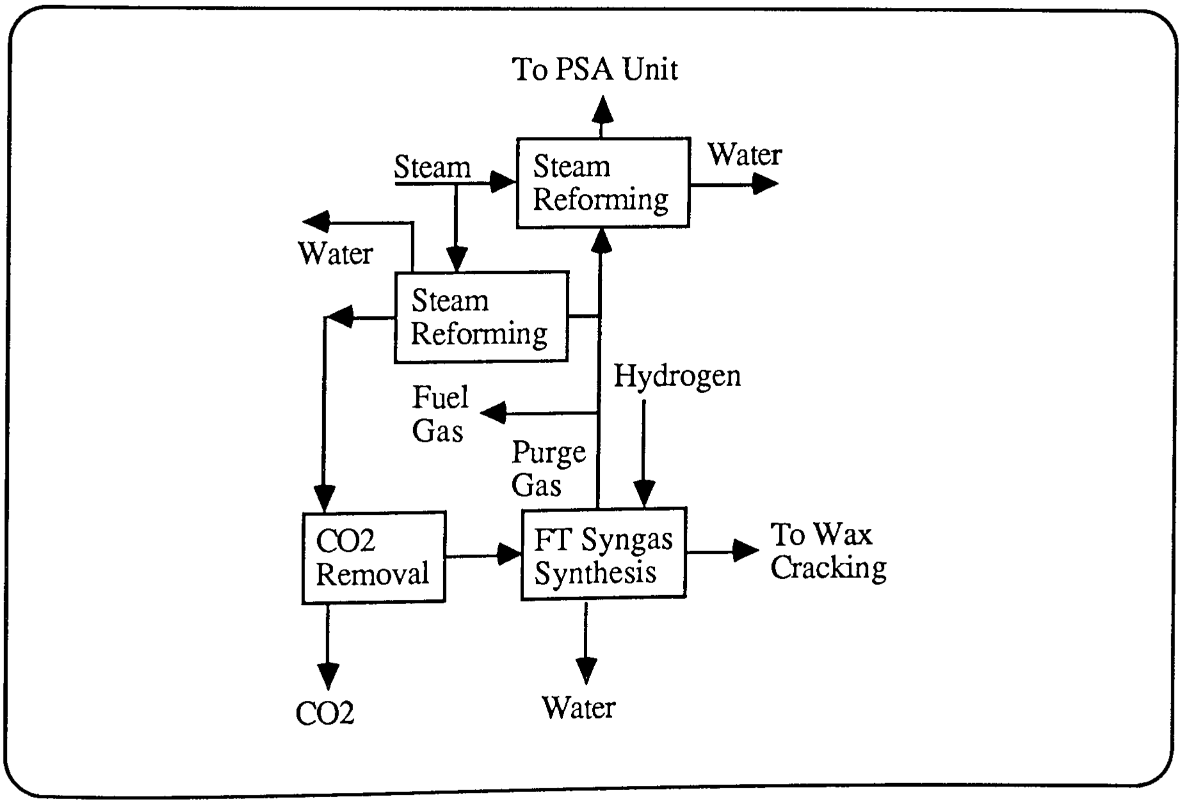

Figure 6.24 Unit Configuration As Used In the Program

b) The recycle ratio [RR], is the molar ratio of the recycle reformer etc, to the purge gas. It is specified as 1 in the program but can be altered by the user to examine its effect on the results.

6.4.5 Simplified Calculation Sequence

A summary of the variables used and the associated equations is given in Appendix C and the derivation of the equations is given in Appendix C. Figures 4.42 to 4.49 show simplified calculation sequence of the mass balance for the SMDS step, including gas shifting, acid gas removal and the associated recycle loops.

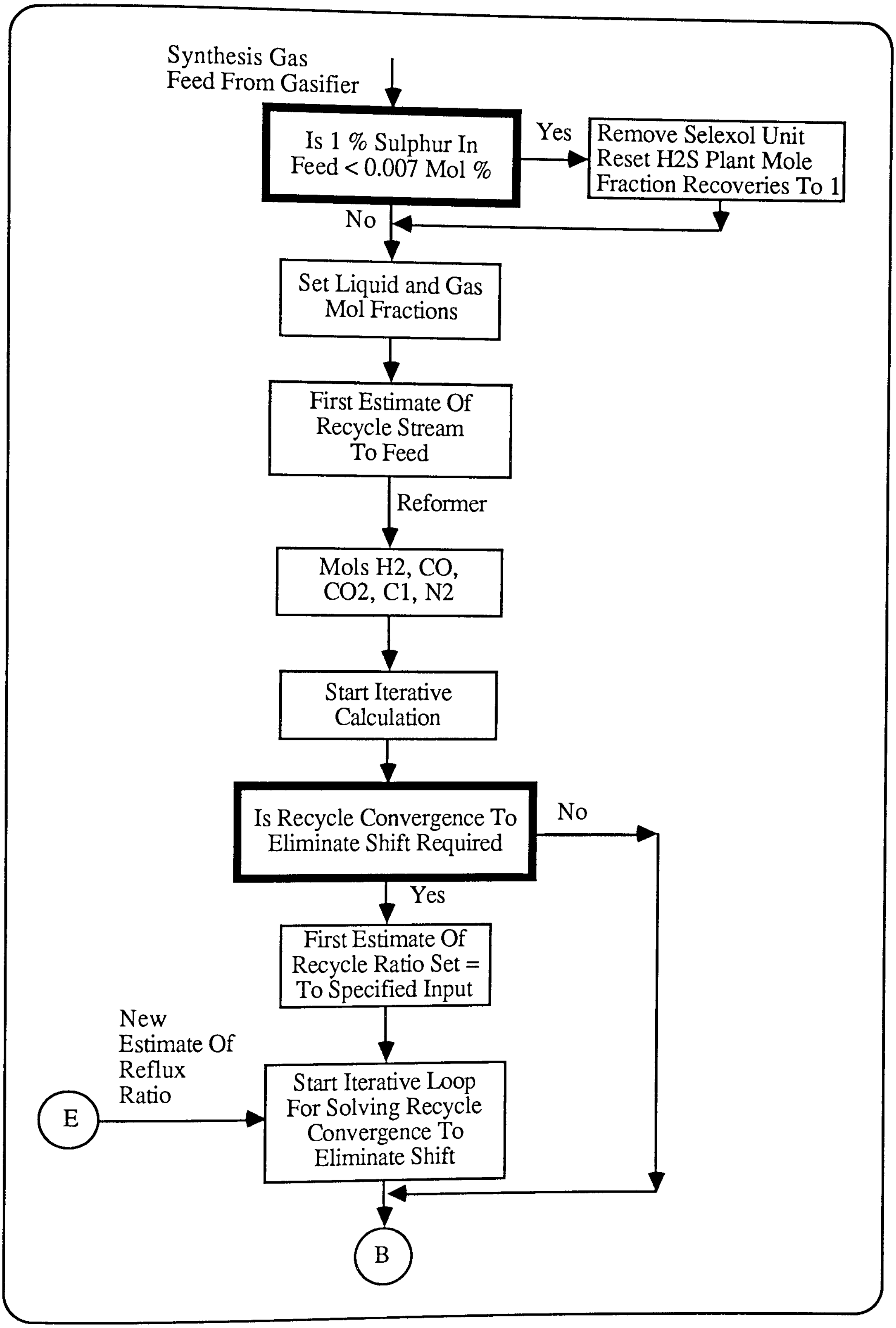

Figure 6.25 SMDS Program Calculation Sequence, Part A

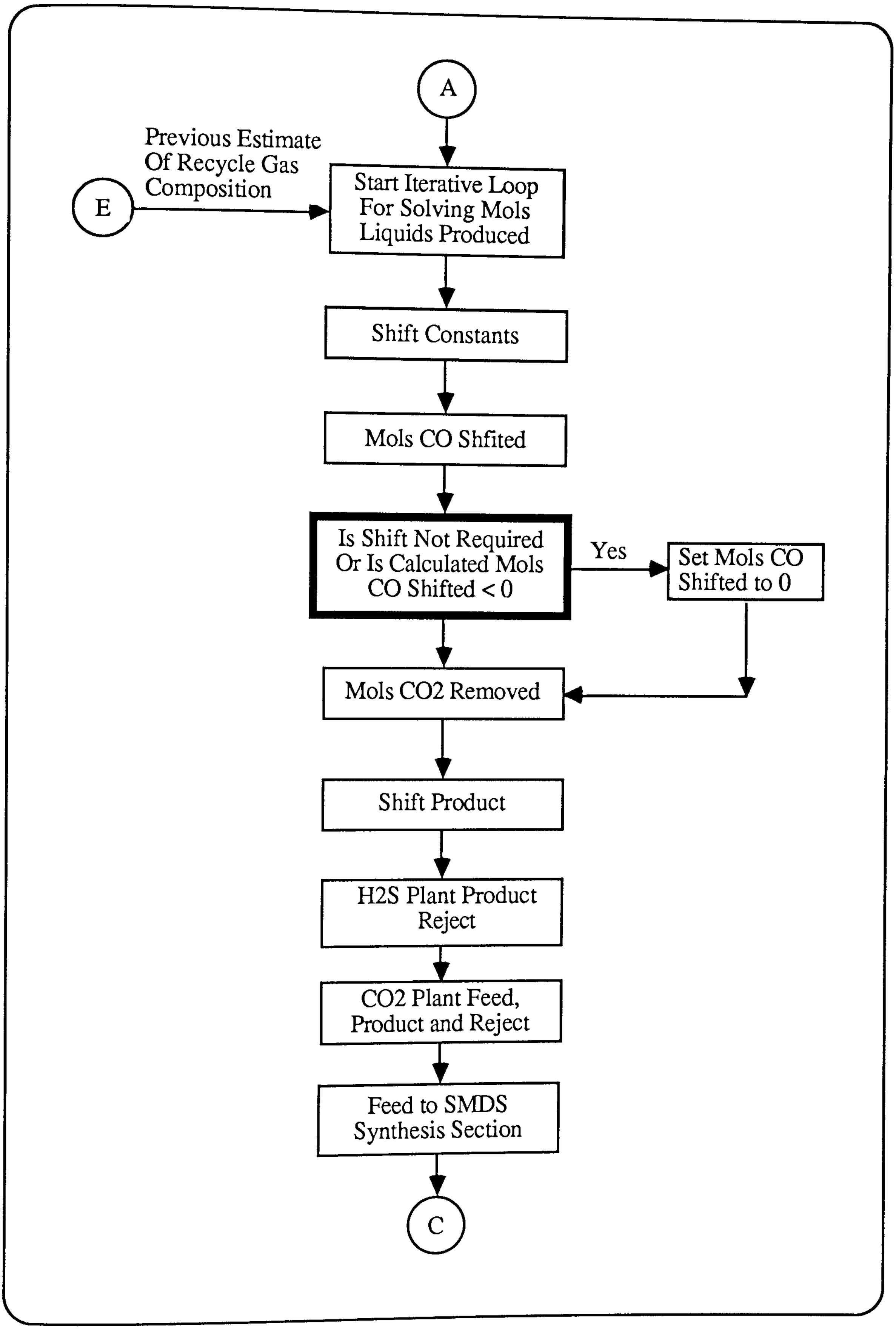

Figure 6.26 SMDS Program Calculation Sequence, Part B

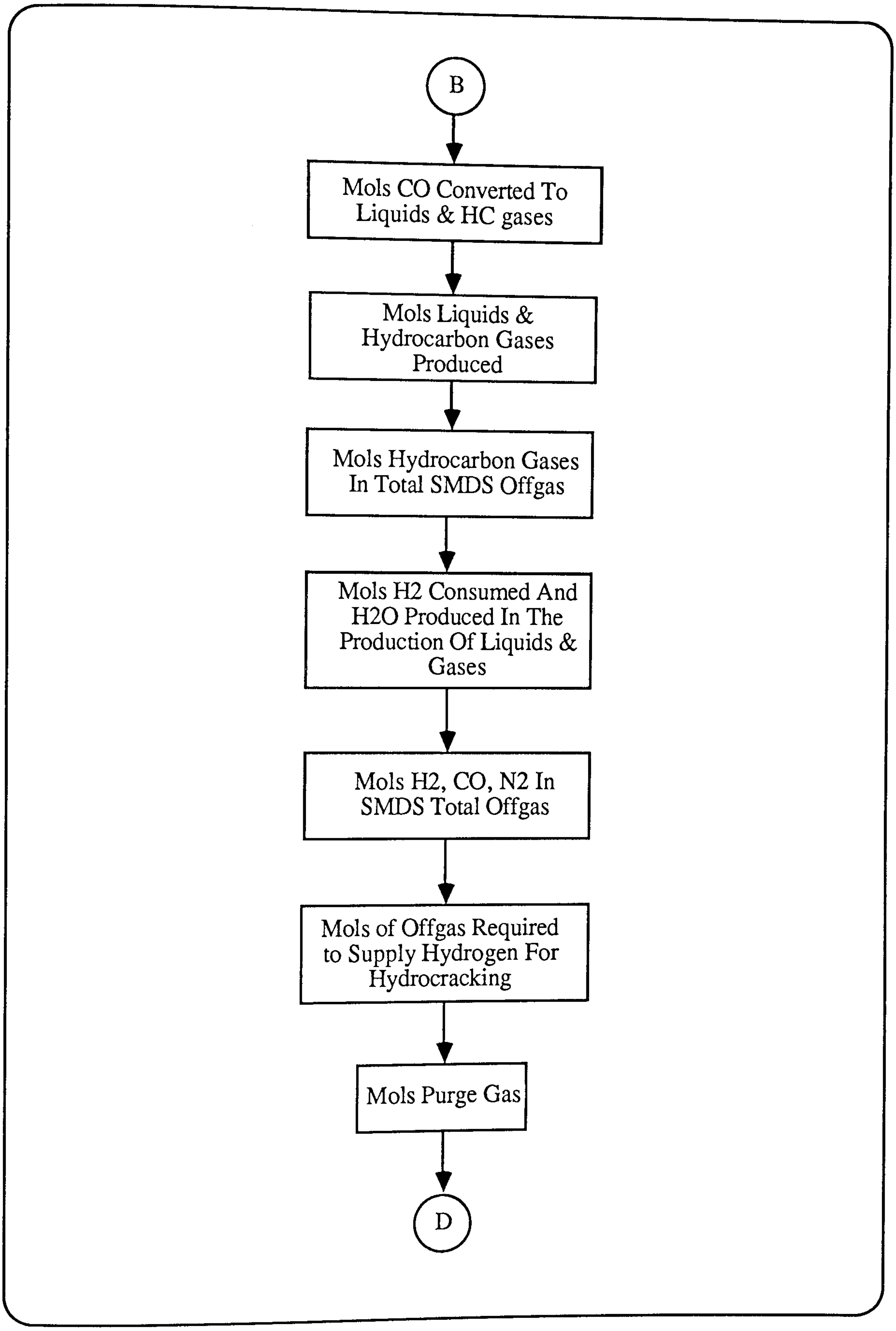

Figure 6.27 SMDS Program Calculation Sequence, Part C

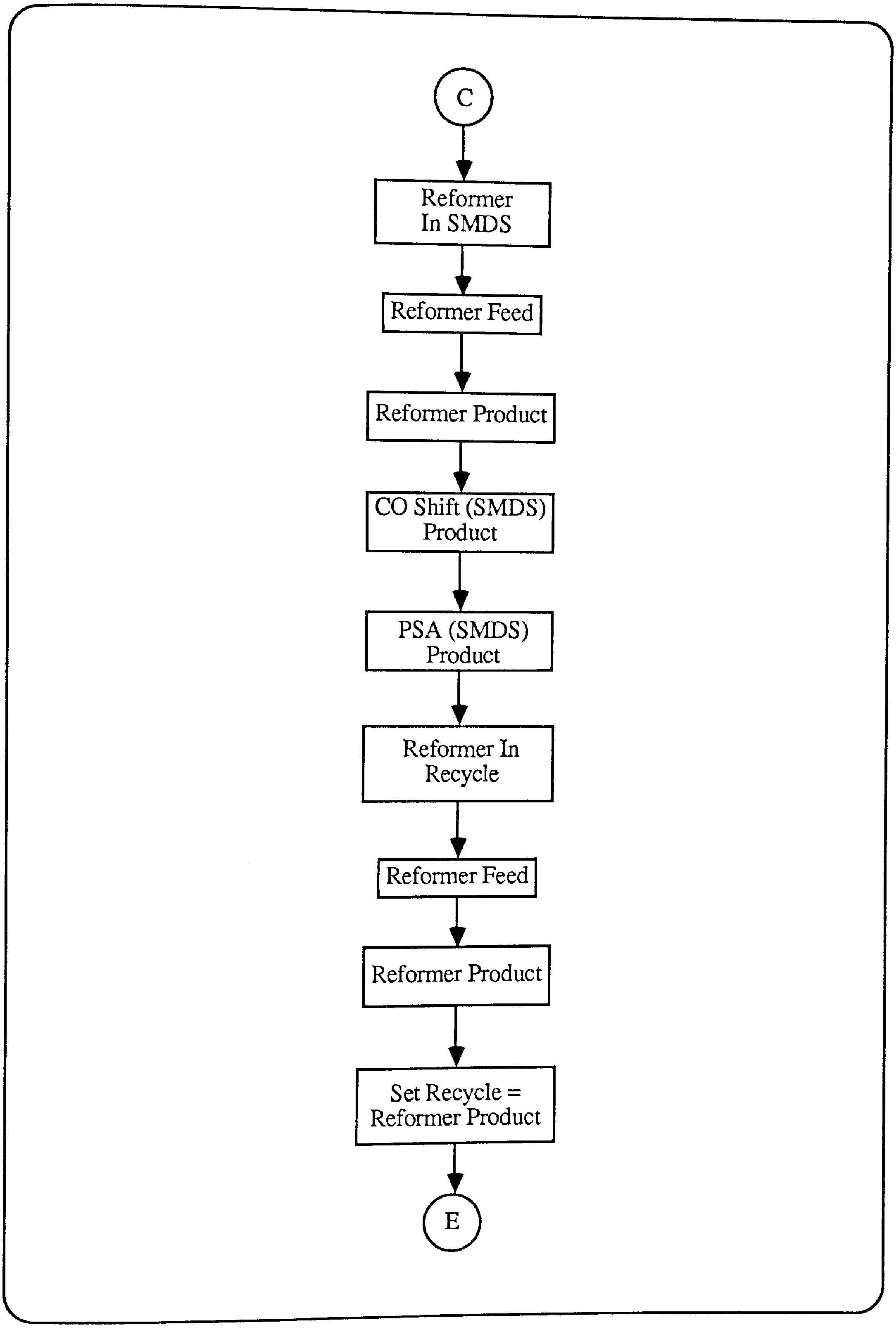

Figure 6.28 SMDS Program Calculation Sequence, Part D

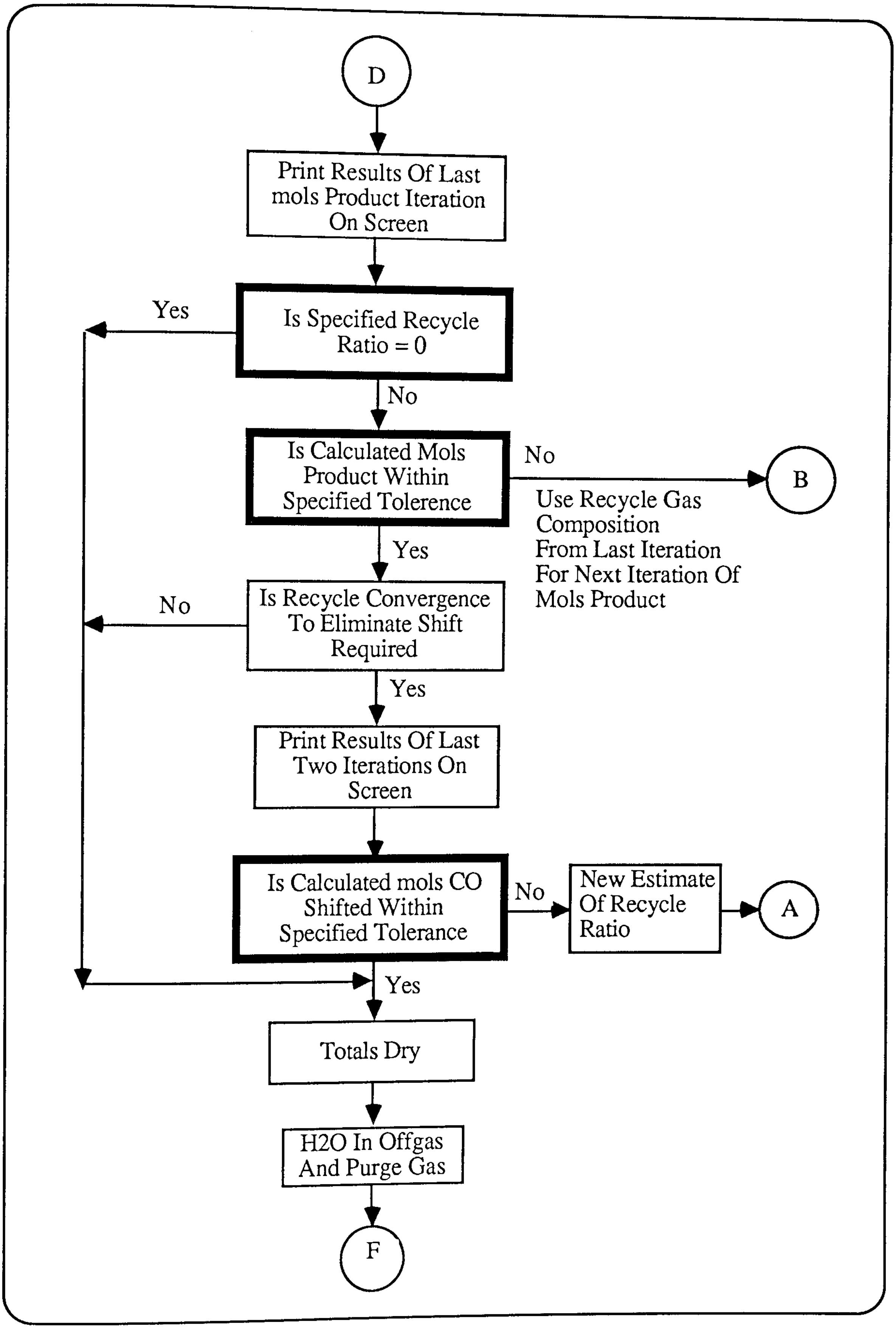

Figure 6.29 SMDS Program Calculation Sequence, Part E

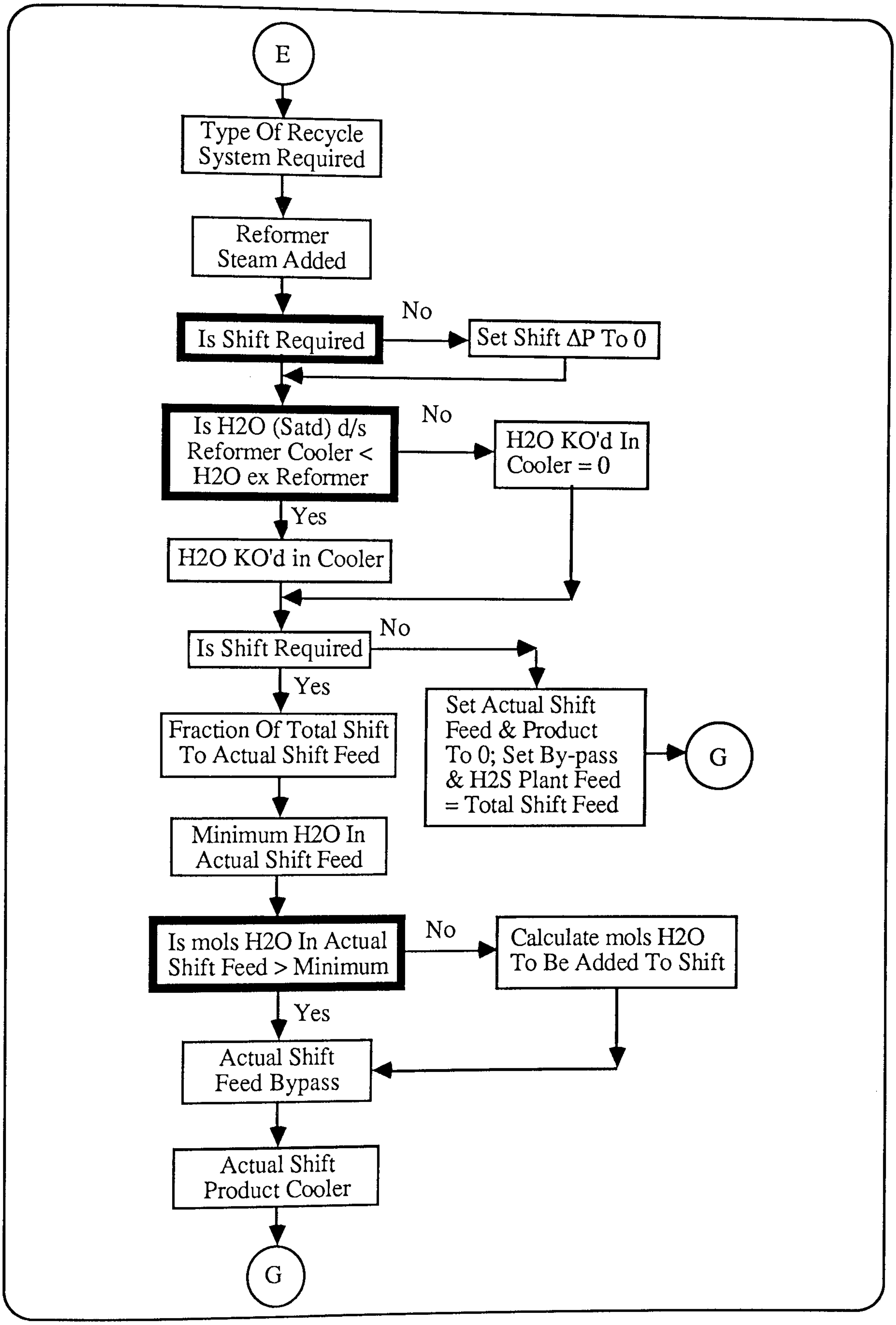

Figure 6.30 SMDS Program Calculation Sequence, Part F

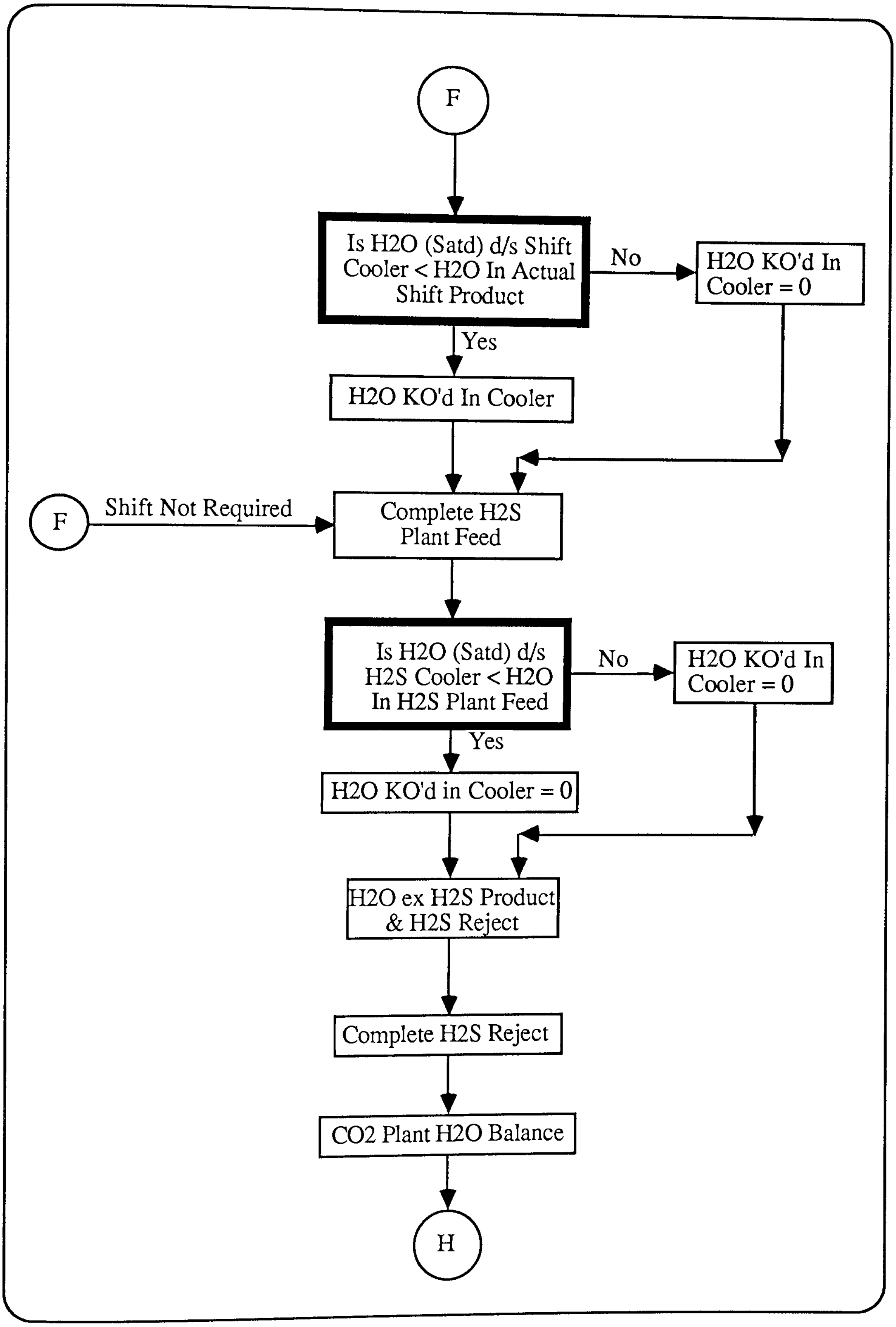

Figure 6.31 SMDS Program Calculation Sequence, Part G

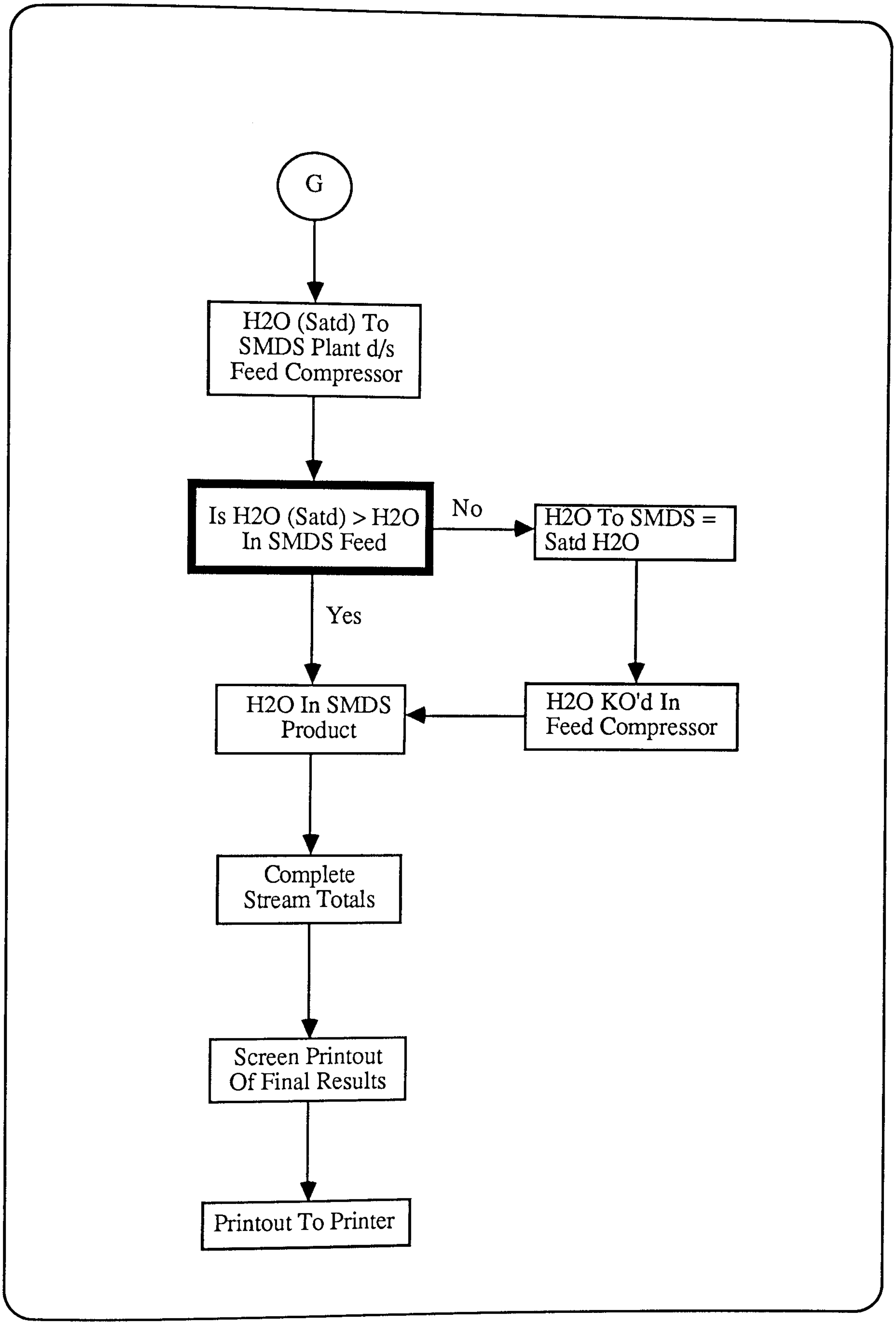

Figure 6.32 SMDS Program Calculation Sequence, Part H

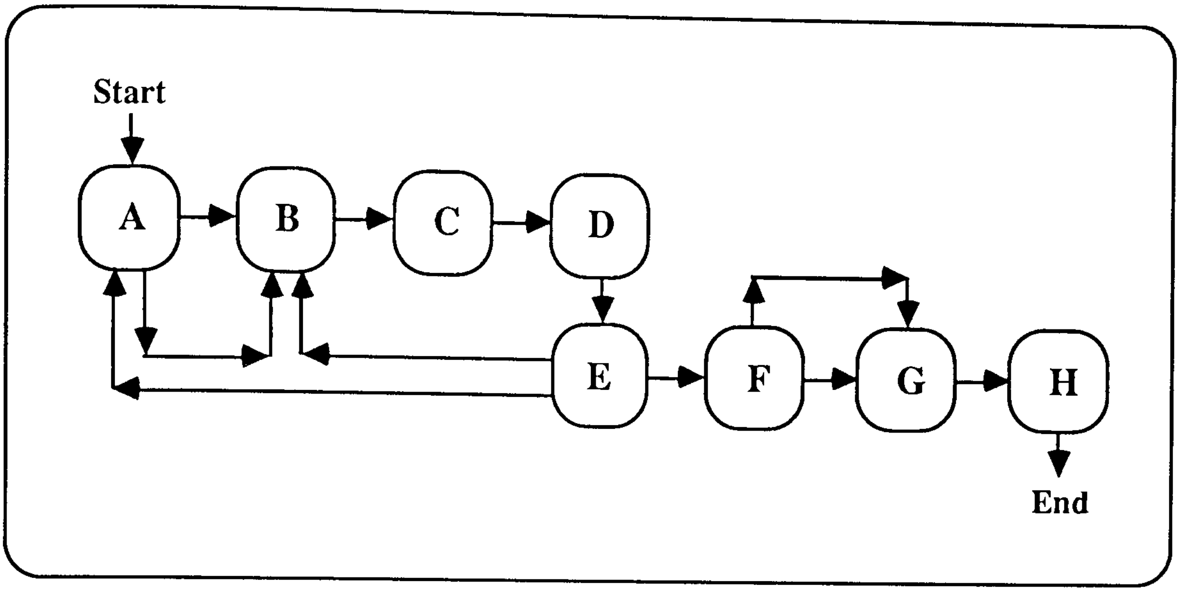

Figure 6.33 Overall SMDS Calculation Procedure

6.4.6 Mass Balance For SMDS Step (With Shell Gasifier)

The following is an example of the model output for the SMDS step including CO shift acid gas removal and alcohol synthesis.

```
MOL% C1 CONVERTED        -4.562
MOL% HC TO REF.          44.452
MOLS TO REFORMER         27.385
MOLS TO PSA               0.000
MOL% H2O EX SHIFT          7.179
CASE: Shell Gasifier
*************************************************
           SYNGAS         ACTUAL**      ACTUAL**      SHIFT
           FEED           SHIFT FEED    SHIFT PROD    BY-PASS
           -----------    -----------   -----------   -----------
H2            319.797       142.415       430.469       177.382
CO            666.837       296.963         8.909       369.874
CO2            25.698        11.444       299.498        14.254
C1              0.631         0.281         0.281         0.350
C2              0.000         0.000         0.000         0.000
N2              4.264         1.899         1.899         2.365
H2O            52.895       341.413        53.360        29.339
H2S             4.975         2.215         2.215         2.759
COS             0.000         0.000         0.000         0.000
SO2             0.000         0.000         0.000         0.000
CS2             0.000         0.000         0.000         0.000
MERCAPTAN       0.000         0.000         0.000         0.000
THIOPHENE       0.000         0.000         0.000         0.000
           -----------    -----------   -----------   -----------
TOTAL        1075.098       796.631       796.631       596.324
```

	H2S PLANT FEED	H2S PLANT REJECT	H2S PLANT PRODUCT	CO2 PLANT FEED
H2	607.851	0.790	607.061	670.133
CO	378.783	0.795	377.987	394.512
CO2	313.752	47.784	265.968	282.821
C1	0.631	0.003	0.628	4.847
C2	0.000	0.000	0.000	0.000
N2	4.264	0.008	4.257	9.056
H2O	82.699	2.066	0.934	1.179
C3	0.000	0.000	0.000	0.000
C4	0.000	0.000	0.000	0.000
C5	0.000	0.000	0.000	0.000
H2S	4.975	4.975	0.000	0.000
COS	0.000	0.000	0.000	0.000
SO2	0.000	0.000	0.000	0.000
CS2	0.000	0.000	0.000	0.000
MERCAPTAN	0.000	0.000	0.000	0.000
THIOPHENE	0.000	0.000	0.000	0.000
TOTAL	1392.955	56.422	1256.834	1362.549

	HPC OFFGAS	SMDS REF. FEED.	SMDS REF PROD	SMDS PSA PRODUCT
H2	0.000	0.000	126.194	113.575
CO	7.874	4.379	0.791	0.000
CO2	21.976	12.231	52.458	0.000
C1	15.586	6.437	6.730	0.000
C2	9.570	5.323	0.000	0.000
N2	9.040	7.657	7.657	0.571
H2O	0.115	0.064	96.837	0.000
C3	7.831	4.356	0.000	0.000
C4	5.941	3.305	0.000	0.000
C5	0.000	0.000	0.000	0.000
TOTAL	77.861	43.753	290.668	114.146

CASE: Shell Gasifier

	PURGE GAS	REFORMER FEED	REFORMER PRODUCT
H2	0.000	0.000	63.072
CO	0.174	2.745	16.525
CO2	0.487	7.667	16.853
C1	0.256	4.035	4.219
C2	0.212	3.337	0.000
N2	0.305	4.800	4.800
H2O	0.003	36.519	0.246
C3	0.174	2.730	0.000
C4	0.132	2.071	0.000
C5	0.000	0.000	0.000
TOTAL	1.743	63.904	105.715

```
               PSA          PSA          PSA          RECYCLE
               FEED         PRODUCT      TO FUEL      TO FEED
               -----------  -----------  -----------  -----------
H2                   0.000        0.000        0.000       63.072
CO                   0.000        0.000        0.000       16.525
CO2                  0.000        0.000        0.000       16.853
C1                   0.000        0.000        0.000        4.219
C2                   0.000        0.000        0.000        0.000
N2                   0.000        0.000        0.000        4.800
H2O                  0.000        0.000        0.000        0.246
C3                   0.000        0.000        0.000        0.000
C4                   0.000        0.000        0.000        0.000
C5                   0.000        0.000        0.000        0.000
               -----------  -----------  -----------  -----------
TOTAL                0.000        0.000        0.000      105.715

LIQ.PROD       NAPHTHA      KEROSINE     DIESEL
--------       ----------   ----------   ----------
MOLS                11.651       10.847       16.920
TOTAL LIQ(D):=      39.418
** WATER MOLS AFTER STEAM ADDITION OR WATER REMOVAL
%ERROR ON CLOSURES-MOLS ALCOHOLS                 0.000
                 -RECYCLE RATIO                  0.000

                  REFORMER     SHIFT        H2S PLANT    ALCOHOL
                  -----------  -----------  -----------  -----------
H20 ADDED              36.479      317.857
H20 REMOVED             4.121        0.000       79.699        0.000
CO SHIFTED                         288.054                    25.572
CO2 REMOVED                                                    0.000

MOL% @ UNIT FEED,DRY                        CO2 PLANT
--------------------                        ----------
N2                     17.527        0.417        0.665        0.823
C1-C5                  44.452                                  0.439
C1-C5,N2                             0.698        1.021        1.262
H2                                                            60.909
CO                                  65.235                    35.829
CO2                                              20.775        2.000


CASE: Shell Gasifier

INPUT SPECIFICATIONS
--------------------

MOLAR H2:CO RATIO               1.700   CO SELECT.LIQUIDS               0.800
MOL FR.CO SHIFTED               0.000   MF CO CONVERTED                 0.980
MOLAR RECYCLE RATIO            15.732
PRESS.,BARA-FEED               50.000   -HP SEPARATOR                  45.000
SVP H20 @ 38 C                  0.066

REFORMER & PSA
--------------
MF C1 IN PRODUCT                0.040   MF HC TO CO                     0.600
STEAM/HC MOL RATIO              3.000   MF PSA H2 RECOVERY              0.900
MF PSA H2 PURITY                0.995

SHIFT
-----
MF FEED CONV.                   0.970   MOLS H20/MOL DRY GAS            0.750
SYNGAS FEED PRESS, BARA        30.000   PRESSURE DROP, BAR              1.000
TEMP C,D/S COOLER             170.000   SVP H20 @ TAMP, BARA            7.920

H2S/CO2 REMOVAL
---------------
MF CO2 IN PRODUCT (MAIN)        0.020   PRESS. DROP H2S, BAR            0.500
```

6.5 Mobil Methanol to Gasoline

The Mobil methanol to gasoline model was based on the information provided by John Brown Engineers and Constructors Ltd and which is given in Appendix A. The mass and utility balance is based on the amount of methanol entering the plant. A block flow diagram is shown in Figure 6.34.

6.6 Mobil Methanol to Olefins, Gasoline and Diesel

The Mobil methanol to Olefins, Gasoline and Diesel model was based on the information provided by John Brown Engineers and Constructors Ltd and which is given in Appendix A. The mass and utility balance is based, similarly to the MTG model, on the amount of methanol entering the plant. A block flow diagram is shown in Figure 6.35.

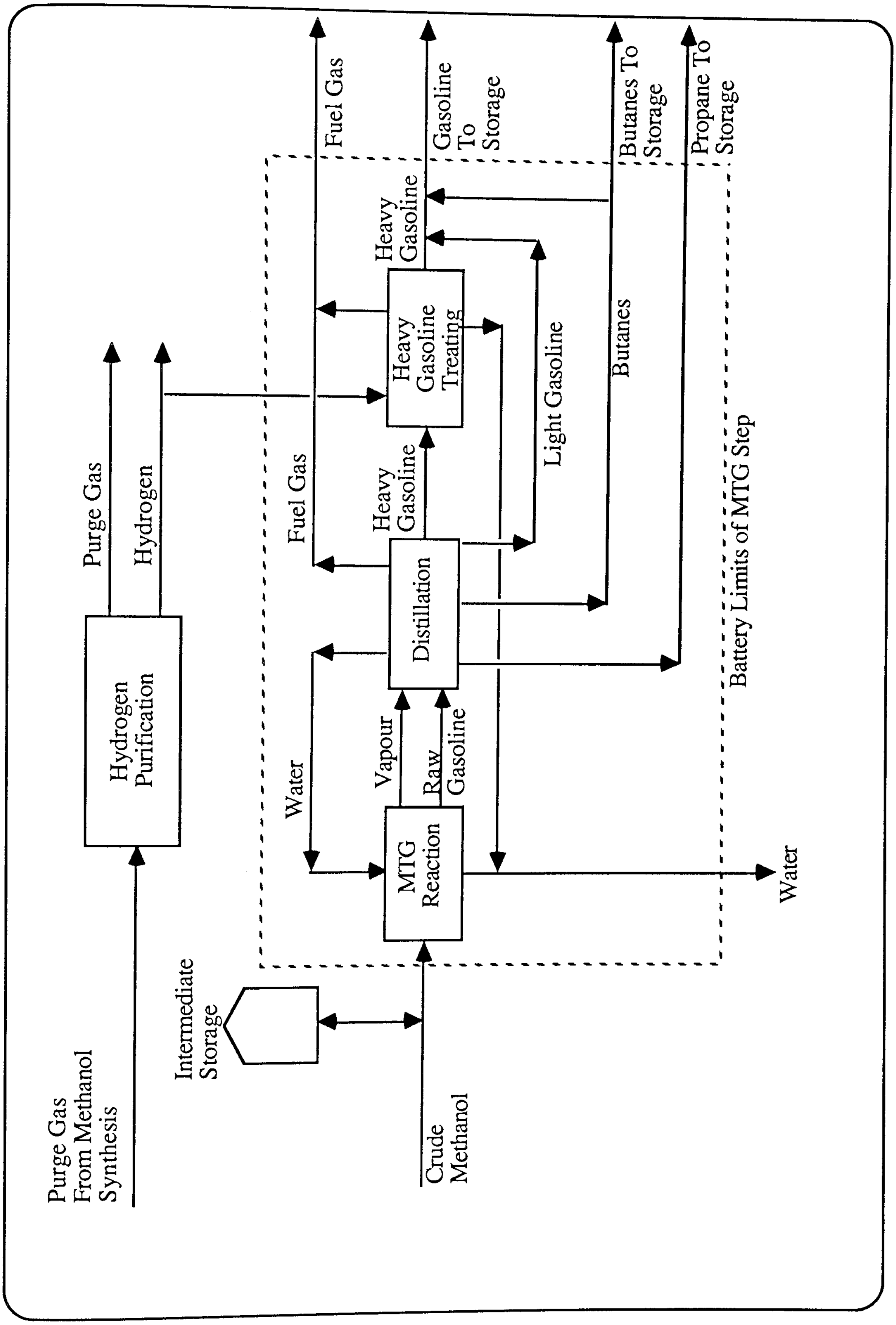

Figure 6.34 Methanol To Gasoline Block Flow Diagram

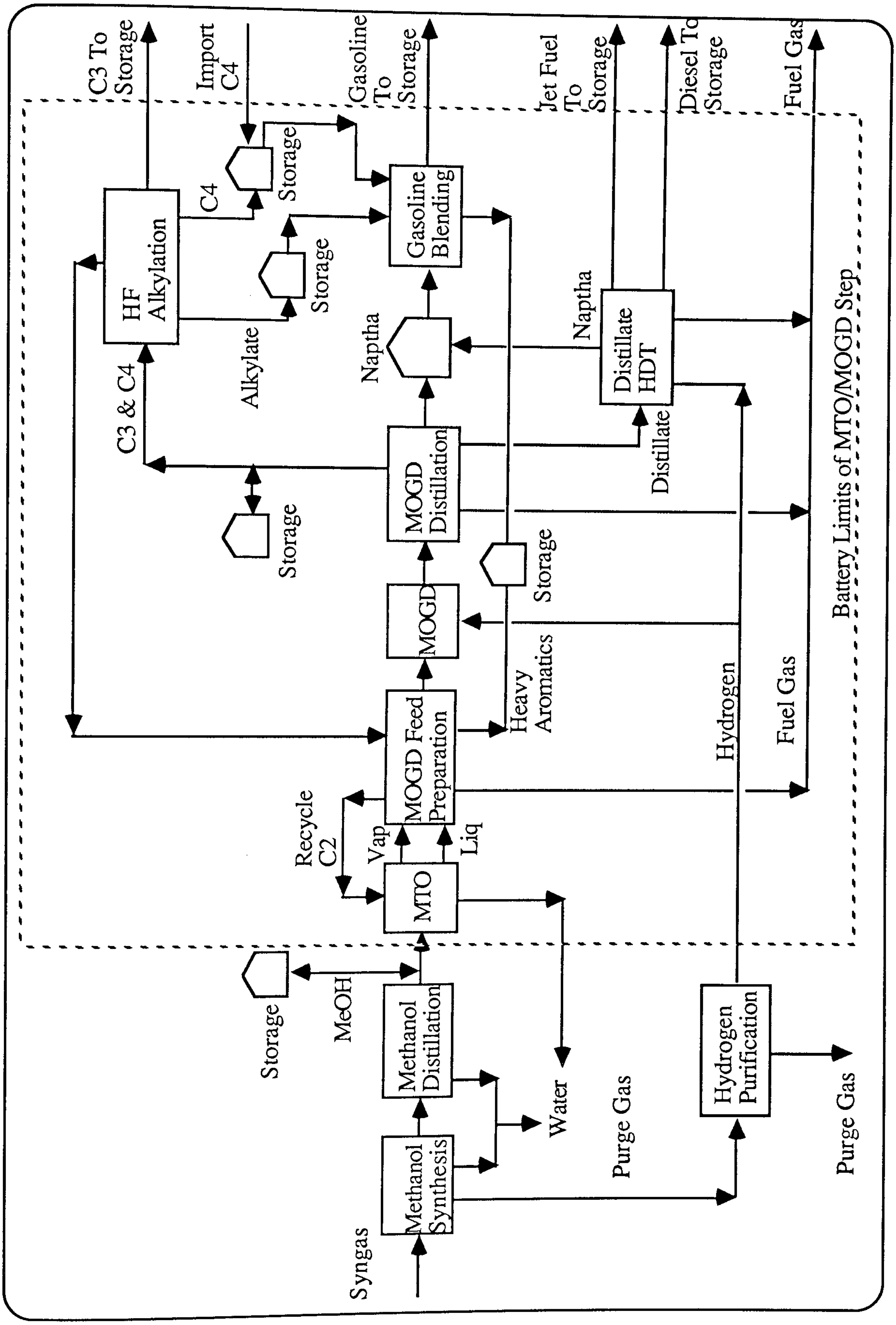

Figure 6.35 MOGD Block Flow Diagram

6.7 Acid Gas Removal and CO Shifting

The Acid Gas Removal Unit for removing H_2S and CO_2 from the raw syngas was specified as the Selexol process. The process operates on the principle of physical absorption using an organic solvent. This process was chosen because:

a The solvent used is H_2S and CO_2 selective;

b It has a lower heat and power requirement than processes using physical solvents, eg Rectisol, which requires refrigeration to operate at low temperatures;

c It operates at or near ambient temperature conditions;

d The solvent is chemically and thermally stable and comparatively non-corrosive.

Selective absorption of H_2S in the first column concentrates this component for subsequent sulphur recovery via the Claus process. A second column is used for bulk absorption of CO_2. The product gas contains less than 1 ppm of H_2S and as low as 10 ppm of CO_2. Figure 6.36 illustrates such a process designed to produce gas with less than 1 ppm of H_2S and 0.5 vol % of CO_2.

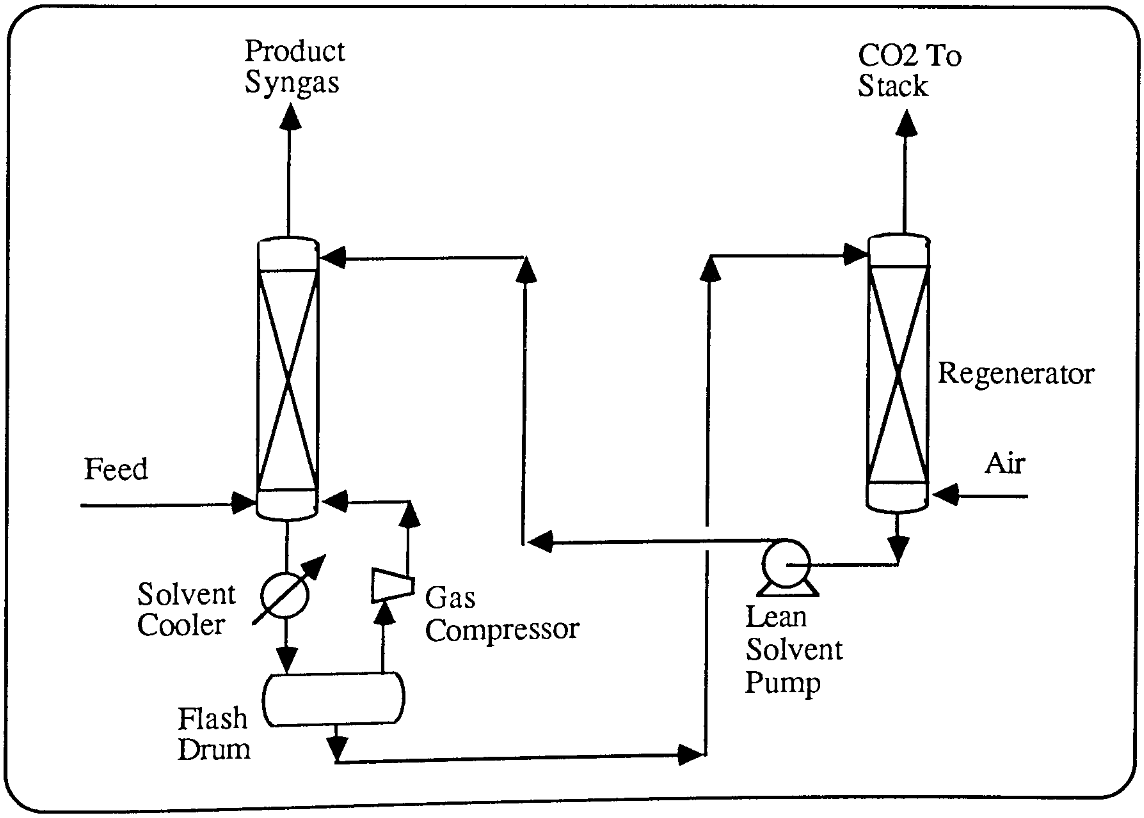

Figure 6.36 CO_2 Removal

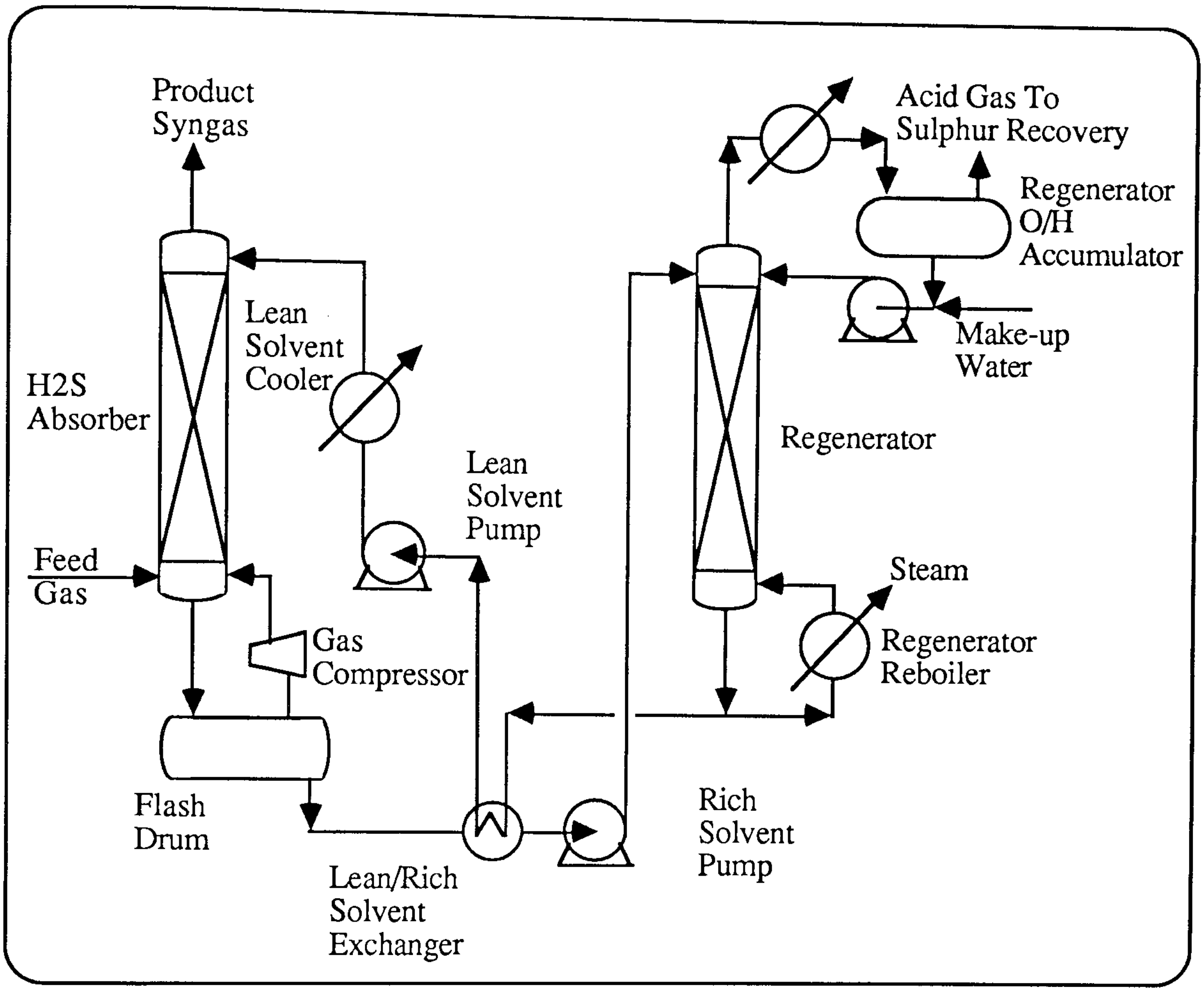

Figure 6.37 H_2S Removal

Steam is used to regenerate the solvent in the H_2S section and air in the CO_2 removal section. The stream conversion factors are given in Table 6.1. The stream conversion factors express the the fraction of a particular gas in the input stream which is found in the main product stream, the remainder being removed by the solvent and exiting in either the acid gas removal stream or the CO_2 removal stream as appropriate.

Table 6.1 Sulphur And CO_2 Removal Stream Conversion Factors

Component	Sulphur Removal, Product Stream Conversion Factor	CO_2 Removal, Product Stream Conversion Factor
H_2	0.9987	0.9987
CO	0.9979	0.9979
CO_2	0.3477	variable
CH_4	0.9952	0.9952
C_2's	0.9691	0.9691
N_2	0.9982	0.9982
H_2O	0.3113	0.3113
H_2S	0.00	-
COS	0.00	-
SO_2	0.00	-
CS_2	0.00	-
Mercaptan	0.00	-
Thiophene	0.00	-

6.7.1 H_2S Removal

A flow diagram for the H_2S removal stream is shown in Figure 6.37.

a) For the high sulphur cases (> 0.5 mol % H_2S), the facilities include:

- Conversion of sulphur complexes to H_2S eg COS*;
- Absorption of H_2S in a Selexol unit;
- Final clean-up with a zinc oxide bed.

* the material balance takes no account of the chemical reactions associated with COS conversion etc, as the impact is insignificant, the concentrations of COS found in the feed gas are insignificant, and usually of the order of 0.1%, about 1/10th of the concentration of H_2S. As the concentration of H_2S cannot easily be predicted by the gasifier models and the effect on the mass balance is negligible, all the sulphur present is assumed to be in the form H_2S.

b) For the low sulphur cases (<< 1 mol % H_2S) a zinc oxide bed only is required. For clarification only, high sulphur cases can be taken to mean all cases where the synthesis gas is derived from coal. Low sulphur cases are taken to refer to biomass derived synthesis gas. The program automatically checks the input stream for the level of H_2S and proceeds accordingly.

c) Input variables

i) The following mole recoveries, [LH[N]], of the light ends over the H_2S plant are used in all cases as shown in Table 6.2. Eg 99.87 mol % of H_2 in the feed appears in the product stream. These allow for the loss of these components in the Selexol absorption liquid. Note that where the Selexol unit is not required eg biomass cases, this model is not used.

Table 6.2 Mole Fraction Recoveries Over H_2S Plant

H_2	CO	CO_2	C_1	C_2	N_2	H_2O
0.9987	0.9979	1.0000	0.9952	0.9691	0.9982	0.3113

ii) Pressure drop across the H2S removal plant [DPH], is specified as 0.5 bar (abs) in all cases

iii) H_2S Plant Required [HQ], is specified by the program automatically depending on the level of H_2S in the feed gas, or by the program user at runtime, as follows:

- 1 if Selexol Unit is required;
- 0 if Selexol Unit is not required.

6.7.2 CO_2 Removal Plant

a) It is assumed that there is no removal of hydrocarbons above C_2 in the Selexol CO_2 removal section.

b) Input variables

i) Mol fraction CO_2 in outlet gas, dry basis [A]. This is specified as 0.02 ie 2 mol % for all cases except for the Lurgi / methanol synthesis combination. This is because the methanol synthesis model is sensitive to the level of CO_2 present in the feed gas. With the Lurgi gasifier there is a surplus of hydrogen available which can be used to convert CO_2 to methanol. Conversion of CO_2 to methanol in this way is normally wasteful of hydrogen due to the production of water and is only suitable if excess hydrogen is present. For this reason the CO_2 content for the Lurgi gas can be set to a higher value when producing methanol, a value of 0.0477 was used in the program. Varying this specification will change the amount of water in the final fuel alcohol and methanol products. The Fuel alcohol and SMDS models are insensitive to the CO_2 level in the feed gas as the conversion of CO_2 to products is not included in the reactions used to specify the steps models. The value should therefore be set at 2 mole % which is the specified concentration for the processes.

ii) The mol fraction recoveries shown in Table 6.3 over the CO_2 plant are used in all cases eg 99.87 mol % of H_2 in the feed appears in the product stream. Note that the CO_2 value is specified as 1.0 solely for simplifying the calculation. The CO_2 removed is calculated from the specification in (i) above.

Table 6.3 Mol Fraction Recoveries Over CO_2 Plant

H_2	CO	CO_2	C_1	C_2	N_2	H_2O
0.9987	0.9979	1.0000	0.9952	0.9691	0.9982	0.3113

iii) Pressure drop across the CO_2 plant [DPC], is specified as 0.5 bar in all cases.

6.7.3 CO Shift Section

The shift unit consists simply of a shift reactor and a by-pass, the amount of shifting performed is controlled with the amount of synthesis gas which is passed through the reactor and which reaches equilibrium. The remainder of the gas by-passes the reactor and the total shift product composition is the sum of the two gas streams. Figure 6.38 shows this arrangement.

a) The mass balance for the shift section is assumed to be due entirely to the water gas shift reaction, with no other significant reactions occurring.

$$CO_2 + H_2O \dashrightarrow CO + H_2$$

b) Zero conversion of COS and other trace sulphur compounds in the shift section to H_2S is assumed.

c) The step includes a shift cooler to cool the shift product and to utilize the energy for steam generation.

d) Input variables:

i) The mol fraction of CO in the shift feed converted to CO_2, dry basis [K1], is specified as 0.97 in all cases, i.e. 97 % mol of CO in actual feed to shift is converted to CO_2.

ii) The minimum mol fraction H_2O / mol dry gas in shift feed [K2], is specified as 0.5 in all cases except the following:

- Shell	0.75
- Prenflo	0.7
- BG / L	0.6

0.5 is the necessary minimum to ensure enough water is present for the water gas shift reaction to convert 0.97 mole % of the CO to CO_2. However this must be increased in the above cases to ensure that the water in the shift product is not negative.

iii) If the shift section is required this is specified in the program as [SQ=]:

- 0 if shift not required;
- 1 if shift required.

The shift section may not be required if the feed gas is already of the correct H_2 / CO ratio.

iv) The feed to the shift unit is either:

- Raw syngas from gasifier, where no feed compression is required;
- Raw syngas from the feed compression step.

v) The feed pressure [PH] (in bar (abs)) is either the pressure from the gasifier if greater then 28 bar (abs), or, 28 bar (abs) if the feed syngas compression step is required. It is considered that a reasonable minimum pressure through the shift, H_2S and CO_2 steps is 28 bar (abs).

vi) The pressure drop through the shift step is specified as 1.0 bar for all cases. For the cases where the shift step is not required, the program will automatically reset this specification to 0.

vii) The temperature of the shift cooler [TS], is specified as 170 °C in all cases.

viii) Saturated vapour pressure [VP2] of H_2O in the discharge stream of the shift cooler, is specified as 7.92 bar (abs) in all cases, and corresponds to the saturated vapour pressure of water at 170°C.

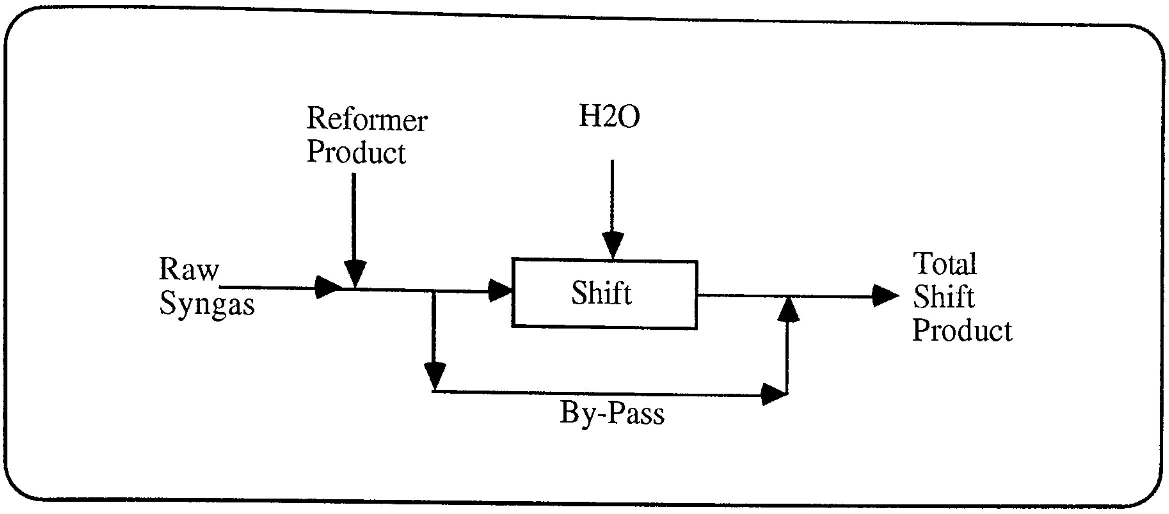

Figure 6.38 CO Shift Unit With By-pass

6.7.4 Scot Sulphur Plant Material Balance

A Scot Plant is included to process the H_2S plant reject stream. The plant converts 99.8 % of the sulphur contained in the feed gases to by-product sulphur. The model is based on the data provided by John Brown Engineers and Constructors Ltd and given in Appendix A.

6.8 Pressure Swing Absorption Unit

The pressure swing absorption unit is used to produce a pure hydrogen product from a gas stream containing CO, CO_2, H_2, N_2, H_2O and traces of other gases such as hydrocarbons. The hydrogen may be used for feed to synthesis processes such as SMDS or MOGD or as a recycle stream. A PSA (Pressure Swing Absorption) Unit is used to recover hydrogen from the fuel alcohol and methanol unit purge gas stream. The hydrogen is recycled back to the feed stream for the alcohol unit. A flow diagram is shown in Figure 6.39.

a) The program for this unit assumes that the only contaminant present in the PSA product is nitrogen. For all cases with no nitrogen in the feed the contaminant is assumed to be methane.

b) Input Variables:

i) Mol fraction hydrogen in PSA product [H3].
This is specified as 0.995 in all cases;

ii) Mol fraction hydrogen recovery over PSA unit [H4].
This is specified as 0.9 in all cases ie 90 % of hydrogen in the PSA feed is recovered in the product.

H_2 Purification Unit Material Balance

Basis :
Mol fraction hydrogen recovery = 0.90
Required hydrogen purity, mol fraction = 0.995

The impurity in the hydrogen product stream is taken to be:

- Nitrogen for all cases with nitrogen in the feed;
- Where there is no nitrogen in the feed, the impurity is taken as methane.

Only a part of the purge gas needs to be fed to the PSA Unit, the balance being routed to fuel gas. The equations used in the mass balance program are described in Appendix A.

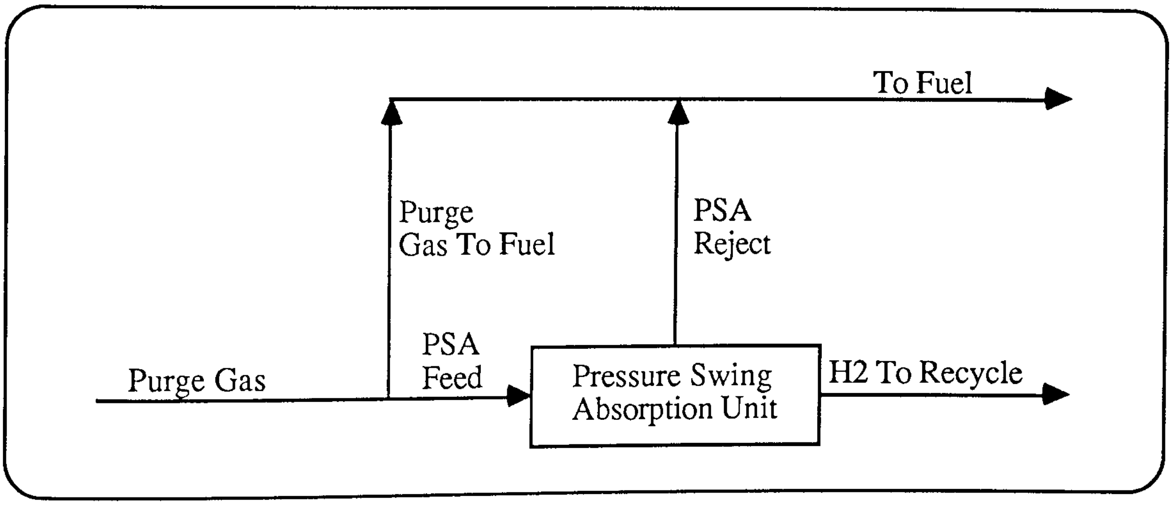

Figure 6.39 Pressure Swing Absorption Unit

6.9 Reformer

The reformer is used to convert methane and higher hydrocarbons in the recycle stream from the synthesis gas conversion processes to a synthesis gas which may be recycled to the main synthesis gas feed.

a) The following equations are used in the mass balance.

$$\begin{aligned}
CH_4 + H_2O &\dashrightarrow CO + 3H_2 \\
C_2H_6 + 2H_2O &\dashrightarrow 2CO + 5H_2 \\
C_3H_8 + 3H_2O &\dashrightarrow 3CO + 7H_2 \\
C_4H_{10} + 4H_2O &\dashrightarrow 4CO + 9H_2 \\
C_5H_{12} + 5H_2O &\dashrightarrow 5CO + 11H_2 \\
C_6H_{14} + 6H_2O &\dashrightarrow 6CO + 13H_2 \\
CO + H_2O &\dashrightarrow CO_2 + H_2
\end{aligned}$$

b) Input Variables

- i) The mol fractions of hydrocarbons [Z] converted to CO are specified as 0.6 in all cases ie 60 mol % of the hydrocarbons are converted to CO, and 40 mol % to CO_2.
- ii) The mol fraction of C_1 in the reformer product [D], dry basis is specified as 0.04 in all cases, ie methane concentration (or methane slip) in the reformer product is 4 mol %.
- iii) The steam / hydrocarbon molar ratio [SH] is specified as 3 in all cases, ie 3 mols steam are required per mol of hydrocarbons in the reformer feed.

CHAPTER 7
RESULTS

7.1 Introduction

Results are presented in this chapter for the main cases for each combination of feed, product, gasifier and gas conversion process. A base case of technical and financial variables is defined in Section 7.2. In addition to these cases a far greater number of variations and sensitivity studies can be performed which are too numerous to include. The Shell gasifier was chosen as the base case as it is capable of accepting virtually any type of coal or lignite feed with good efficiency with all feeds. It also has the advantage of having relatively clean gas with no tars or oils, methane or higher hydrocarbons. It is therefore convenient to use for comparison against gasifiers of limited feeds or more difficult gas cleaning/processing problems.

For similar reasons the Methanol process was chosen as the base case conversion process as the process is simple in that only one product is produced and the data for the methanol model may be assumed to be the most reliable due to the commercial experience with the process of the suppliers of the process and cost information.

Point of Ayr coal is used in the base case as it represents a typical low value bituminous coal. This coal was recommended by British Coal as being a suitable coal to use. A throughput of 10 000 te per day of dry ash free coal was used as the base case throughput, as above about 5 000 te per day very limited economies of scale were apparent. This is because at these throughputs, multiple streams of gasifiers and synthesis processes are used and hence there is very little associated economy of scale. The throughput of 10 000 te per day represents a throughput which was approximately mid range for the range of throughputs included in the model and was sufficiently high that only a small drop in production cost was observed for increasing throughputs.

The financial data values were chosen to be the same as those used by British Coal. The price of Point of Ayr coal was taken as that of sized coal as available for bulk purchase from British Coal.

7.2 Multiple Product Processes

As several synthesis gas conversion processes produce multiple products, either as by-products or more significantly as major products of the process, it is necessary to describe the basis by which multiple product processes are handled by the program in terms of the calculation of the product costs of production of the products.

For processes where there is one major product and one or more by-products of relatively low impact on the process economics (these are taken as those with a value of less than 1 % of the total process product value) then the by-products may be assigned a value equal to the current market rate.

For processes where the by-products are financially significant, or where there are several major products of similar impact on the process economics, then the calculation of the products costs of production must be performed in a different way. For these cases the products were assigned a relative value compared to gasoline, based on typical market rates for the products and their individual values calculated from the cost of production of the entire output of the process.

The ratios used for the products were calculated by John Brown Engineers and Constructors Ltd[123] for mid June 1989 and were as given in Table 7.1:

Table 7.1 Relative Value of Products Compared to Gasoline

Product	Relative Value
Gasoline Unleaded	1.000
Gasoil	0.901
Naphtha	0.895
LPG	0.851
Kerosine	1.014
Low Sulphur Fuel Oil (<1 %)	0.539

The calculated value of the products will therefore depend on the value used for these ratios. The ratios were typical for North West Europe FOB ARA (Free On Board, Amsterdam-Rotterdam-Antwerp).

7.3 Base Case Results

The results presented are all based on the financial, economic and technical data shown in Table 7.2.

Table 7.2 Base Case Data

A) Financial and Economic

Project Life, years	20
Days per year of operation	340
Real Interest Rate, %	10.0
Inflation Rate, %	4.0
Feedstock Cost, £/tonne	54.3
Labour Unit Cost, £/year	15000
Maintenance, % Capital Cost/year	2.5
Overheads, % Capital Cost/year	5.0

Utilities	
5 bar steam £/t	5.0
50 bar steam £/t	10.0
Process water £/t	1.0
Cooling water £/t	0.040
Fuel gas £/GJ	3.0
Hydrogen £/t	1500
Oxygen £/t	40.0
Power £/MW	30.0

B) Technical

Feedstock:	Point of Ayr coal	Gasifier:	Shell
Feed throughput:	10 000 te/day DAF	Product :	Methanol

7.3.1 Output of Model for Base Case

The summary output of the program is given below for the base case. A detailed mass balance for the methanol synthesis section of the model is given in section 4.4.2.6.

Table 7.3 Base Case Model Output

```
*******************************************************************************

                        ASTON LIQUID FUELS PRODUCTION MODEL


*******************************************************************************

 Run : Shell,POA,1000

 Feedstock       : Point of Ayr
 Product         : Methanol

 Throughput      : 10000.00 tonnes daf feedstock / day


 THE STEPS ARE ARRANGED IN THE FOLLOWING ORDER

    101     Reception and Storage
    241     Pulverizing/Drying
    304     Shell Gasifier
    431     Methanol Synthesis
    432     Methanol Distillation
    500     Product Storage
```

```
          SUMMARY OF PROCESS STREAMS
          ==========================

 OUTLET STREAM from step 101 Reception and Storage
  Flow =13422.8184 tonnes / day
  Composition, mass fraction:
    Coal MAF       H2O   Ash etc
      0.7450    0.1500    0.1050
  Mass flows of each component:
    Coal MAF       H2O   Ash etc
     10000.0    2013.4    1409.4


 OUTLET STREAM from step 241 Pulverizing/Drying
  Flow =11642.2402 tonnes / day
  Composition, mass fraction:
    Coal MAF       H2O   Ash etc
      0.8589    0.0200    0.1211
  Mass flows of each component:
    Coal MAF       H2O   Ash etc
     10000.0     232.8    1409.4


 OUTLET STREAM from step 304 Shell
  Flow = 1075.0978 Mmol / day
  Composition, mole fraction:
          H2        CO       CO2       CH4  C2+ H/c  N2/Ar    H2S/COS       H2O
      0.2975    0.6203    0.0239    0.0006   0.0000   0.0040    0.0046    0.0492
  Mole flows of each component:
          H2        CO       CO2       CH4  C2+ H/c  N2/Ar    H2S/COS       H2O
       319.8     666.8      25.7       0.6      0.0      4.3       5.0      52.9


 OUTLET STREAM from step 431 Methanol Synthesis
  Flow =  297.5589 Mmol / day
  Composition, mole fraction:
 Methanol       H2        CO       CO2       CH4     N2/Ar       H2O   CH3OCH3   C2+ Alcs
  0.9924    0.0003    0.0002    0.0044    0.0003    0.0000    0.0000    0.0012    0.0013
  Mole flows of each component:
 Methanol       H2        CO       CO2       CH4     N2/Ar       H2O   CH3OCH3   C2+ Alcs
   295.3       0.1       0.0       1.3       0.1       0.0       0.0       0.4       0.4


 OUTLET STREAM from step 432 Methanol Distillation
  Flow = 9449.0723 tonnes / day
  Composition, mass fraction:
    Methanol       H2O  CH3OCH3  C2+ Alcs
      1.0000    0.0000   0.0000    0.0000
  Mass flows of each component:
    Methanol       H2O  CH3OCH3  C2+ Alcs
      9449.1       0.0      0.0       0.0


 OUTLET STREAM from step 500 Product Storage
  Flow = 9449.0723 tonnes / day
  Composition, mass fraction:
    Methanol       H2O  CH3OCH3  C2+ Alcs
      1.0000    0.0000   0.0000    0.0000
  Mass flows of each component:
    Methanol       H2O  CH3OCH3  C2+ Alcs
      9449.1       0.0      0.0       0.0


          SUMMARY OF AUXILIARY INLET STREAMS
          ==================================


  NO AUXILIARY INLET STREAMS
```

```
         SUMMARY OF BYPRODUCT STREAMS
         ==========================

  3 : 304 Shell                         Flow = 1459.605 tonnes / day of Ash
Value = £      0.00 / tonne

  4 : 431 Methanol Synthesis            Flow =  159.197 tonnes / day of Sulphur
Value = £     75.00 / tonne


         SUMMARY OF UTILITIES USAGE
         ========================


                             Low Pr High Pr Process Cooling   Waste  Fuel   Oxygen Power
Step                         Steam  Steam   Water   Water     Water  Gas
                             t/day  t/day   t/day   t/day     t/day  GJ/day t/day   MW

101 Reception and Storage    0.00   0.00    0.00    0.00      0.00   0.00   0.00    0.78

241 Pulverizing/Drying    1990.37   0.00    0.00    0.00      0.00   0.00   0.00    9.77

304 Shell                    0.00 -2016.3 408.79    0.00      0.00   0.00 10026.5   7.14

431 Methanol Synthesis  -3818.91  561.31    0.00 195299.53    0.00 -14898.6 0.00    1.39

432 Methanol Distillation 4624.0  0.00      0.00 21090.33     0.00   0.00   0.00    1.64

500 Product Storage          0.00   0.00    0.00    0.00      0.00   0.00   0.00    0.00

                          =====   =====    =====   ======  ======  ====== ====== ======

 TOTALS                   2795.5 -1455.0  408.79  216390    0.00  -14899  10027   20.7

 COAL TONNES EQUIVALENT  285.62 -138.68     --      --        -- -701.40     -- 159.74

 UTILITY UNIT COST         5.00   10.00    1.00    0.04    1.00    3.00  40.00  30.00

 UTILITY COST / DAY    13977.27  -14550  408.79 8655.59    0.00  -44696 401060 622.06

 TOTAL                   365477.00
                        ===========


          CAPITAL COST SUMMARY
         ==================


  Step                           Installed

                                   k£         %

  1 : 101   Reception and Storage   5416.8    1.1

  2 : 241   Pulverizing/Drying     44506.2    8.7

  3 : 304   Shell                 210036.4   41.1

  4 : 431   Methanol Synthesis    131208.6   25.7

  5 : 432   Methanol Distillation 102815.5   20.1

  6 : 500   Product Storage        17461.9    3.4

                                  ========

 TOTAL                            511445.3
```

```
          FINANCIAL SUMMARY
          =================

     Input data for calculation was as follows:
     ------------------------------------------

     Financial Case                Runname
     Project Life, years             20
     Days per year of operation     340.0000
     Real Interest Rate, %           10.0000
     Inflation Rate, %                4.0000
     Feedstock Cost, £/tonne         54.3000
     Labour Unit Cost, £/year     15000.0000
     Maintenance, % CapCost/year      2.5000
     Overheads, % CapCost/year        5.0000
     Required real ROI, %             0.0000
     Utilities costs:
     5 Bar     50 Bar    Process   Cooling     Fuel    Hydrogen    Oxygen     Power     Feed
     Steam     Steam     Water     Water       Gas                                      Fines
     £/t       £/t       £/t       £/t         £/GJ      £/t        £/t       £/MWh     £/t
     5.000     10.000    1.000     0.040       3.000   1500.000    40.000     30.000    50.00

     Breakdown of Annual Costs
     -------------------------

                                              £              %

         Capital Amortisation            58782808.0        14.6

         ROI per year                           0.0         0.0

         Feedstock Cost                 184620000.0        45.8

         Utilities Cost                 124262184.0        30.8

         Maintenance Cost                12786133.0         3.2

         Overheads Cost                  25572266.0         6.3

         Labour Cost                       960000.0         0.2

         Additional Process Inputs              0.0         0.0

         Byproduct Credits                4059514.0        -1.0

         Other Costs                            0.0         0.0

                                         ==========

         TOTAL ANNUAL COSTS          £  402923872.0

                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

   RUN: Data:Shell Res Folder:Sh   FINANCIAL CASE : Runname

   FEEDSTOCK:
   Point of Ayr              10000.0 daf t/d,    13422.8 raw t/d

   PRODUCTS:                     Flow    % mass   % energy    % C.Conv.
                                  t/d     yield     yield        Effic.
   Methanol                     9449.1     94.5      63.1         42.4

   TOTAL ENERGY PRODUCTS        9449.1     94.5      63.1         42.4

   PRODUCTION COSTS
                                  £/t     ECU/t
   Methanol                      125.4    188.1

   PLANT CAPITAL COST            511.4 M pounds,     767.2 M ECU
```

```
BASED ON THIS DATA:

Project Life, years              20
Days per year of operation     340.0000
Real Interest Rate, %           10.0000
Inflation Rate, %                4.0000
Feedstock Cost, £/tonne         54.3000
Labour Unit Cost, £/year     15000.0000
Maintenance, % CapCost/year      2.5000
Overheads, % CapCost/year        5.0000

Utilities costs:
     LP        HP   Process  Cooling     Fuel Hydrogen    Oxygen     Power       Feed
  Steam     Steam     Water    Water      Gas                                   Fines
    £/t       £/t       £/t      £/t     £/GJ      £/t       £/t     £/MWh        £/t
  5.000    10.000     1.000    0.040    3.000  1500.00    40.000    30.000      50.00

 THE STEPS ARE ARRANGED IN THE FOLLOWING ORDER

    101    Reception and Storage
    241    Pulverizing/Drying
    304    Shell
    431    Methanol Synthesis
    432    Methanol Distillation
    500    Product Storage
```

7.4 Current Fuel prices and costs

Current fuel prices are shown in Table 7.3 for some traditional hydrocarbon fuels. However market prices and production costs are generally difficult to obtain with a high degree of certainty and can fluctuate over a wide range of ± 30% or more, varying with time and/or location. This effect is exacerbated by the recent situation (1990/1991) of uncertain oil supplies. These values can only, therefore, be taken as indicative. It is also important to note that considerable differences can arise between cost of production and market price. For methanol, for example, the market price is depressed at up to 50% below the production cost of a current state of the art plant due to excess capacity. Crude oil, conversely, carries a price that is considerably above the cost of production which also affects downstream fuel product prices, and these are also subject to market forces in their own right. Cost and price comparisons between fossil and synthetic fuels therefore need to be carefully evaluated.

Table 7.4
Wholesale Prices and Production Costs of Fuels, September 1990

Product	Gasoline	Diesel	Medium fuel oil	Heavy fuel oil	Methanol	Fuel alcohol
Wholesale price, tax free, £/te[124]	260	183	99	79	75	N/A
Production cost, tax free, £/te	-	-	-	-	141[125]*	182 **

* Estimated current cost of production from natural gas using state of the art technology
** Estimated equivalent cost of production

7.5 Effect of Feed Coal

The results shown in Figure 7.1 show the effect of increasing the feedstock cost on the product production cost and the relative cost of production for three different feed qualities, based on a throughput of 10 000 te/d, using a Shell gasifier. As expected, the highest quality feed gives the lowest cost product due to higher conversion efficiencies. The UK coal price is the typical price charged by British Coal for Point of Ayr coal and is typical of the price of a British coal feedstock. The world coal price is representative for which coal may be bought on the open international market. The German coal cost is the cost of production of a typical German coal rather than the price normally asked for purchase[126].

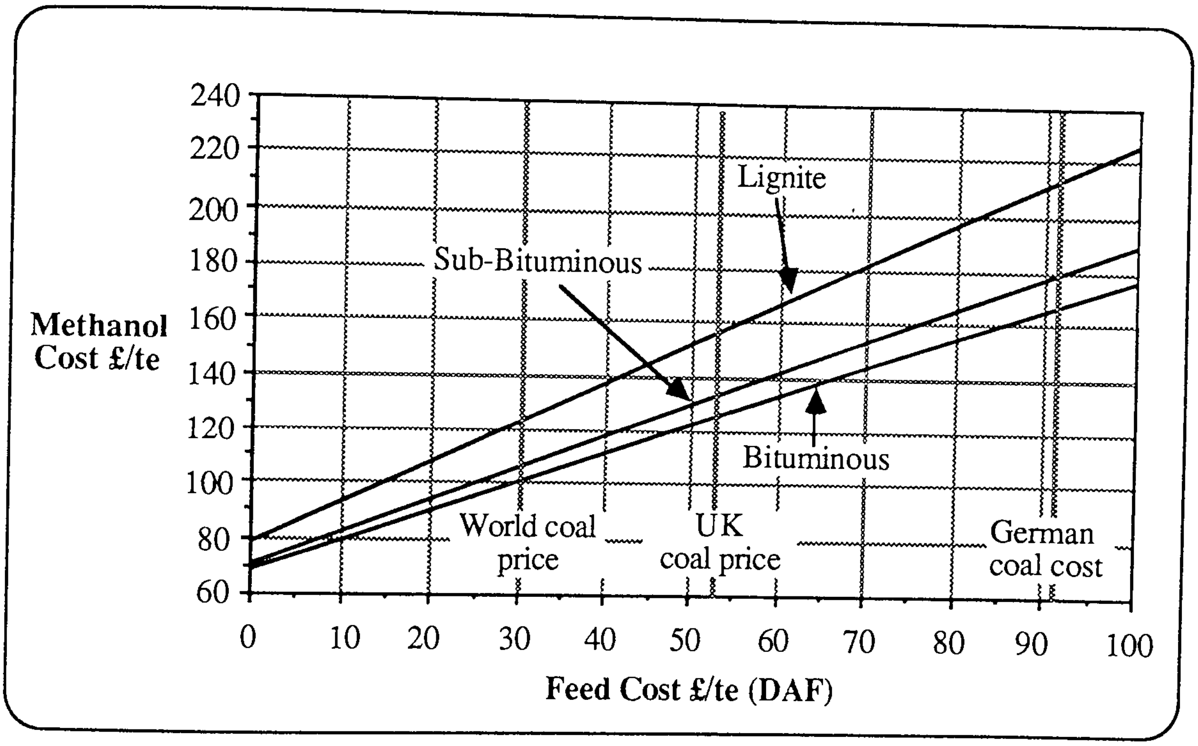

Figure 7.1 Methanol Cost for Different Feeds (Shell Gasifier at 10 000 te/d)

For the same base case, the data when plotted with cost / unit of energy as the independant variable, shows that the conversion of feed energy to product energy is more efficient for higher rank feeds, this is shown in Figure 7.2. This is due to the higher ash and water content in lower rank coals which lowers the amount of useful energy contained in the feed. For the bituminous and sub-bituminous feeds included in this thesis the energy efficiency is very similar, however, for the lignite included, the energy efficiency is significantly lower.

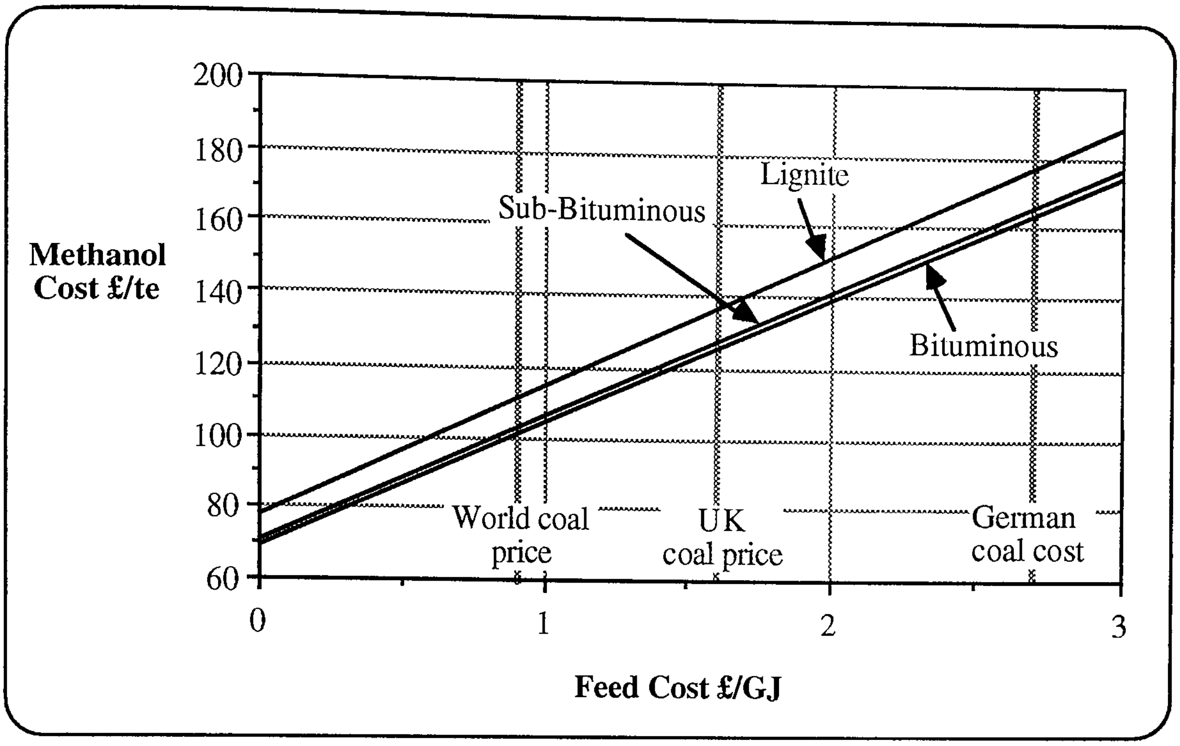

Figure 7.2 Methanol Cost for Different Feeds (Shell Gasifier at 10 000 te/d)

Although the energy content per tonne of different coal grades is different and therefore a useful criteria for comparing feedstocks might be £/GJ of energy, the presentation of results on this basis offers few advantages over using £/tonne as the basis for presentation. All coal costs of production, transport and preparation are more strongly dependant on the mass throughput than the energy throughput contained in the coal. Sale prices in contrast depend strongly on energy content (for feedstocks intended for power generation). For presentation of the results in this thesis, £/tonne have been used for the feedstock price. This is done to provide parity with the oil industry where oil production, refining and oil product marketing are frequently integrated within single organisations, to reduce the impact of market fluctuations on specific sections of the integrated corporate structure. Therefore £/tonne is more useful as production costs and not sale prices should be the basis of the feedstock cost.

7.6 Effect of Gasification Technology

Figure 7.2 shows a comparison of methanol production cost for several gasifiers using Point of Ayr coal feed. The lowest cost comes from using the British Gas / Lurgi gasifier. This can be attributed to the combination of low oxygen consumption of the gasifier and high cold gas thermal efficiency. The cold gas thermal efficiency of the gasifier gives an indication of the cehmical energy of the gasifier which is potentially convertable to liquid fuels, a low efficiency indicates large quantities of steam are produced which is wastefull of the energy available for conversion.

The cost of fuel production from the Lurgi gasifier is high in comparison to the other gasifiers. This is due to the choice of feed coal and hence operating conditions producing a gas with a higher H_2 / CO ratio than that required for the methanol synthesis process, leading to excess CO_2 and hydrogen being removed from the system and therefore a reduced overall carbon conversion to methanol.

The KRW fluidised bed gasifier has the second lowest product production cost and this is also attributable to a low oxygen consumption and high cold gas efficiency. The entrained gasifiers have a higher production cost due to a high oxygen consumption and a lower cold gas efficiency, more of the energy being recovered as high, medium or low pressure steam and hence of lower usefulness and value than a liquid fuel.

The Texaco is higher than the Shell Gasifier production costs due to the slurry fed nature of the Texaco gasifier which reduces the cold gas thermal efficiency of the gasifier and requires the recovery of more of the energy as steam. Significantly more of the energy contained in the coal is required to evaporate the water in the feed slurry. The higher the quantity of water in the feed the more pronounced this effect becomes, as shown in Figure 6.11.

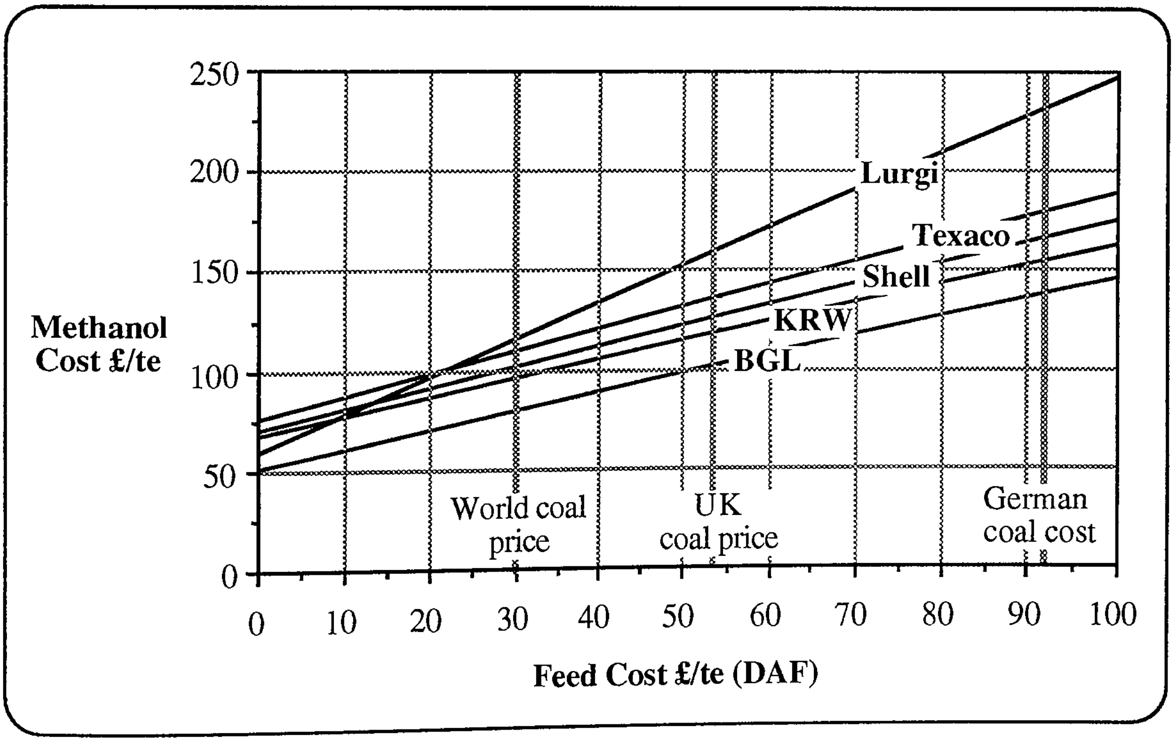

Figure 7.2 Methanol Cost for Different Gasifiers (Point of Ayr Feed, 10000 te/day)

7.7 Effect of Different Products

The results presented in Figures 7.3 and 7.4 show a comparison of product costs for several different products and processes using the Shell gasifier at 10 000 t / d. Figure 7.3 shows the costs per tonne and Figure 7.4 shows the costs per GJ to reflect the different heating values of the fuels. By either criterion, alcohol fuels are more attractive, although diesel fromm the SMDS process is competitive at low coal prices.

7.8 Comparison of Product Costs to Current Prices

Table 7.4 compares product costs to current prices showing that methanol is the most attractive product.

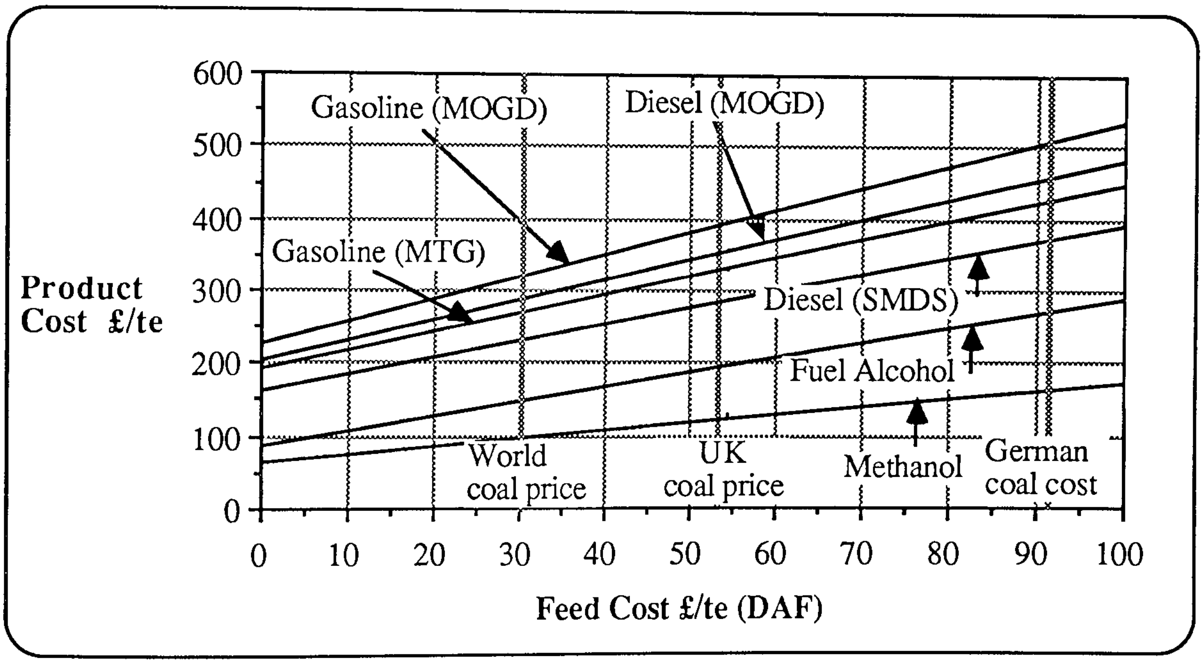

Figure 7.3 Product Costs for Different Conversion Processes, (Point of Ayr Coal, Shell Gasifier, 10 000 te/d)

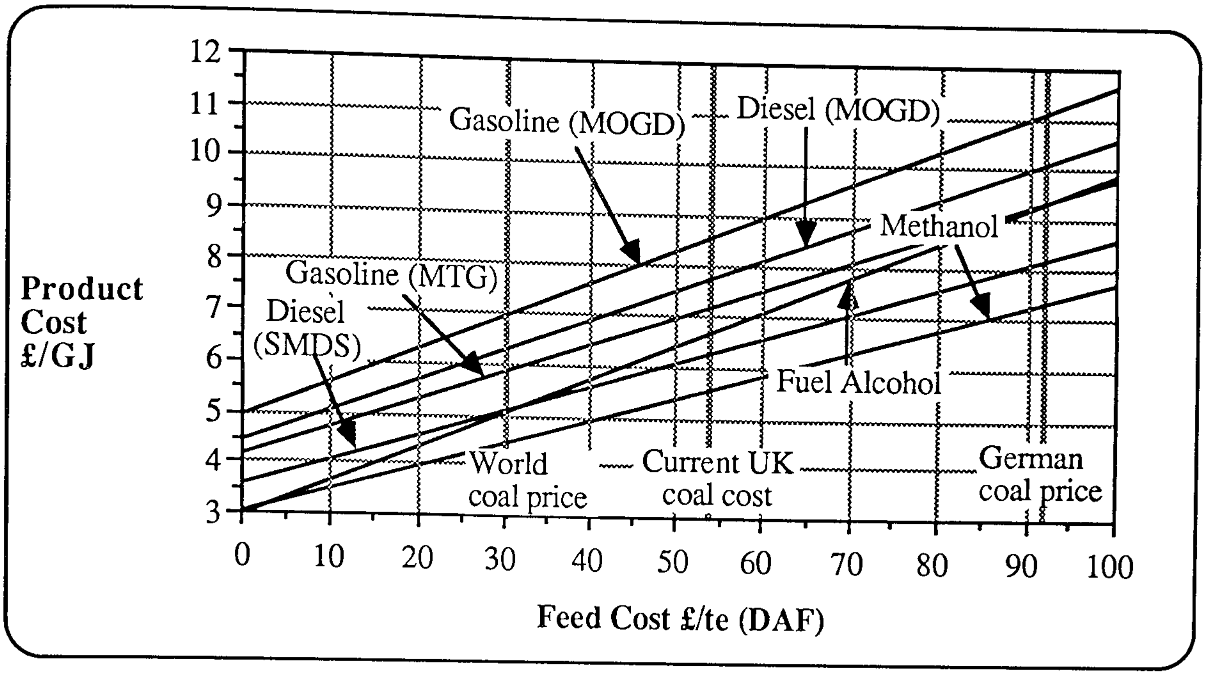

Figure 7.4 Product Costs for Different Conversion Processes, (Point of Ayr Coal, Shell Gasifier, 10 000 te/d)

Table 7.5
Ratio of Fuel Production Costs to Prices

Fuel	Typical UK coal (54.3 £/te) Ratio: Cost / Price	World Bit.Coal (30 £/te) Ratio: Cost / Price
Methanol	0.89	0.71
Fuel alcohol*	1.08	0.81
Gasoline (MTG)	1.27	1.04
Gasoline (MOGD)	1.52	1.23
Diesel (MOGD)	1.94	1.58
Diesel (SMDS)	1.57	1.26

Basis: 10 000 te/d feed - Shell gasifier
* based on estimated current cost of production - see Table 7.3

From Table 7.5 it can be seen that MTG would only become economic using Point of Ayr coal at crude prices well over 30 $/bbl for Brent crude. Similarly MOGD and SMDS fuel production costs are equivalent to a product selling price for which Brent crude would be also significantly over 30 $/bbl. For cheaper coal at 30 £/te MTG production costs at 230 £/te equate to a Gasoline selling price for which Brent Crude would be approximately 37 $/bbl. SMDS could become viable for Brent crude prices at around 30 $/te and higher using cheap imported coal. Therefore with Brent crude at 18 $/bbl a doubling of the crude oil price would be required before any of the processes producing traditional hydrocarbon fuels would begin to be economically viable. Accurate assessments above 30 $/bbl are difficult to make due to increased uncertainty in predicting product prices for crude prices above 30 $ / bbl. These uncertainties are due to alternative fuels suppressing price increases in fuel oils for example and changes in the differential costs of different fuels at high crude prices.

Table 7.6[127]
Predicted Oil products Prices At Various Brent Crude Prices

Brent Crude Price $/bbl	Gasoline £/te*	Kerosine £/te	Naphtha £/te	Gasoil £/te
14	97	86	75	74
18	119	100	119	118
22	141	121	109	105
26	167	145	130	126
30	189	169	147	143
* (@ 1.75 $/£) Base Case Values £/te				
MTG	331.5	NA	NA	NA
MOGD	394.5	NA	NA	355.1
SMDS	NA	323.2	287.2	285.3

7.9 Effect of scale

Figure 7.5 shows the effect of increasing plant size on the production cost of methanol using the Shell gasifier. The effect of scale becomes relatively small after a output size of approximately 5000 te / day of methanol. This is due to the use of multiple streams for the major steps for sizes larger than this. For example the largest sizes of methanol plant built to date in a single stream are around 3000 te/day. The largest gasification plant possible in a single stream is likely to produce enough gas for around 2000 te/d of methanol.

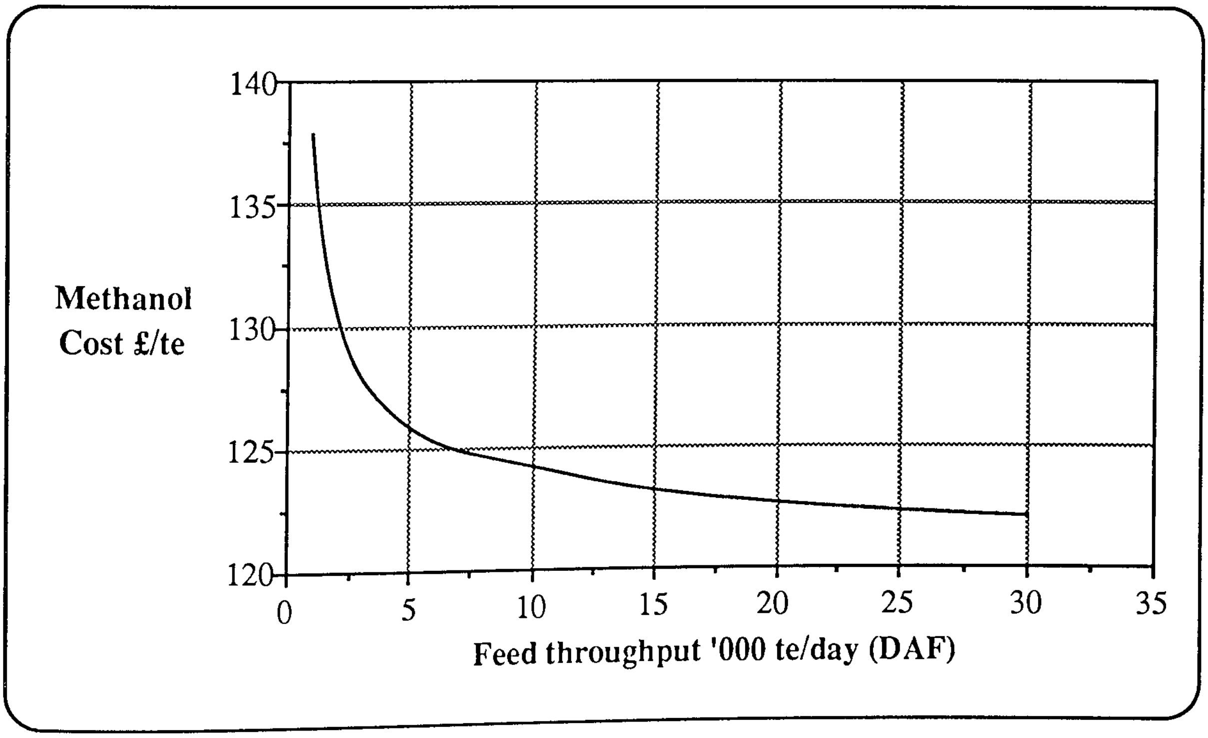

Figure 7.5 Methanol Cost for Different Feed Throughputs, (Point of Ayr Coal, Shell Gasifier, 10 000 te/d)

7.10 Comparison of BGL and Shell Gasifiers

As the base case for the comparisons given here is taken as the Shell gasifier with a throughput of 10 000 tonnes per day of dry ash free Point of Ayr coal, a detailed analysis of this gasifier against the British Gas / Lurgi gasifier is shown. The BGL gasifier is used for comparison as this gave the lowest cost for nearly all cases and for all products. Table 7.6 gives a comparison of capital costs for the two gasifiers and the associated processes to produce methanol from the feed coal. It can be seen that the total capital costs for the process routes differ by less then 6 %. Table 7.7 gives a comparison of the yearly costs.

Table 7.6 Comparison of Capital Costs at 10 000 te/d of Feed

Step	Shell Million £	Shell %	BG/L Million £	BG/L %
Reception and Storage	5.4	1.1	5.4	1.1
Feed Preparation	44.5	8.7	13.9	2.9
Gasification	210.0	41.1	162.9	33.7
Methanol Synthesis	131.2	25.7	172.3	35.6
Methanol Distillation	102.8	20.1	109.9	22.7
Product Storage	17.4	3.4	19.2	4.0
	========		========	
TOTAL	511.4		483.8	

Table 7.7 Comparison of Yearly Costs at 10 000 te/d of Feed

	Shell Miilion £	Shell %	BG/L Million £	BG/L %
Capital Amortization	58.8	14.6	55.6	15.3
ROI per year	0.0	0.0	0.0	0.0
Feedstock Cost	184.6	45.8	184.6	50.8
Utilities Cost	124.2	30.8	89.5	24.7
Maintenance Cost	12.8	3.2	12.1	3.3
Overheads Cost	25.6	6.3	24.2	6.7
Labour Cost	1.0	0.2	1.0	0.3
Additional Process Inputs	0.0	0.0	0.0	0.0
By-product Credits	-4.1	-1.0	-3.8	-1.1
Other Costs	0.0	0.0	0.0	0.0
	==========		==========	
TOTAL ANNUAL COSTS	£ 402.9		£ 363.2	

Table 7.8 Comparison of Yields and Costs

	Shell	BG/L
Flow t/d	9449.1	10395.0
% mass yield	94.5	103.9
% energy yield	63.1	66.0
% Carbon Conversion Efficiency.	42.4	46.7
Methanol production cost (£/t)	125.4	102.8

At this throughput their the economy of scale is small therefore the annual costs equalized to an output of 10 000 tonnes per day of methanol are as shown in Table 7.9.

Table 7.9 Comparison of Equalized Yearly Costs at 10 000 te/d of Methanol

	Shell		BGL	
	Million £	%	Million £	%
Capital Amortization	62.2	14.6	53.5	15.3
ROI per year	0.0	0.0	0.0	0.0
Feedstock Cost	195.4	45.8	177.6	50.8
Utilities Cost	131.5	30.8	82.9	24.7
Maintenance Cost	13.5	3.2	11.6	3.3
Overheads Cost	27.1	6.3	23.3	6.7
Labour Cost	1.0	0.2	0.9	0.3
Additional Process Inputs	0.0	0.0	0.0	0.0
By-product Credits	-4.3	-1.0	-3.7	-1.1
Other Costs	0.0	0.0	0.0	0.0
	==========		==========	
TOTAL ANNUAL COSTS	£ 435.0		£ 349.2	

The difference in production cost can then be broken down approximately into the following main factors as given in Table 7.10.

Table 7.10 Main Yearly Cost Differences Between BGL and Shell to Produce Methanol

	Additional cost of Shell Gasification System*
Utilities cost	14.3 £ / te of methanol
Feedstock cost	5.0 £ / te of methanol
Capital amortization	2.6 £ / te of methanol
Others	0.7 £ / te of methanol
	===============
Total	22.6 £ / te of methanol

* Note: The BG/L gasifier has the lower value in all cases

From Table 7.7 the total cost difference is 125.4 - 102.8 = 22.6 £ / tonne, with the B/L gasifier having the lower cost. The main factor can be seen from the above to be the utilities cost difference for the two gasifiers, as shown in Table 7.10, this is discussed below in section 7.10.1.

7.10.1 Utility Balance

The daily utility requirements of the BG/L and Shell gasifiers are given in Table 7.11. The BG/L gasifier is a net user of fuel gas in the methanol synthesis stage because it is used in the steam reforming section of the plant to reform methane produced in the gasifier into recycleable synthesis gas. The Shell gasifier is a net producer of fuel gas in the methanol section as the purge gas from the methanol synthesis step is usable as fuel gas and the process does not requires fuel gas for steam reforming as methane as not produced in the Shell gasifier.

Table 7.11 Comparison of Utility Costs

BG/L GASIFIER	Low Pr Steam	High Pr Steam	Process Water	Cooling Water	Waste Water	Fuel Gas	Oxygen	Power	Tars
Step sequence	t/day	t/day	t/day	t/day	t/day	GJ/day	t/day	MW	GJ/day
Reception	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.78	0.00
Fixed Bed Prep.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.69	0.00
BG/Lurgi	-550.0	-124.8	7327.6	0.00	367.0	0.00	6612.4	2.50	-17995.4
Methanol Syn.	-5113.8	-7796.1	0.00	325265.1	0.00	27879.8	0.00	4.06	0.00
Methanol Dis.	5086.9	0.00	0.00	23201.6	0.00	0.00	0.00	1.81	0.00
Product Storage	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
COST / DAY (£)	-2884	-79208	7327	13938	367	83639	264494	325	-24653
SHELL GASIFIER									
Step sequence									
Reception	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.78	0.00
Pulveriz./Dry.	1990.4	0.00	0.00	0.00	0.00	0.00	0.00	9.77	0.00
Shell	0.00	-2016.3	408.8	0.00	0.00	0.00	10026.5	7.14	0.00
Methanol Syn.	-3818.9	561.3	0.00	195299.5	0.00	-14898.6	0.00	1.39	0.00
Methanol Dis.	4624.0	0.00	0.00	21090.3	0.00	0.00	0.00	1.64	0.00
Product Storage	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
COST / DAY (£)	13977	-14549	408	8655	0.00	-44695	401059	622	0.00

From Table 7.11 it can be seen that the oxygen cost is the biggest overall single utility cost. When normalized to a methanol production rate of 10 000 te/d of methanol the comparative oxygen costs are as shown in Table 7.12.

Table 7.12 Comparison of Daily Oxygen Costs

BGL	Shell
254 000 £ / te	424 000 £ / te

This is equivalent to a difference of 17 £/te of product (11% of the methanol cost) between the BGL and the Shell gasifier with the other utilities reducing this overall effect to 14.3 £ / te methanol. The biggest single factor influencing the product price differences is, therefore, in this case the oxygen cost and the oxygen consumption of the gasifier. Furthermore it can be seen that the comparison between the two gasifiers is insensitive to the cost of oxygen assumed, an under estimate of 50 % in the assumed cost of oxygen would still make it the biggest single factor for the product cost difference for the criteria used in this analysis. This indicates that a major factor in comparing the relative economic efficiencies of the gasification processes is the oxygen consumption.

7.11 Non Base Case Results

Figures 7.6 to 7.9 shows the cost of production of methanol against feed price with different feeds for alternative gasifiers to the base case. In all cases the methanol has the lowest production cost with the Point of Ayr (bituminous) feed when compared on a cost per dry ash free tonne. This is due to the higher energy content of the higher rank coals and the higher conversion to methanol per dry ash free tonne of feed.

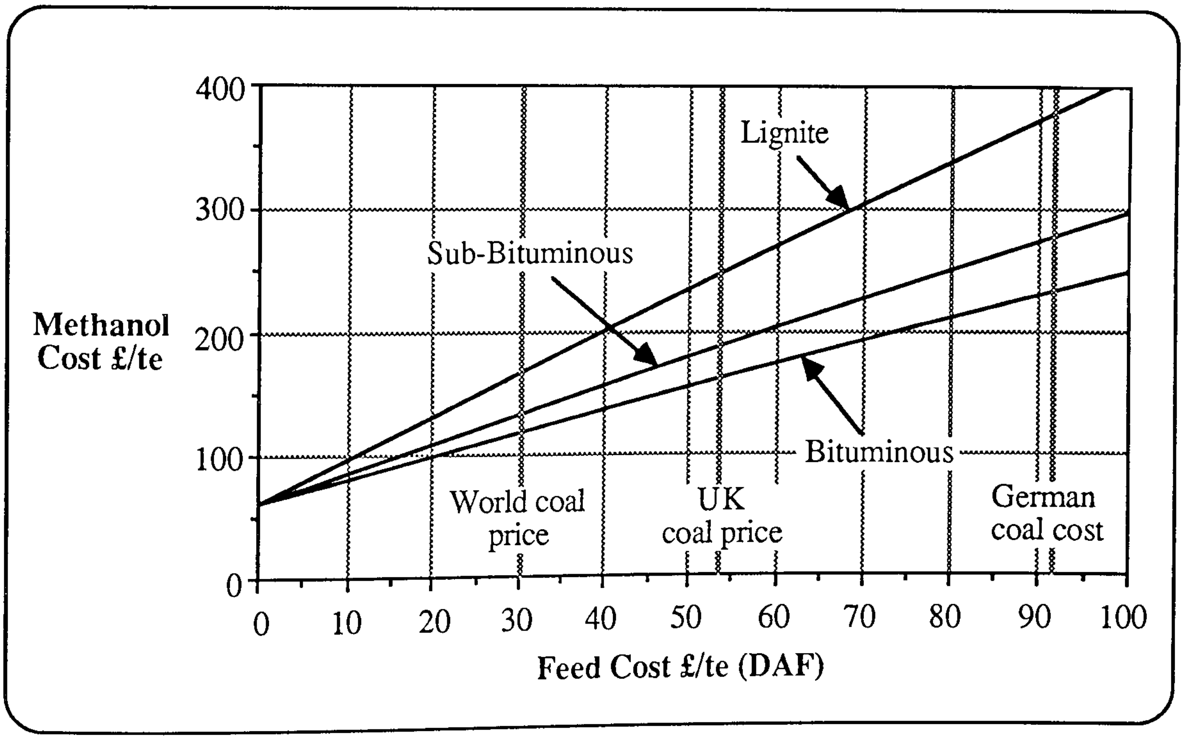

Figure 7.6 Methanol Cost for Different Feeds, Lurgi Gasifier

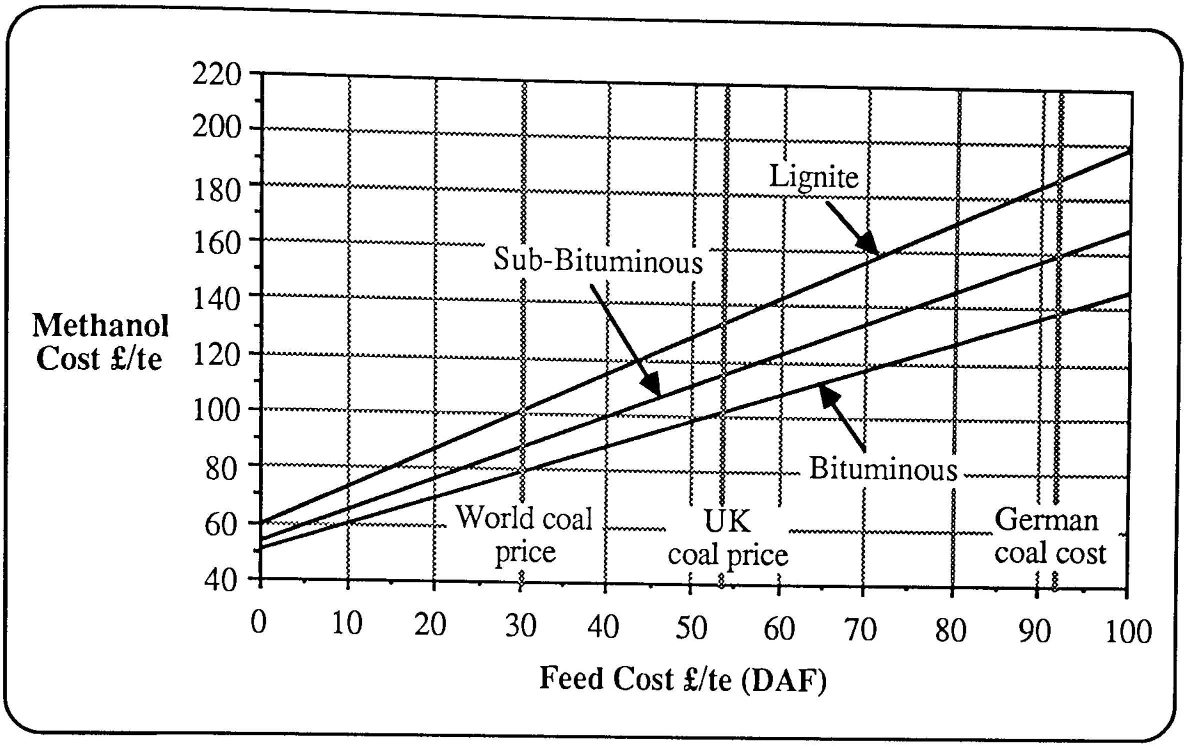

Figure 7.7 Methanol Cost for Different Feeds, BGL Gasifier

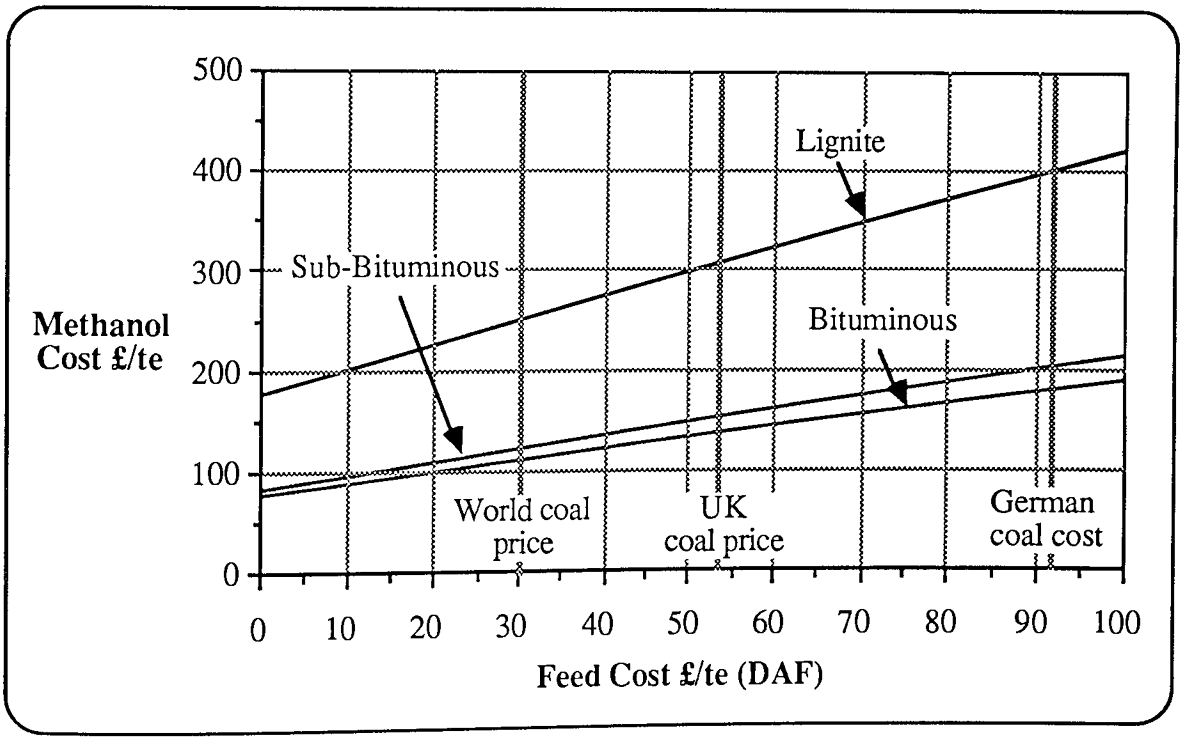

Figure 7.8 Methanol Cost for Different Feeds, Texaco Gasifier

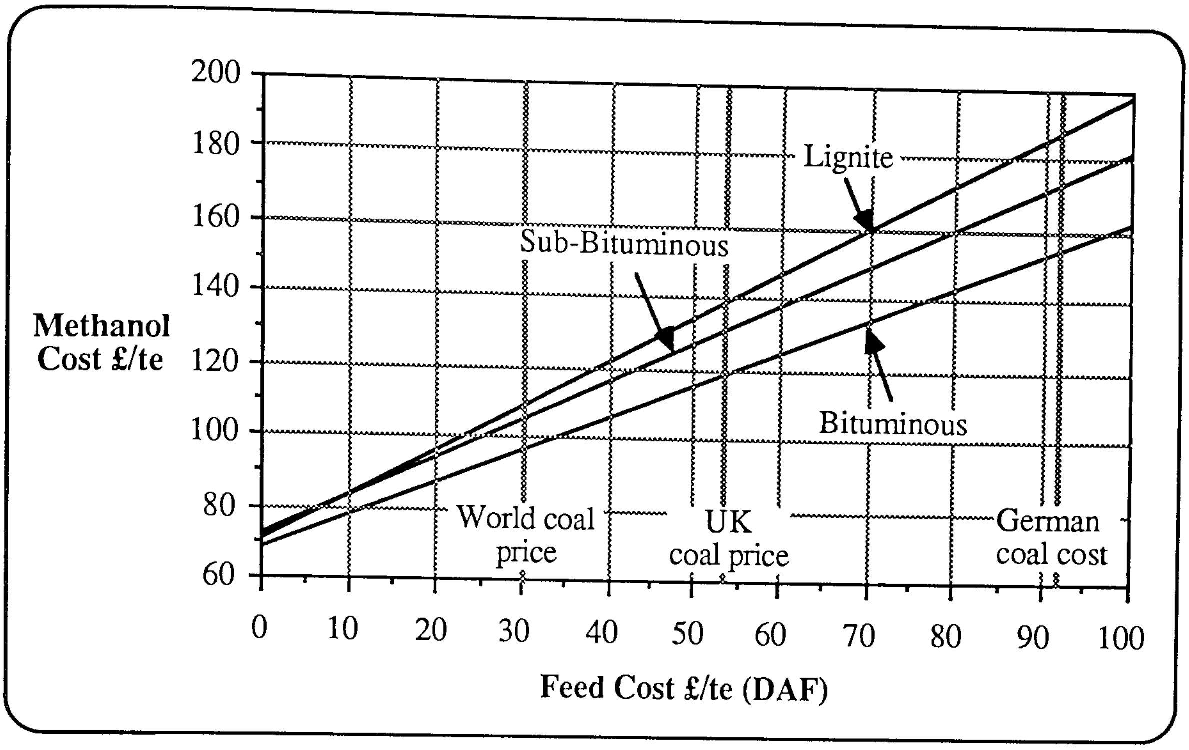

Figure 7.9 Methanol Cost for Different Feeds, KRW Gasifier

Figures 7.11 to 7.16 show the cost of production of Fuel Alcohol against feed cost for different ranks of feed and alternative gasifiers to the base case. The bituminous coal feed gives the lowest cost product for similar reasons to the methanol cases discussed earlier.

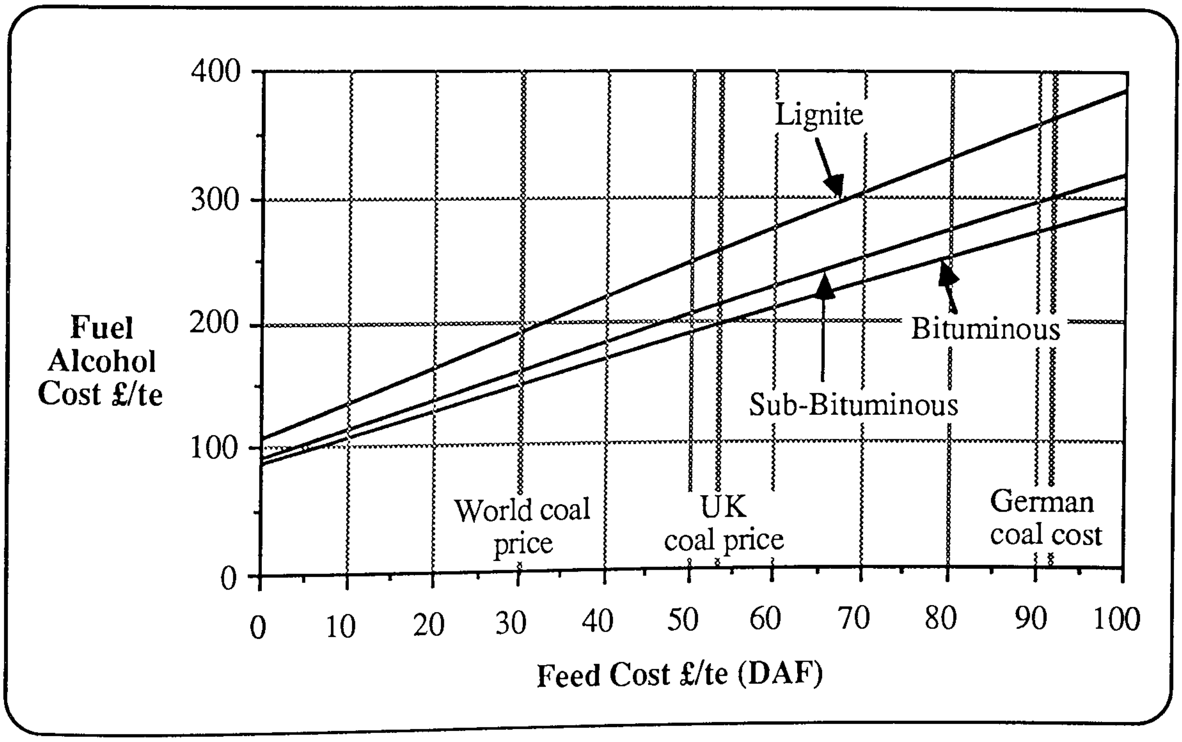

Figure 7.10 Fuel Alcohol Production Costs, Shell Gasifier

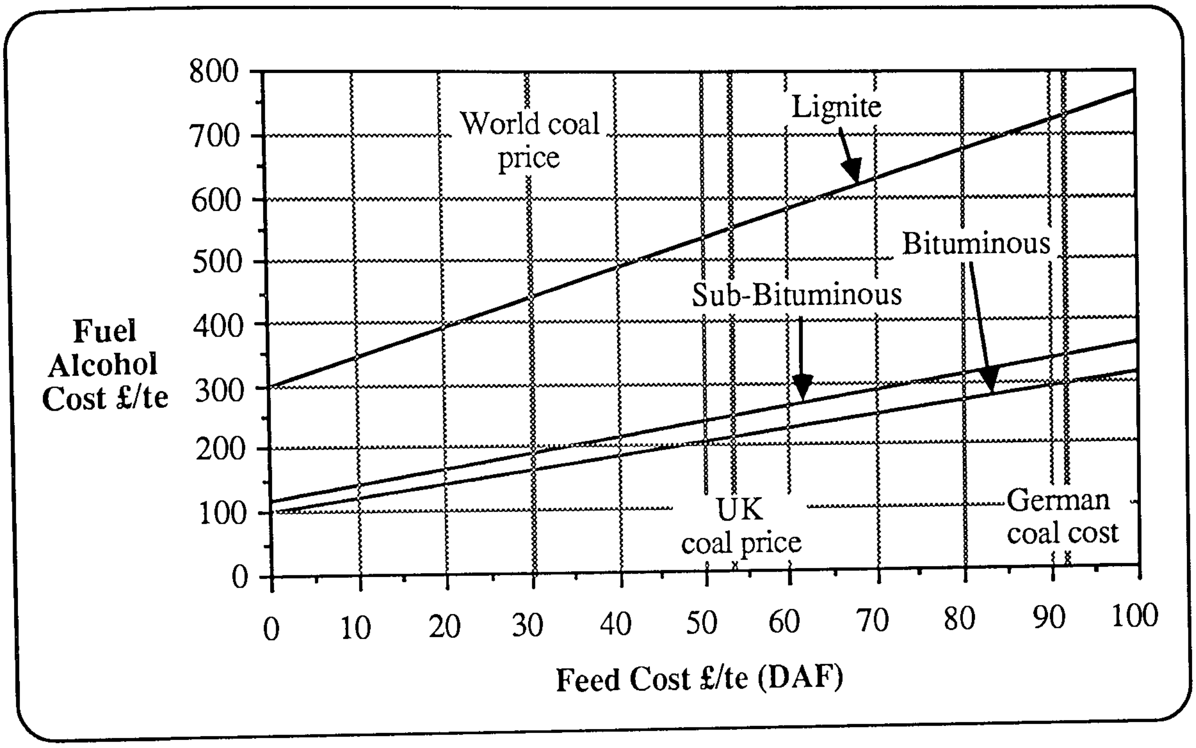

Figure 7.11 Fuel Alcohol Production Costs, Texaco Gasifier

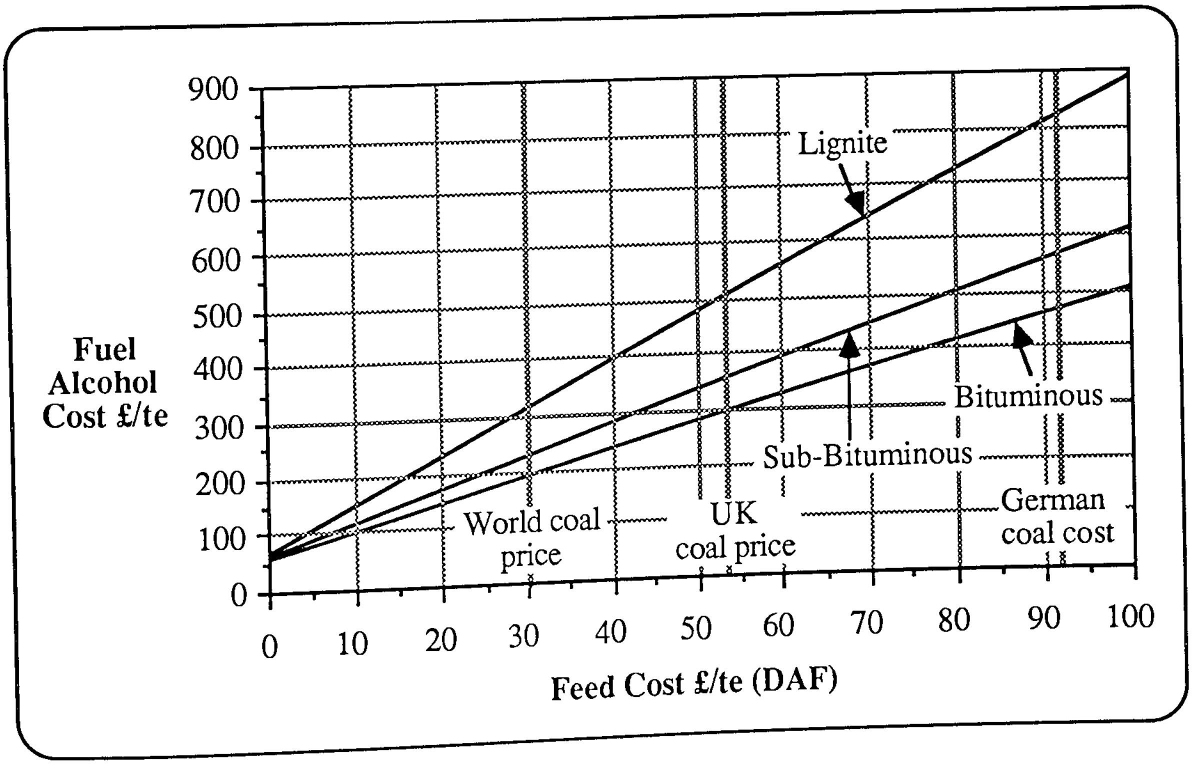

Figure 7.12 Fuel Alcohol Production Costs, Lurgi Gasifier

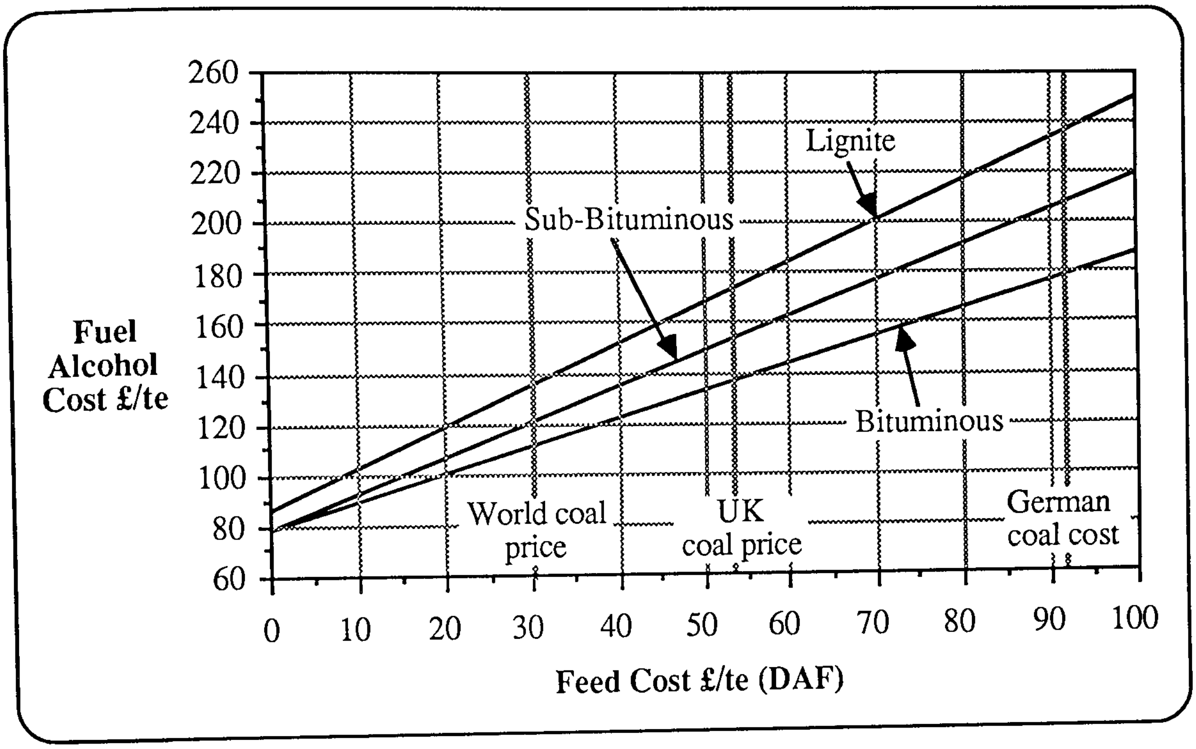

Figure 7.13 Fuel Alcohol Production Costs, BGL Gasifier

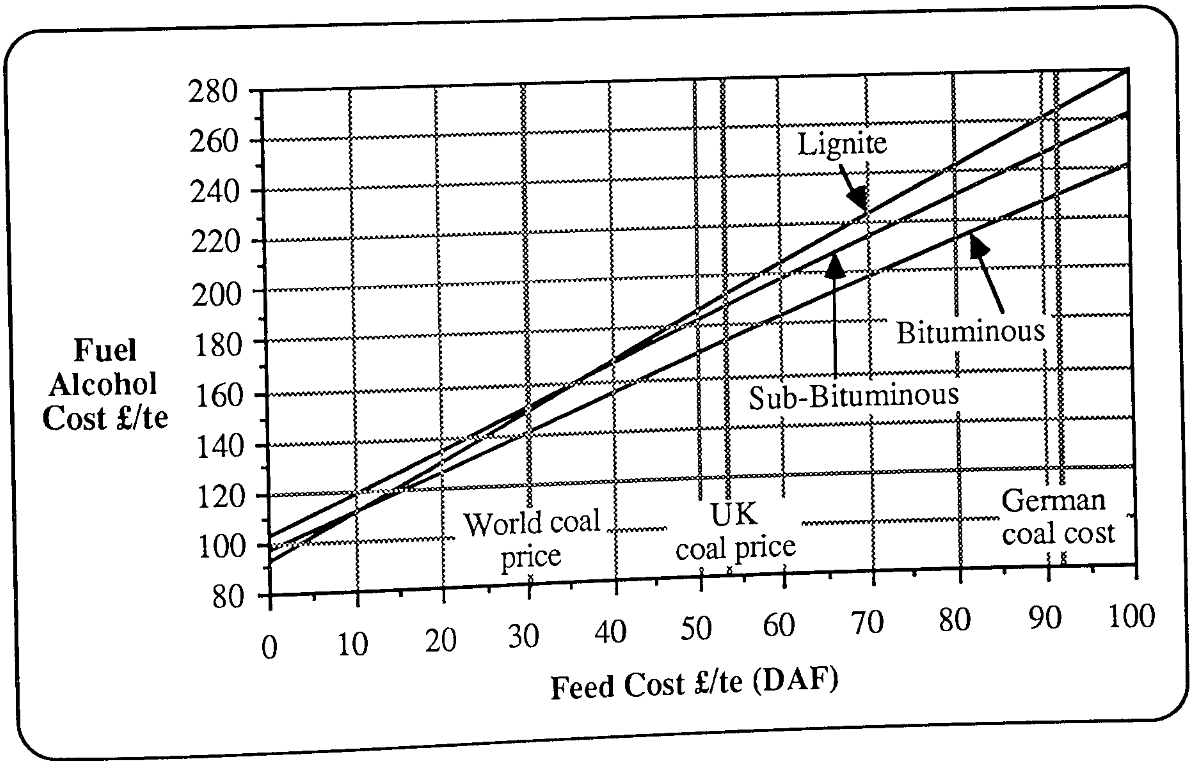

Figure 7.14 Fuel Alcohol Production Costs, KRW Gasifier

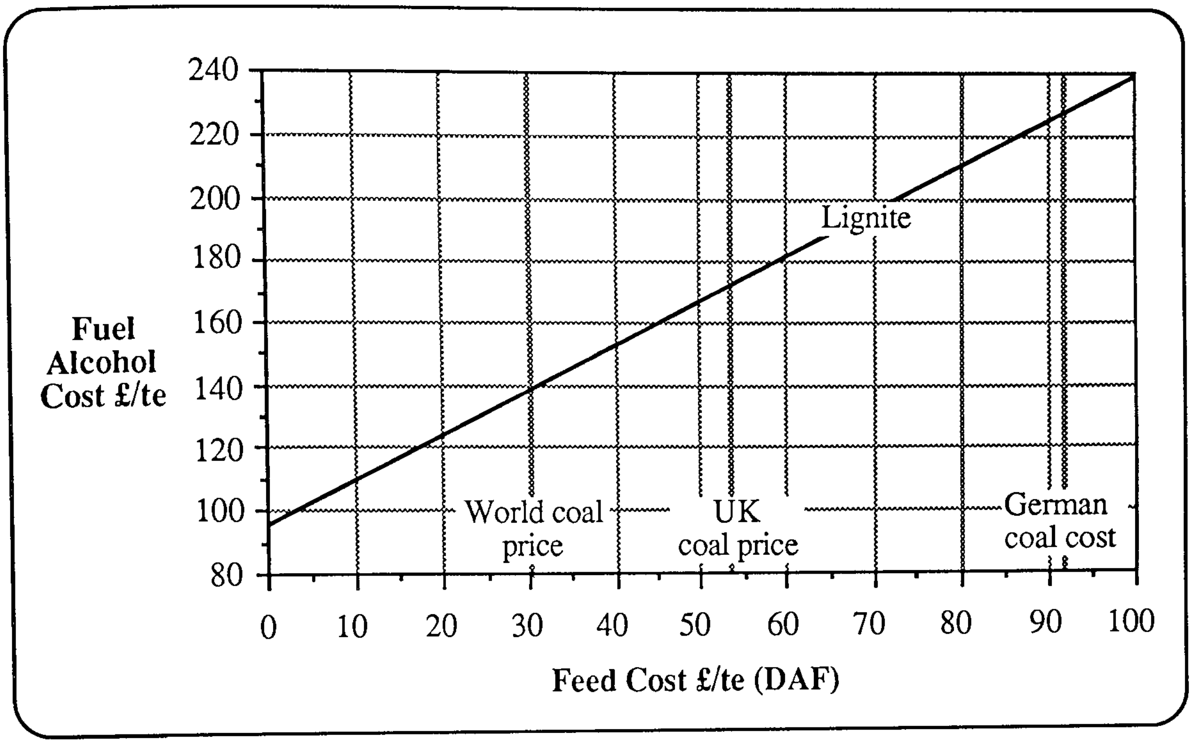

Figure 7.15 Fuel Alcohol Production Costs, HTW Gasifier

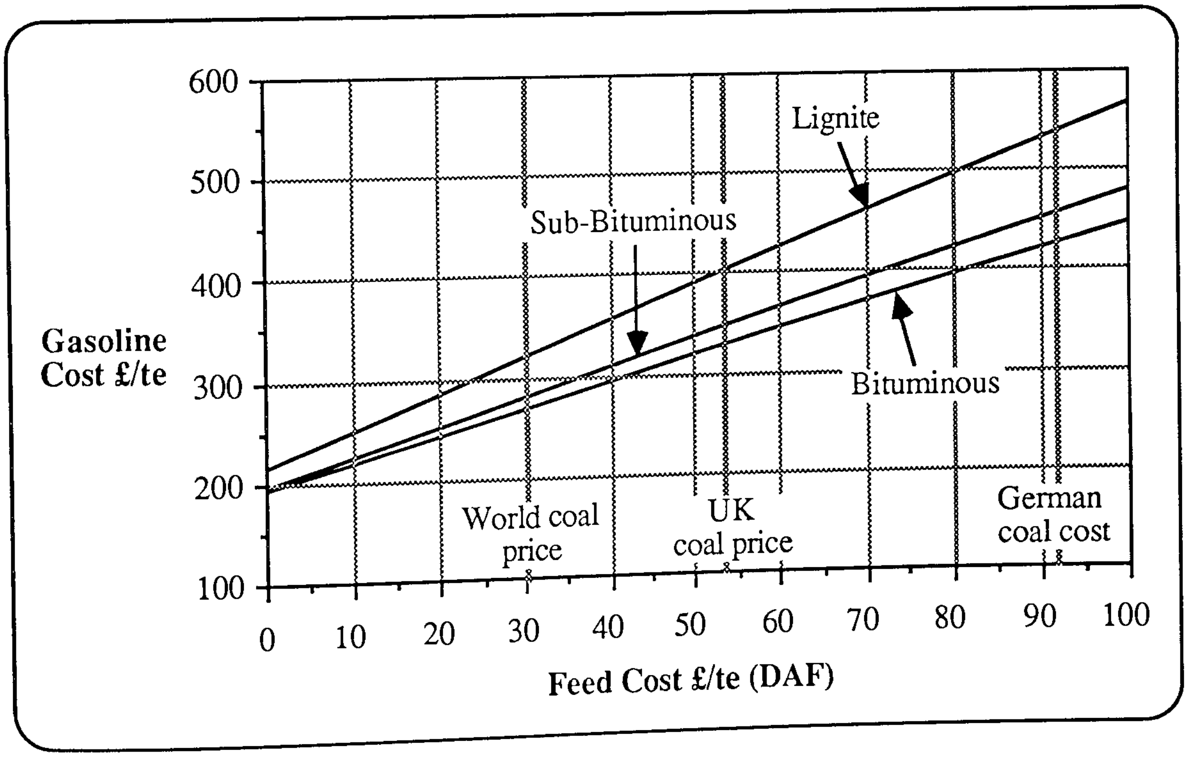

Figure 7.16 Gasoline Costs, MTG process, Shell Gasifier

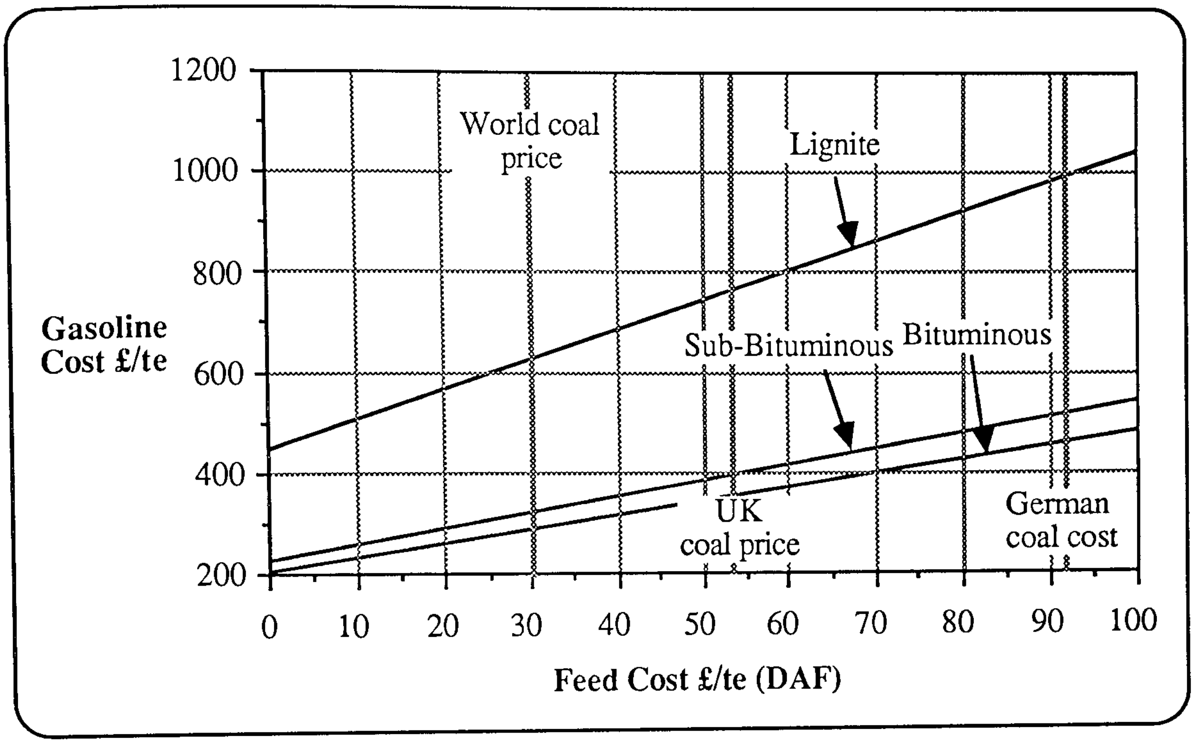

Figure 7.17 Gasoline Costs, MTG process, Texaco Gasifier

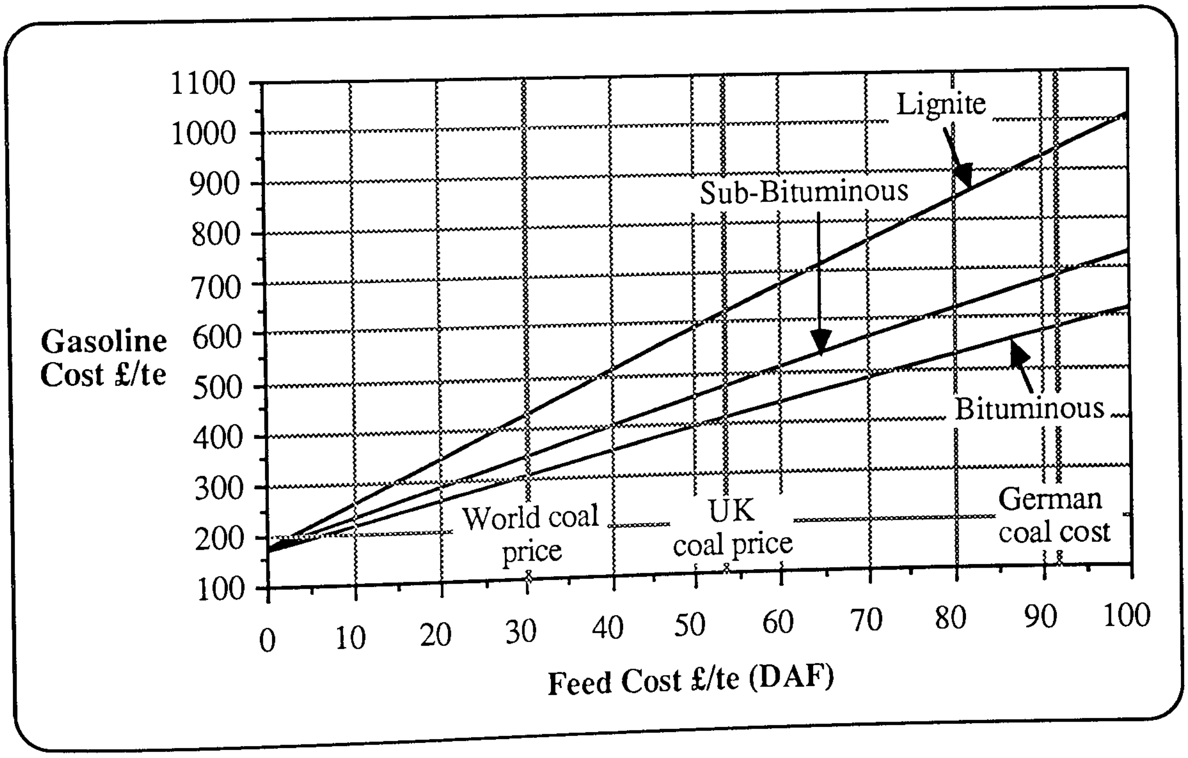

Figure 7.18 Gasoline Costs, MTG process, Lurgi Gasifier

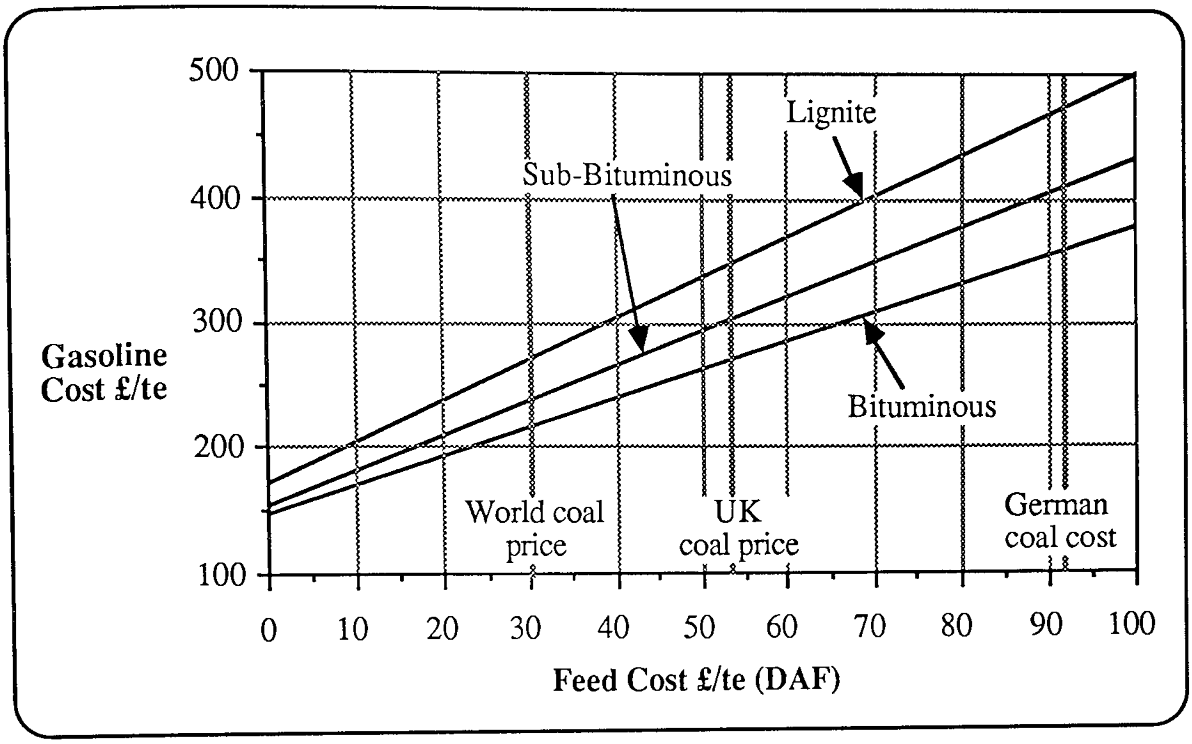

Figure 7.19 Gasoline Costs, MTG process, BGL Gasifier

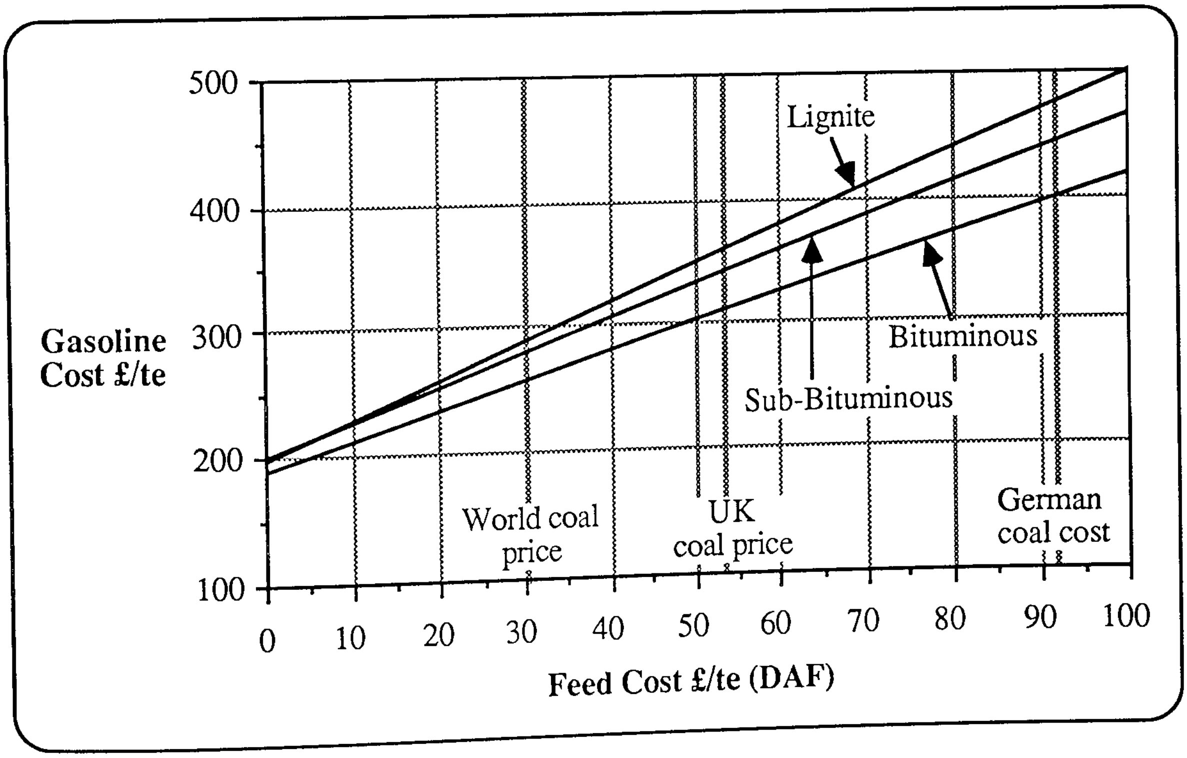

Figure 7.20 Gasoline Costs, MTG process, KRW Gasifier

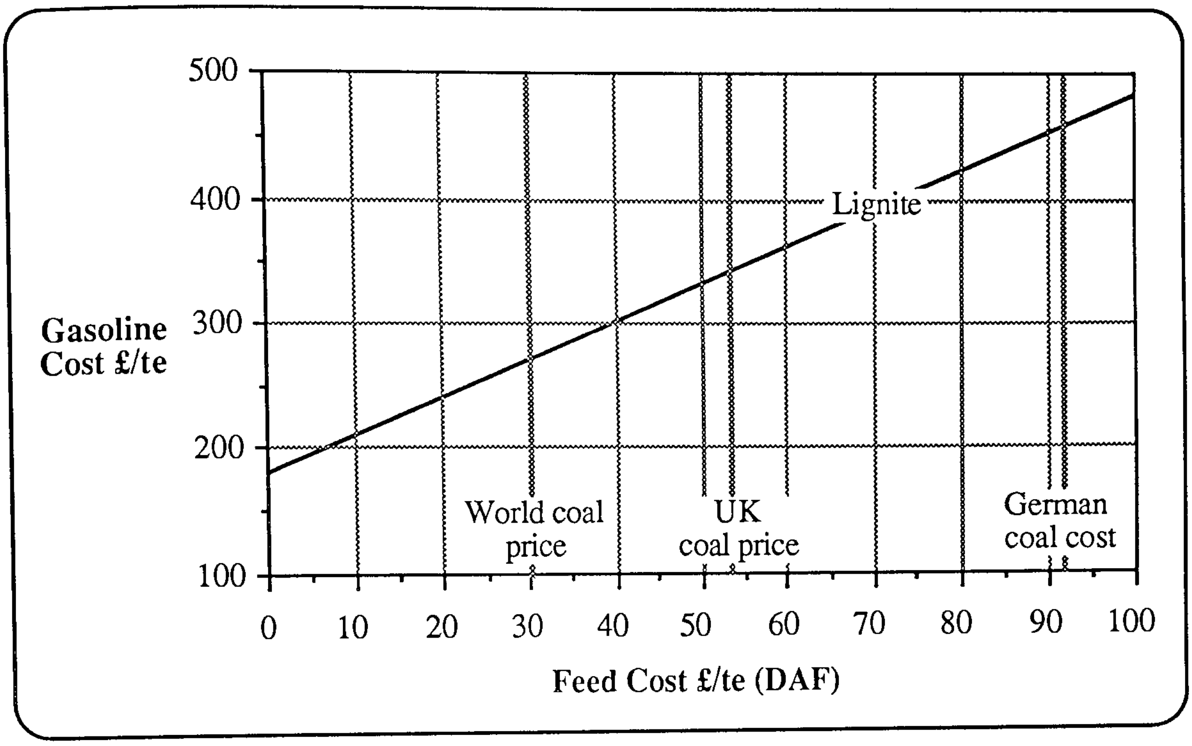

Figure 7.21 Gasoline Costs, MTG process, HTW Gasifier

Figures 7.23 to 7.28 show the cost of production of Gasoline, via the MOGD Process, against feed cost for different ranks of feed and for alternative gasifiers to the base case. The bituminous coal feed gives the lowest cost product for similar reasons to the methanol cases discussed earlier.

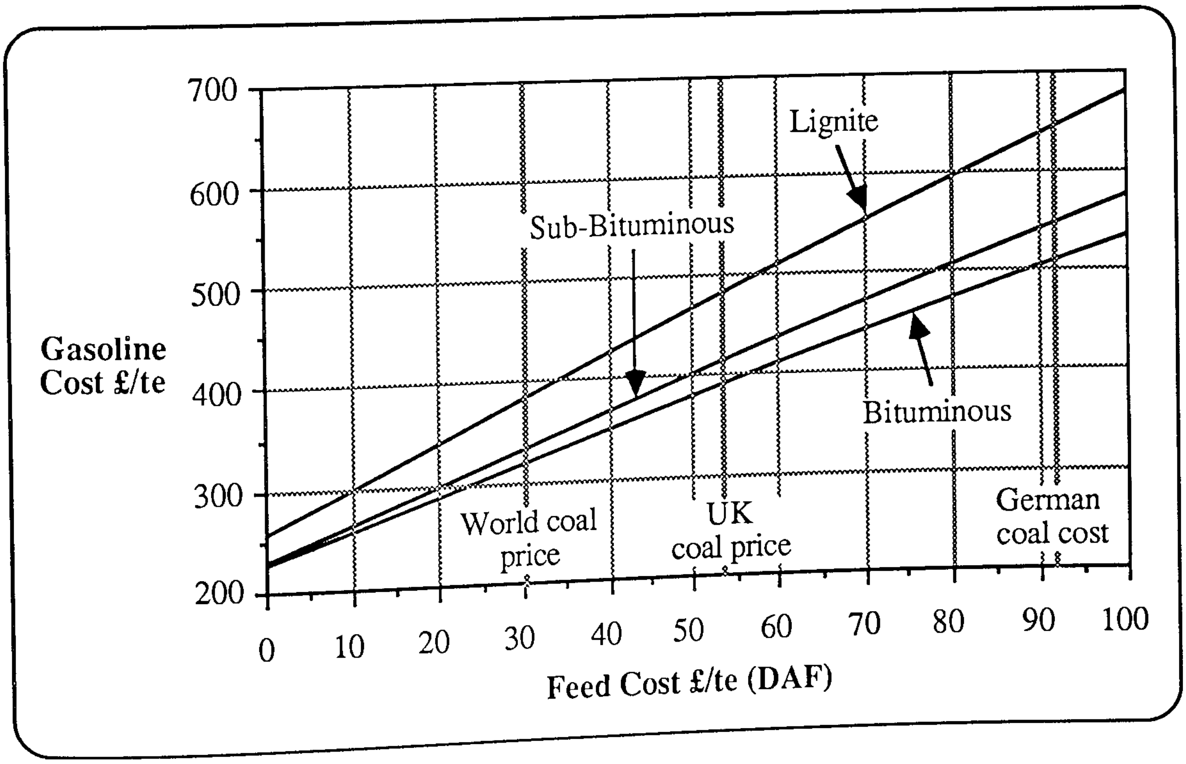

Figure 7.22 Gasoline Costs, MOGD process, Shell Gasifier

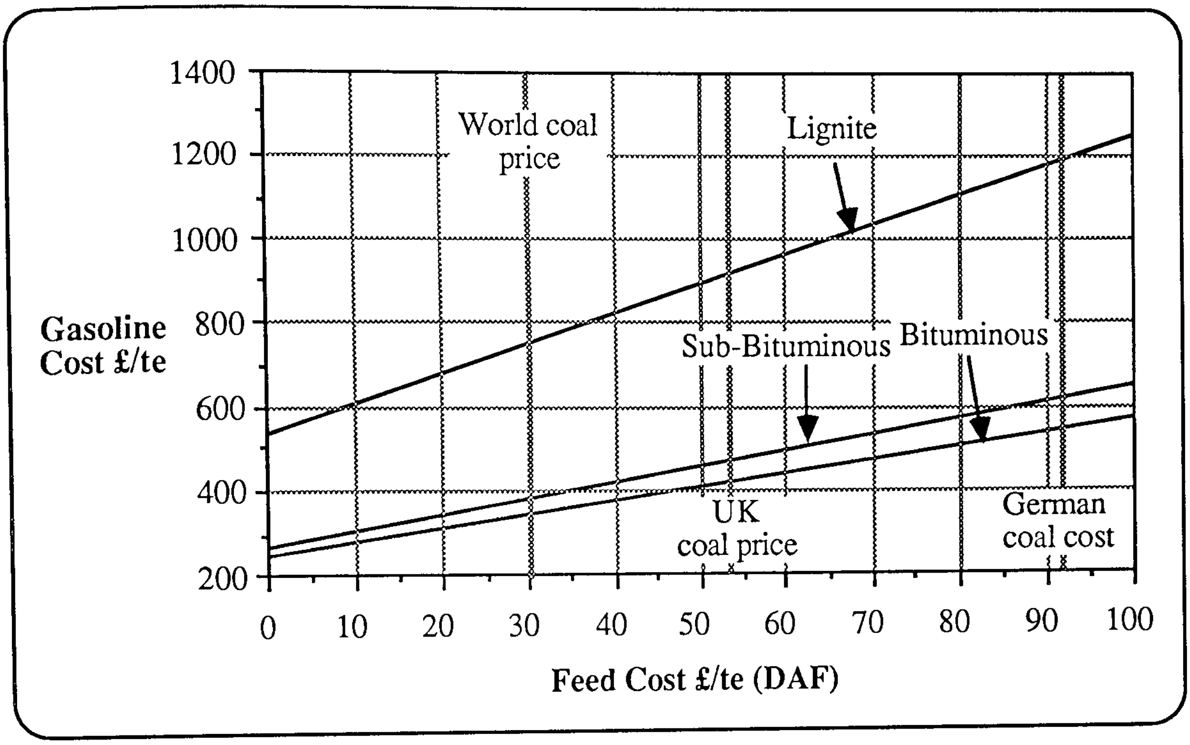

Figure 7.23 Gasoline Costs, MOGD process, Texaco Gasifier

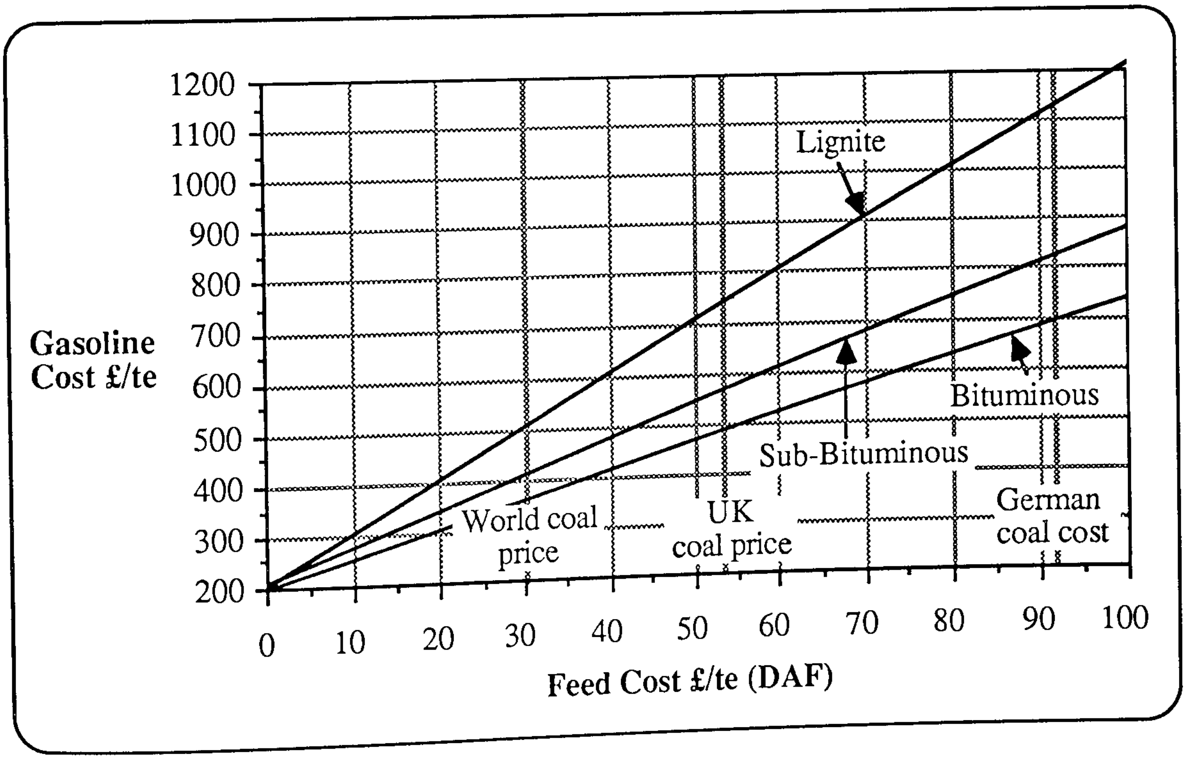

Figure 7.24 Gasoline Costs, MOGD process, Lurgi Gasifier

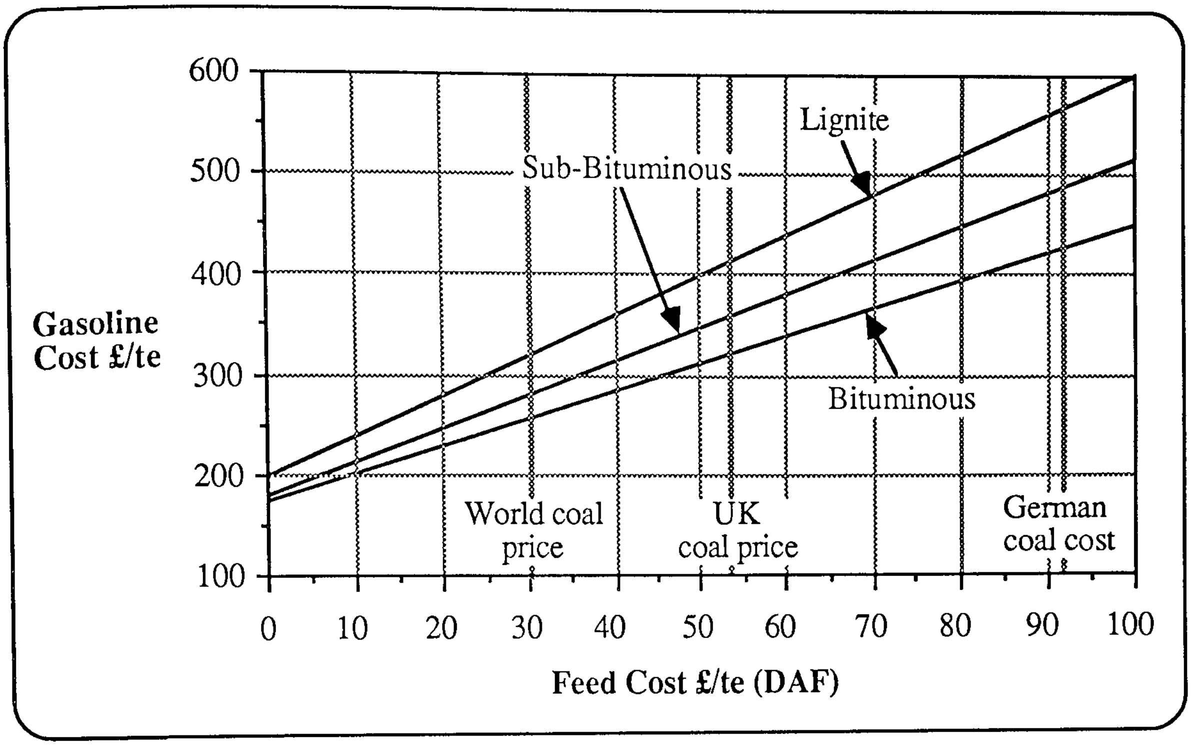

Figure 7.25 Gasoline Costs, MOGD process, BGL Gasifier

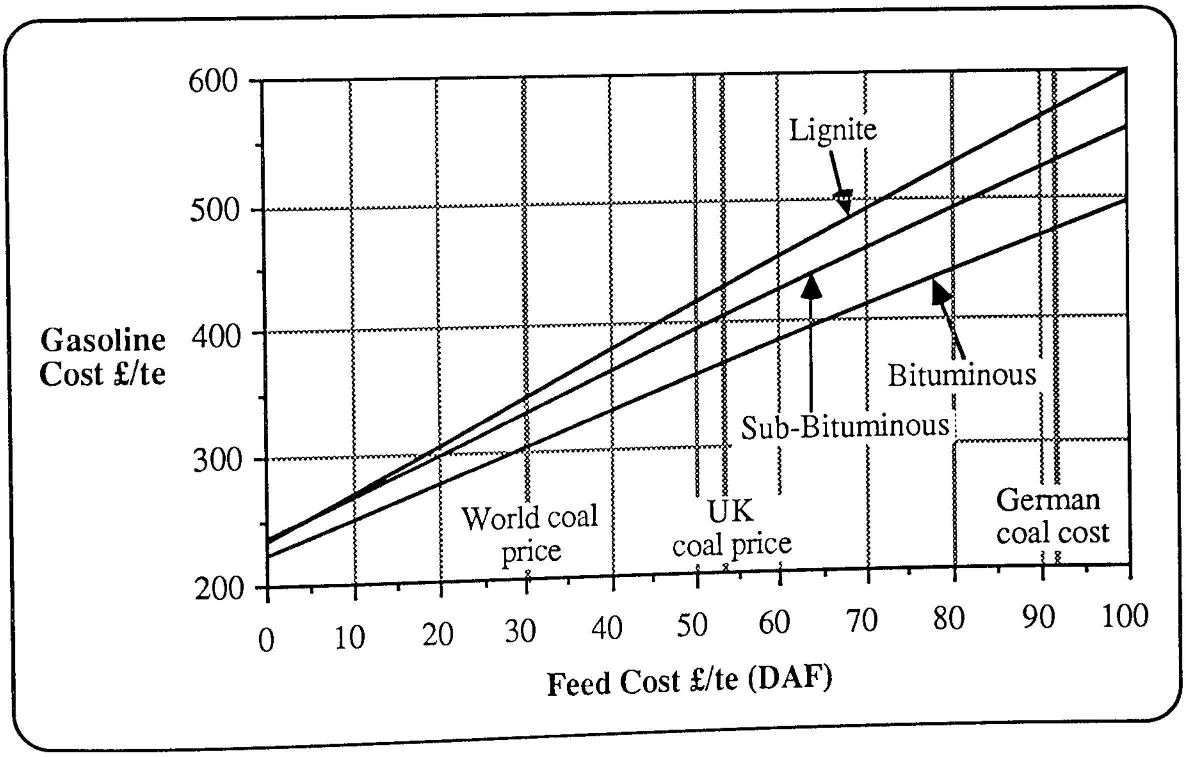

Figure 7.26 Gasoline Costs, MOGD process, KRW Gasifier

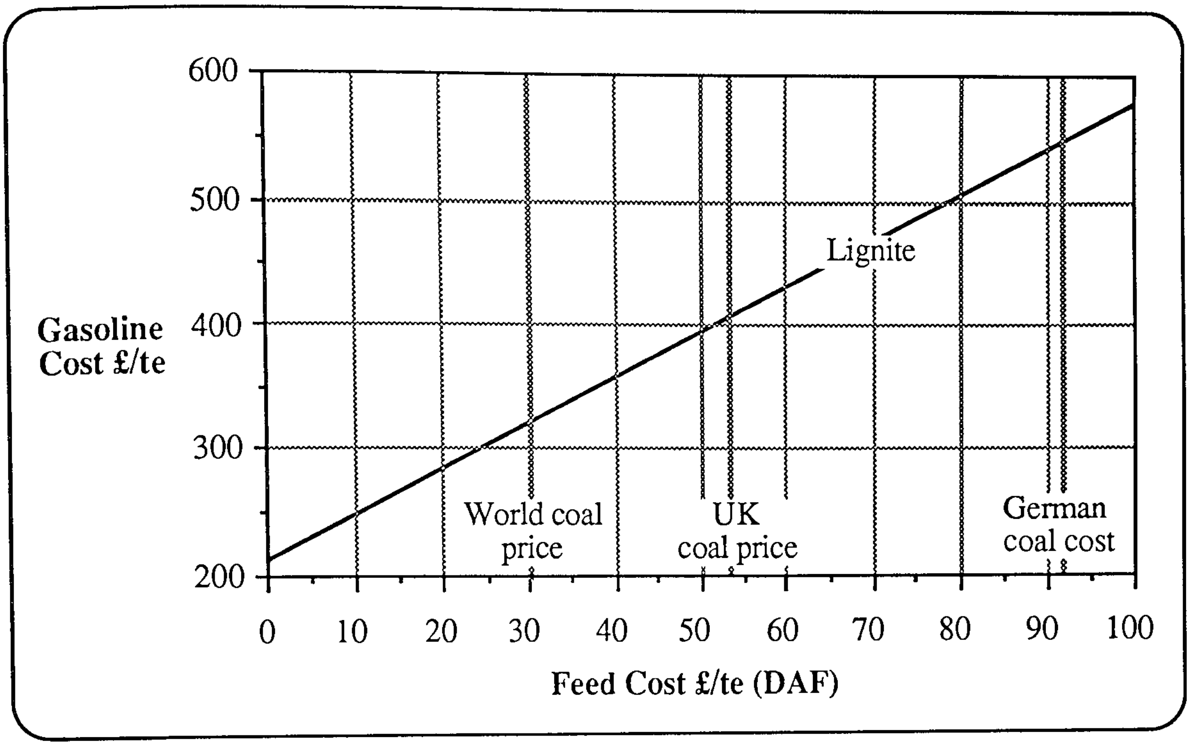

Figure 7.27 Gasoline Costs, MOGD process, HTW Gasifier

Figures 7.29 to 7.34 show the cost of production of Diesel, via the MOGD Process, against feed cost for different ranks of feed and for alternative gasifiers to the base case. The bituminous coal feed gives the lowest cost product for similar reasons to the methanol cases discussed earlier.

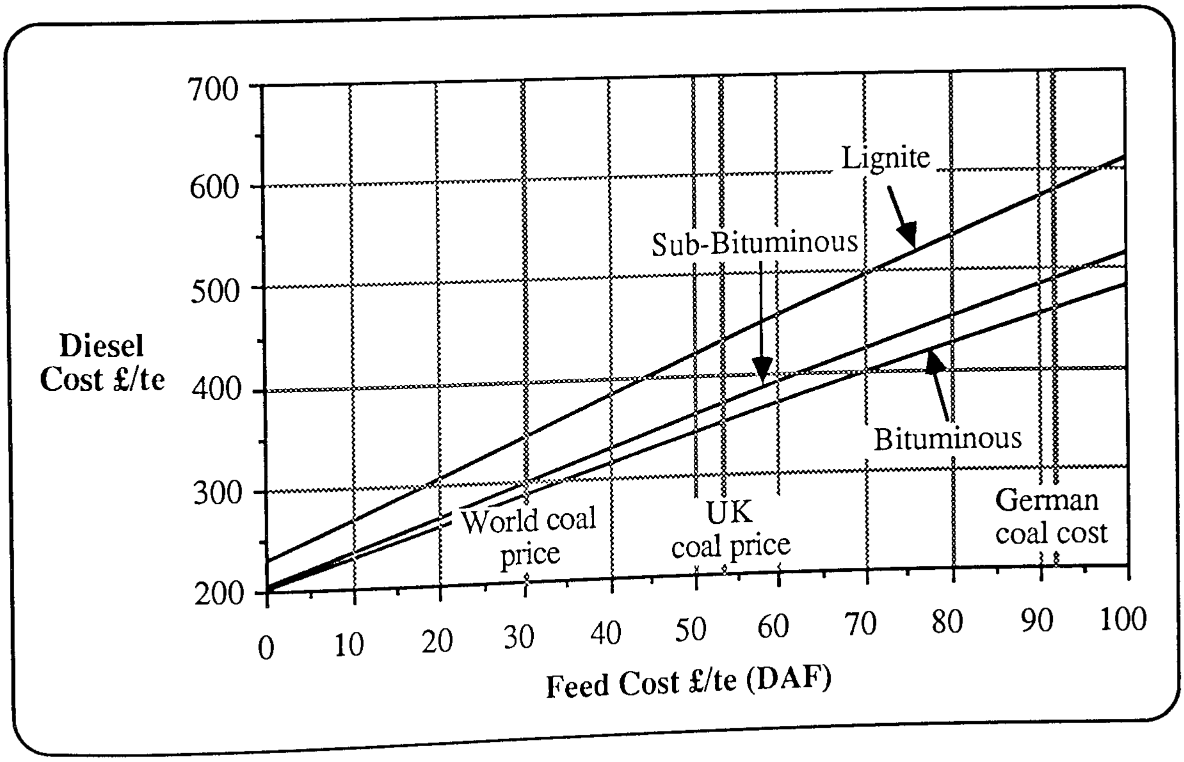

Figure 7.28 Diesel Costs, MOGD process, Shell Gasifier

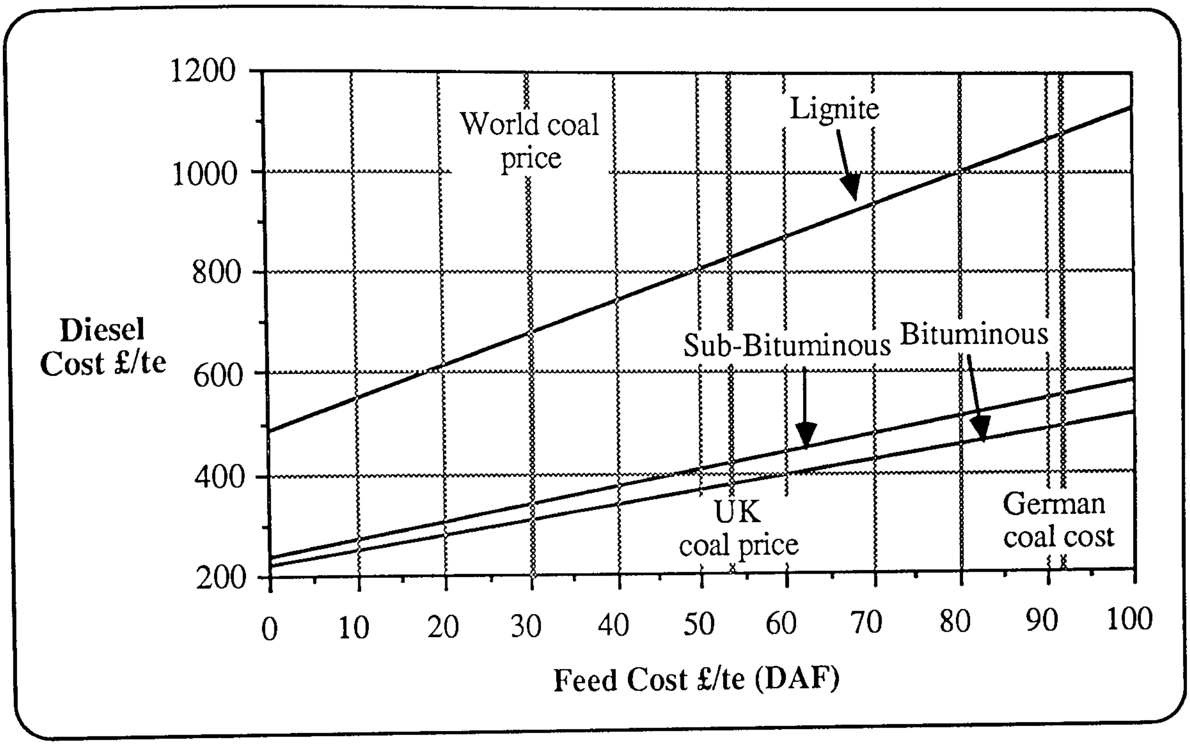

Figure 7.29 Diesel Costs, MOGD process, Texaco Gasifier

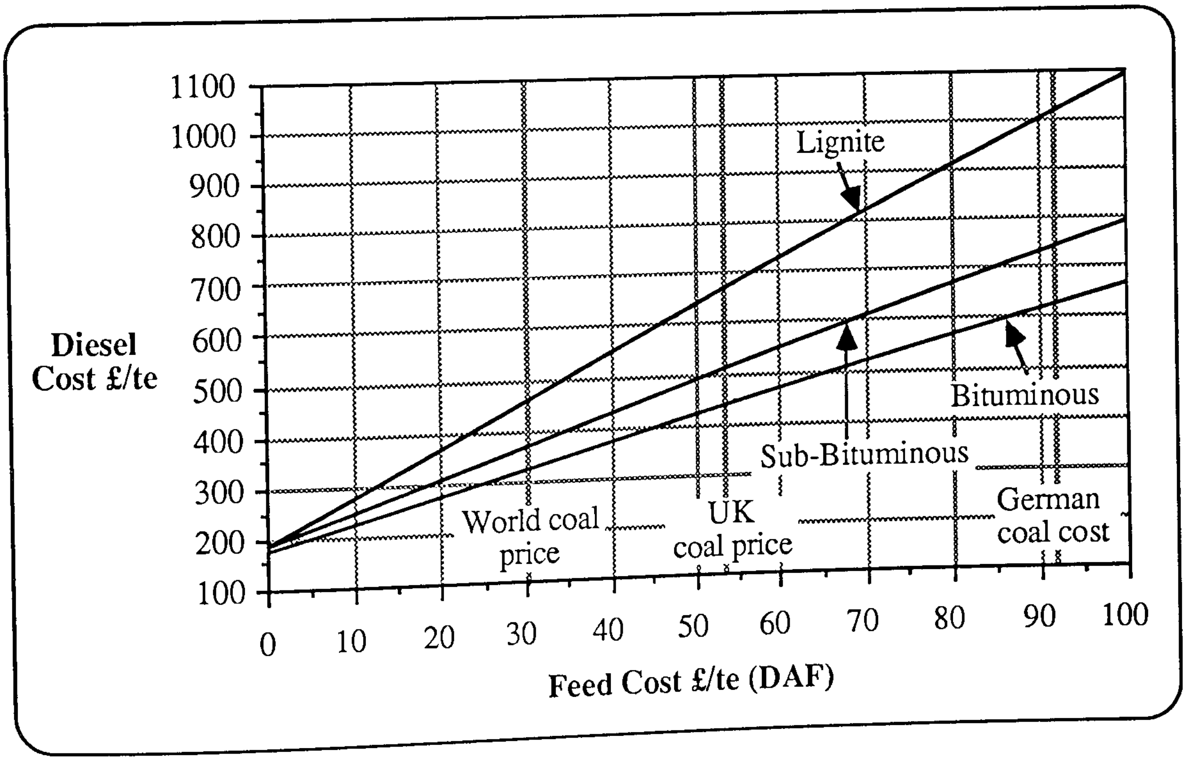

Figure 7.30 Diesel Costs, MOGD process, Lurgi Gasifier

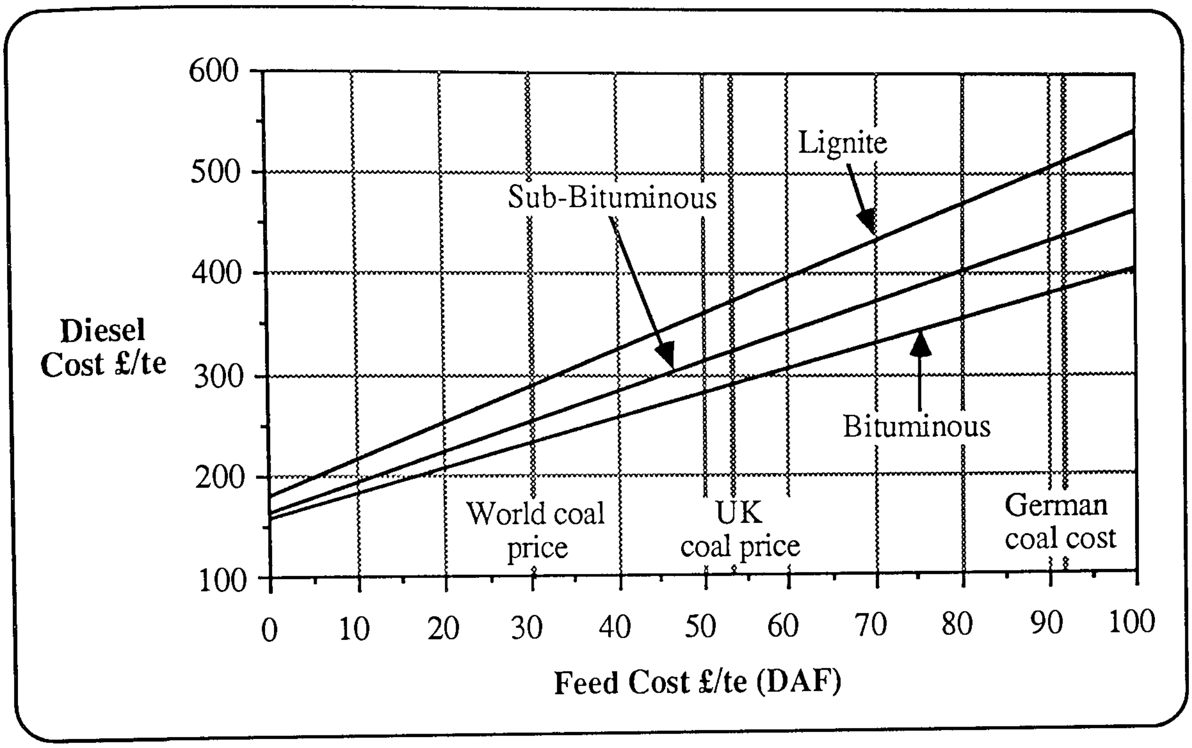

Figure 7.31 Diesel Costs, MOGD process, BGL Gasifier

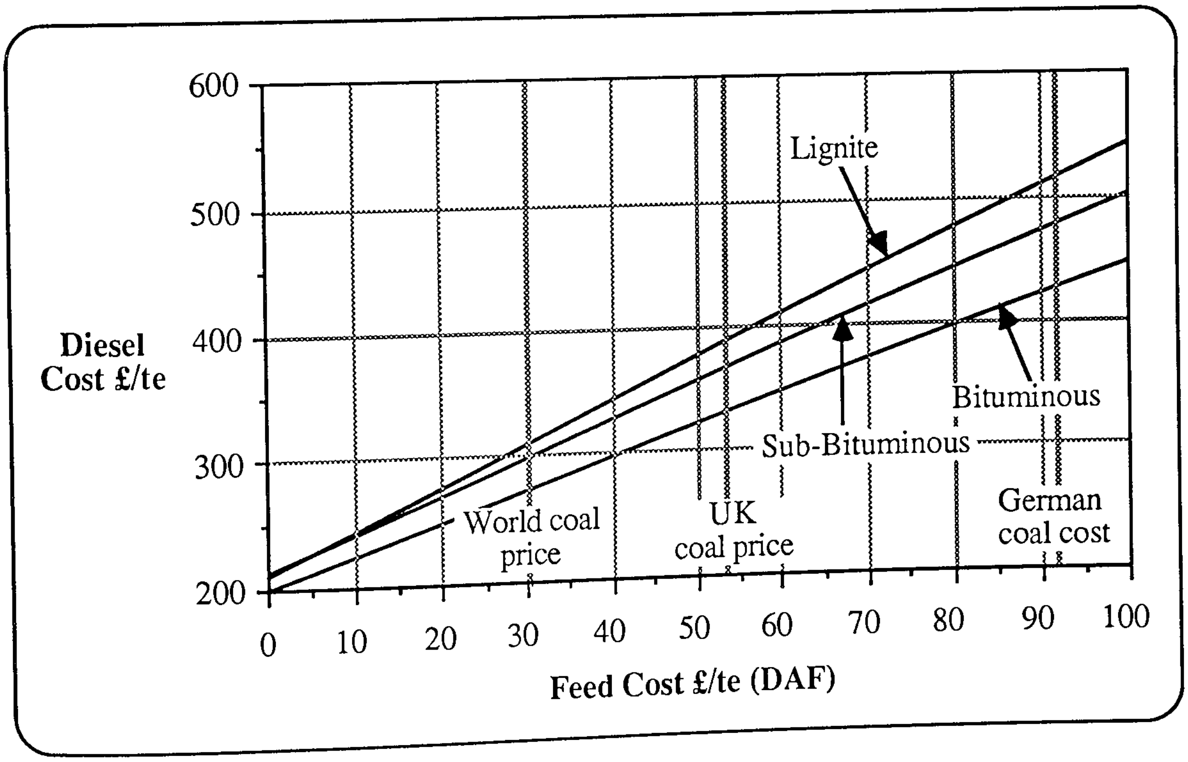

Figure 7.32 Diesel Costs, MOGD process, KRW Gasifier

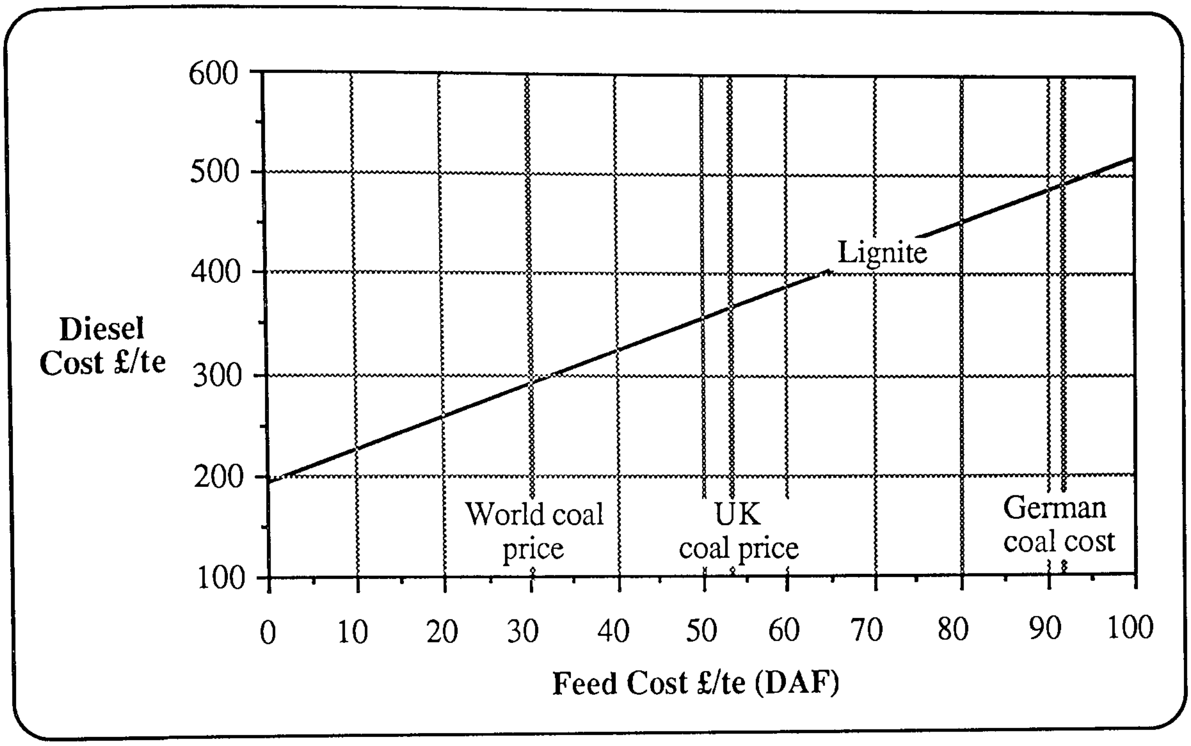

Figure 7.33 Diesel Costs, MOGD process, HTW Gasifier

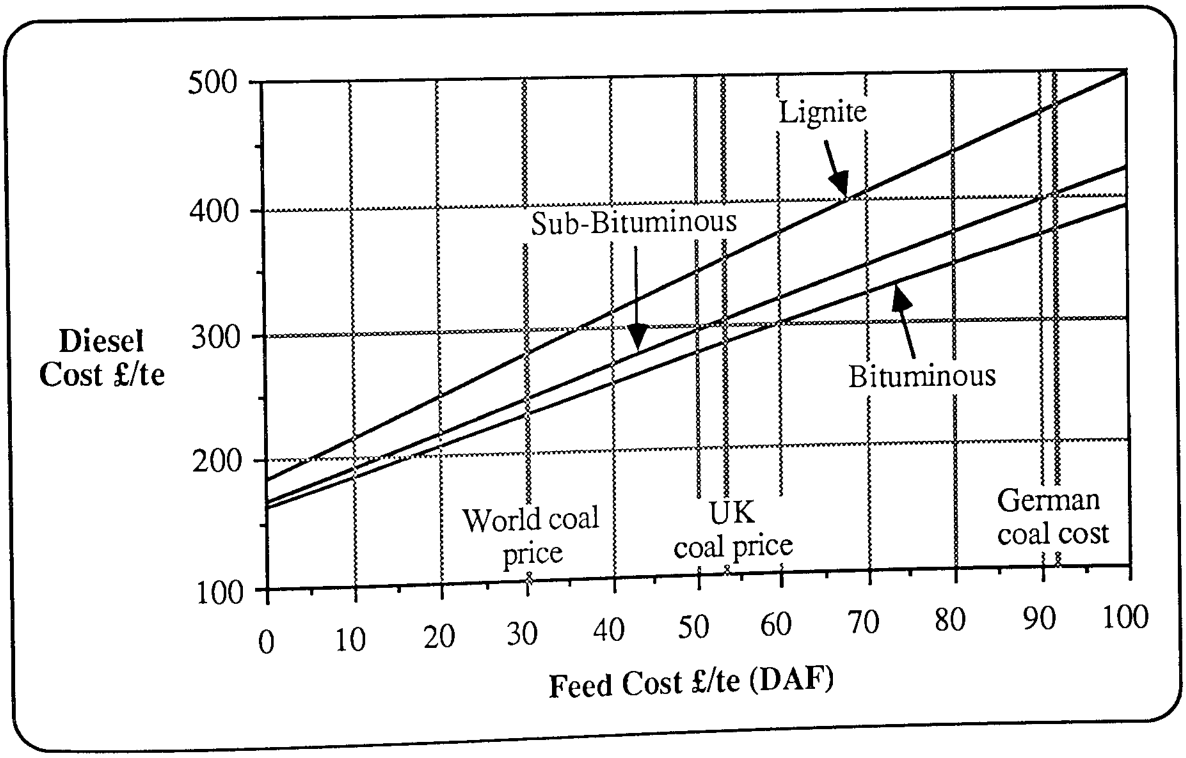

Figure 7.34 Diesel Costs, SMDS process, Shell Gasifier

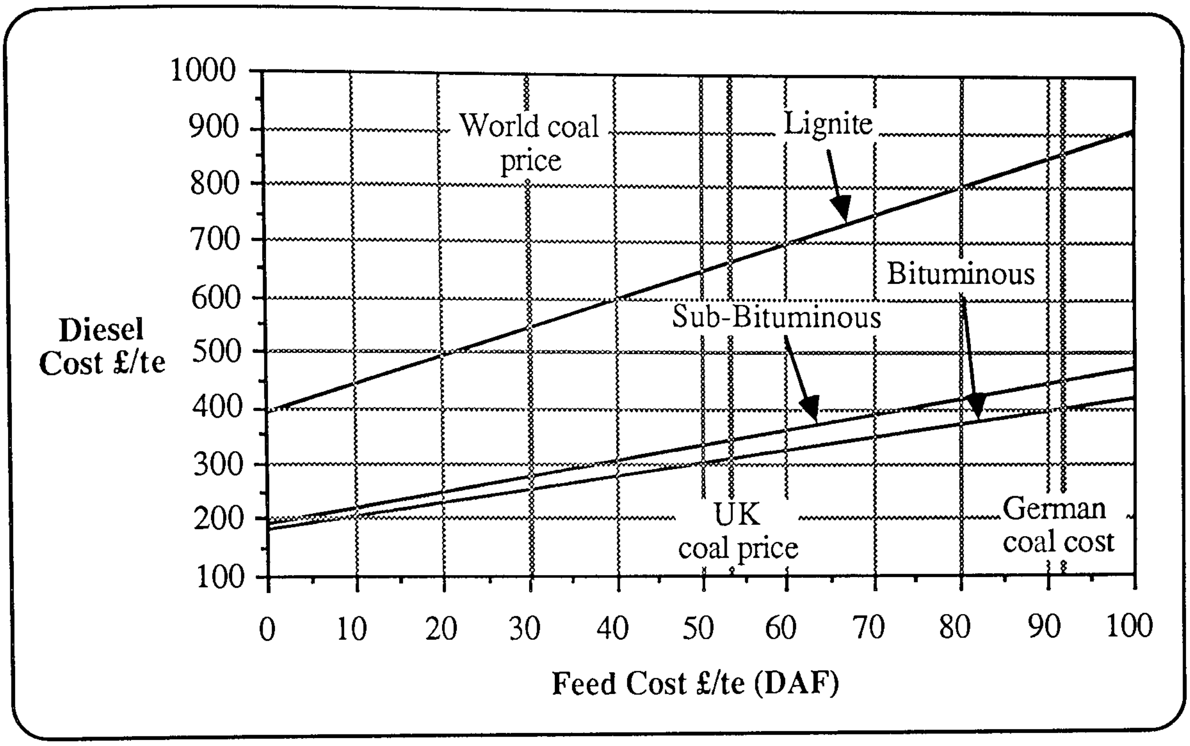

Figure 7.35 Diesel Costs, SMDS process, Texaco Gasifier

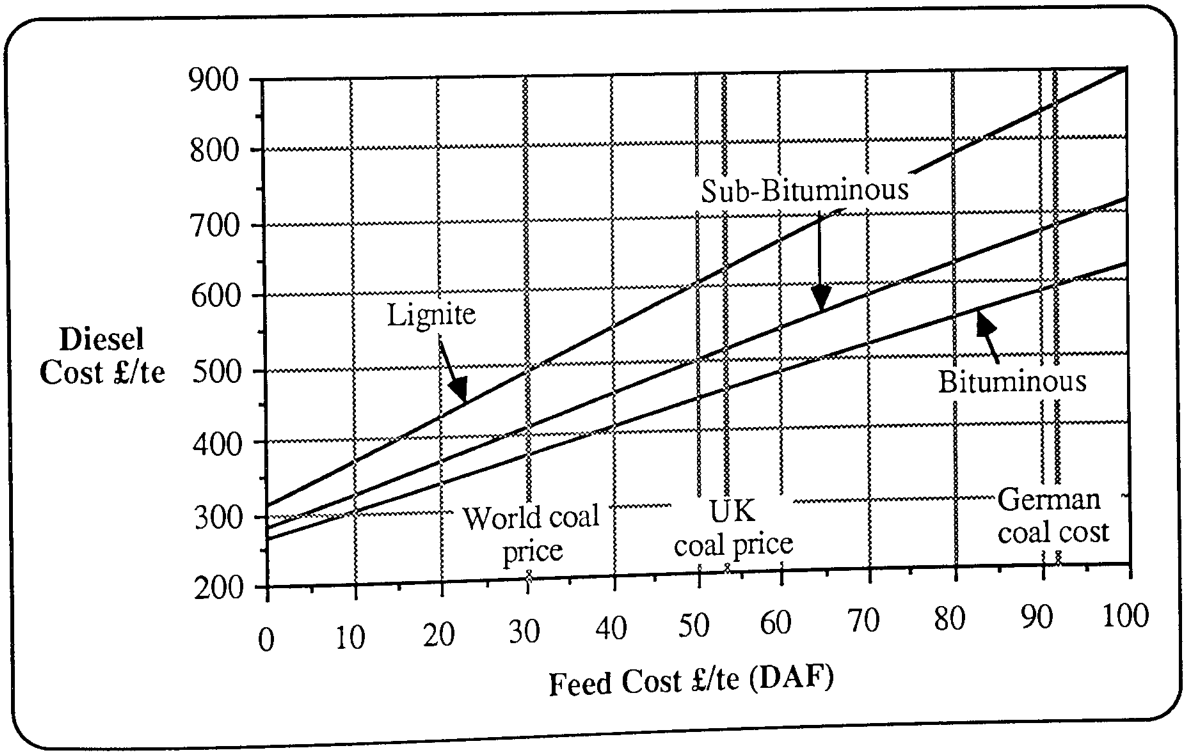

Figure 7.36 Diesel Costs, SMDS process, Lurgi Gasifier

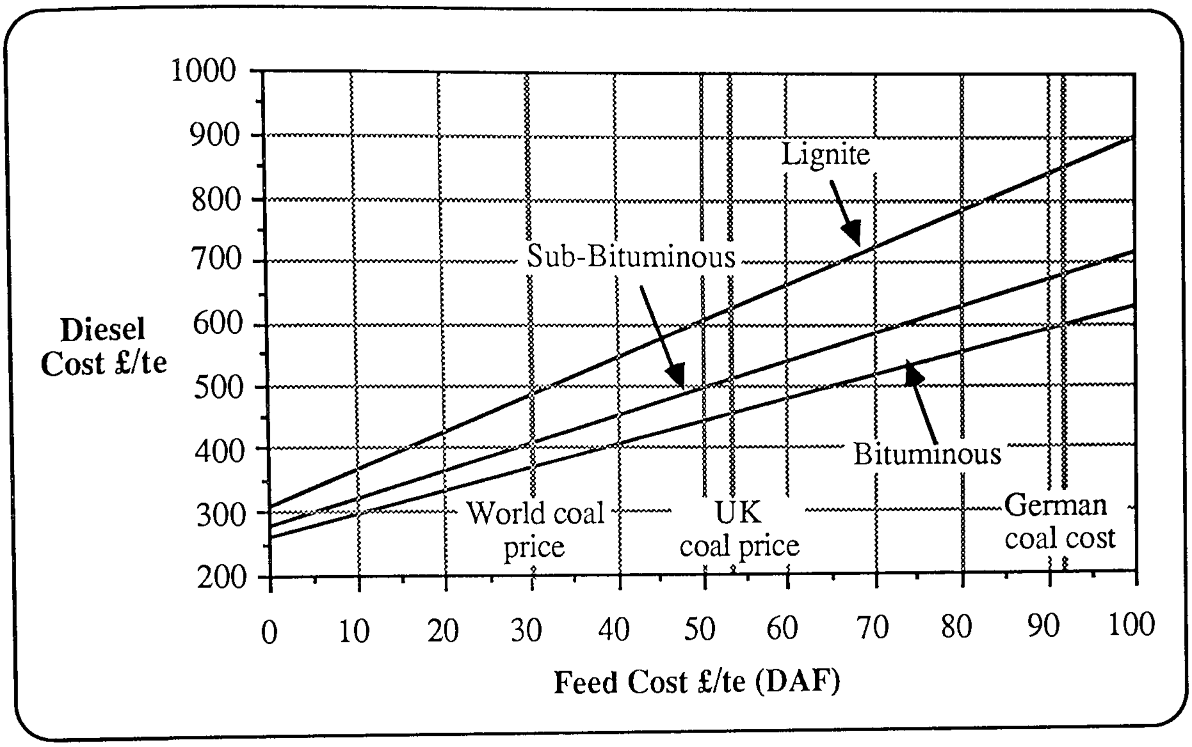

Figure 7.37 Diesel Costs, SMDS process, BGL Gasifier

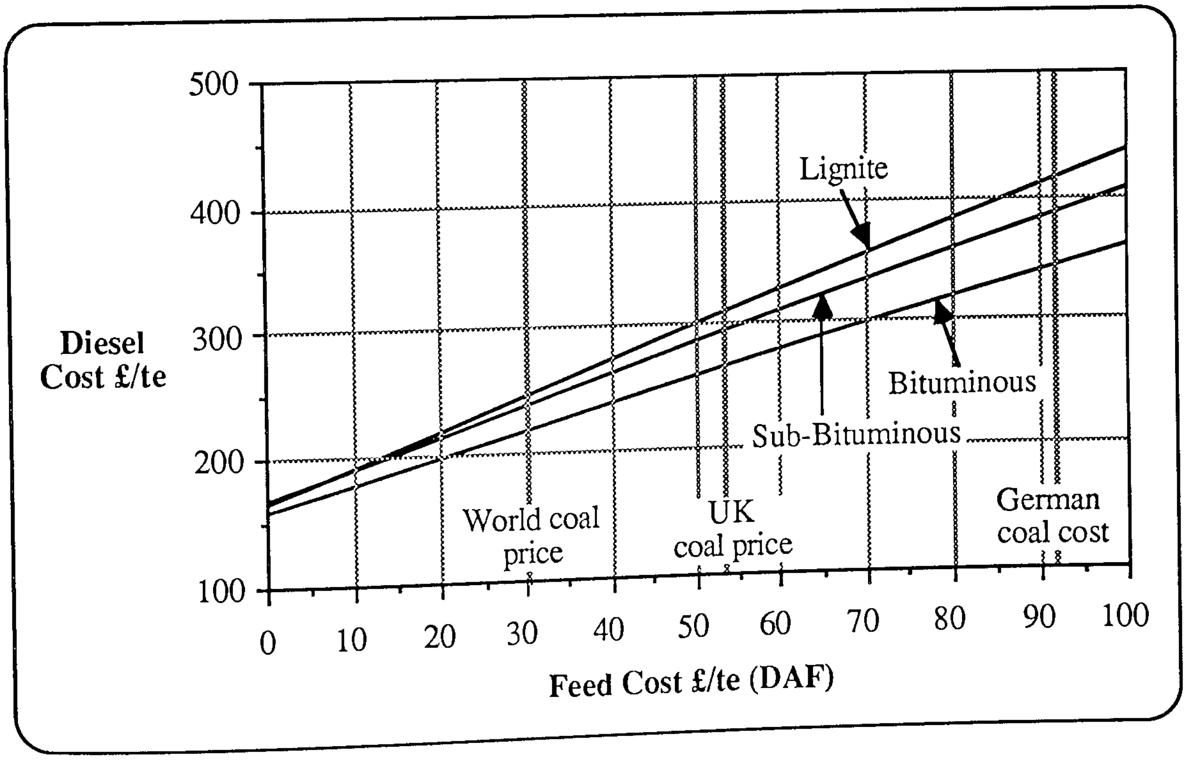

Figure 7.38 Diesel Costs, SMDS process, KRW Gasifier

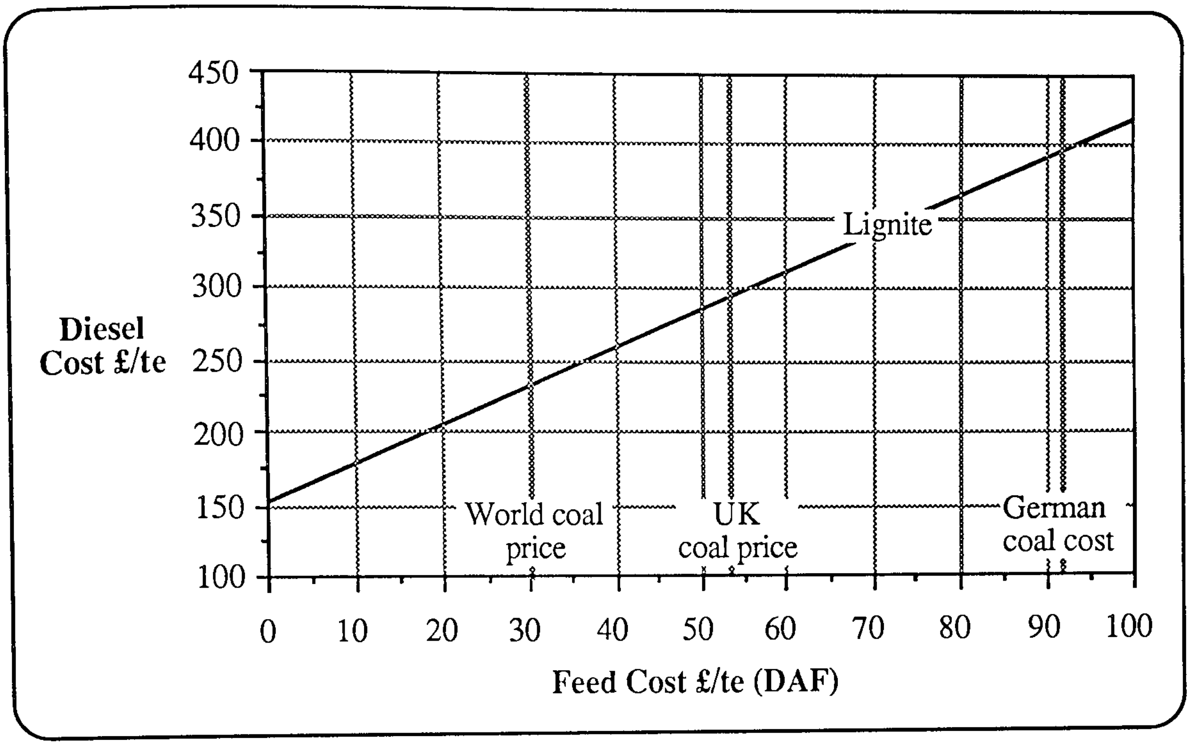

Figure 7.39 Diesel Costs, SMDS process, HTW Gasifier

Figures 7.41 to 7.45 show the cost of production of diesel, gasoline and fuel alcohol against feed cost for different gasifiers. In all cases the BGL gasifier is shown to give the lowest cost of production for each product. As discussed in section 7.5, this is due to a combination of low oxygen requirement and high thermal efficiency. The Lurgi gasifier has the highest production cost due to the unsuitability of the synthesis gas for conversion due to a high H_2 / CO content. With some feedstocks which allow operating conditions where less steam is required the Lurgi gasifier may produce a gas suitable for use in a methanol synthesis process, but the gas would be unlikely to have a low enough H_2 / CO ratio to be suitable in the fuel alcohol or SMDS processes. The results for the Lurgi gasifier are shown on the graphs for comparison only.

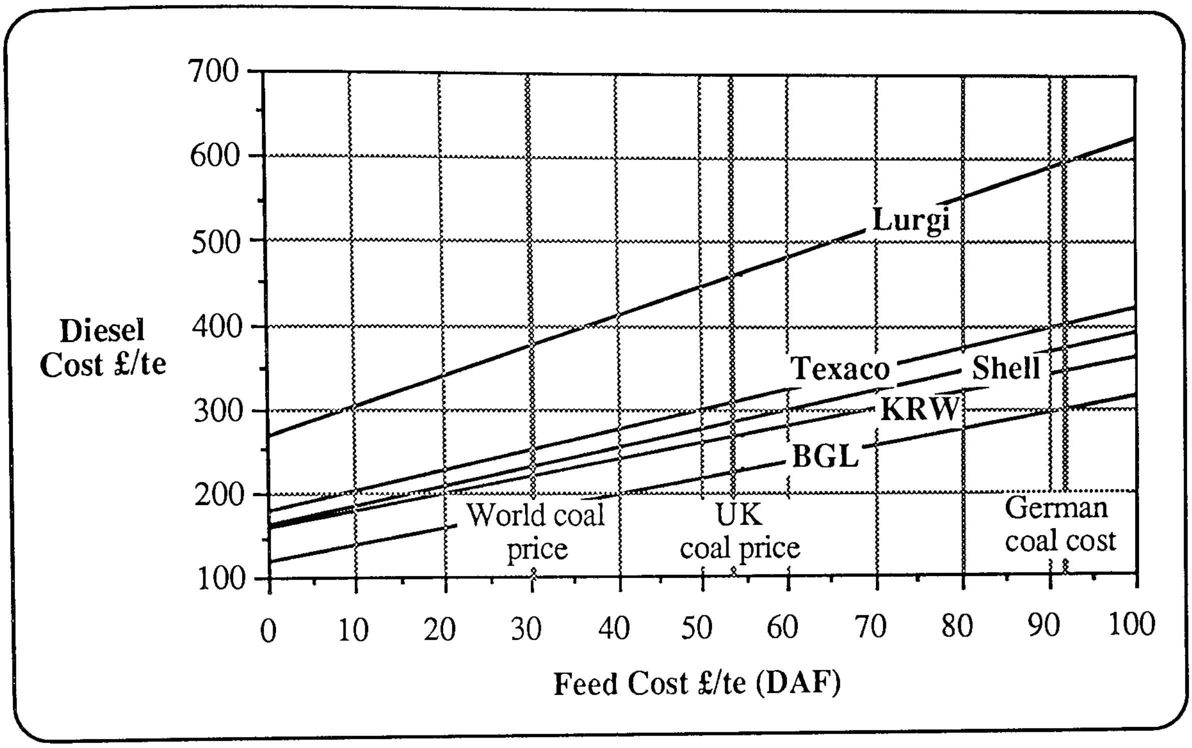

Figure 7.40 Diesel Costs, SMDS process, Alternative Gasifiers

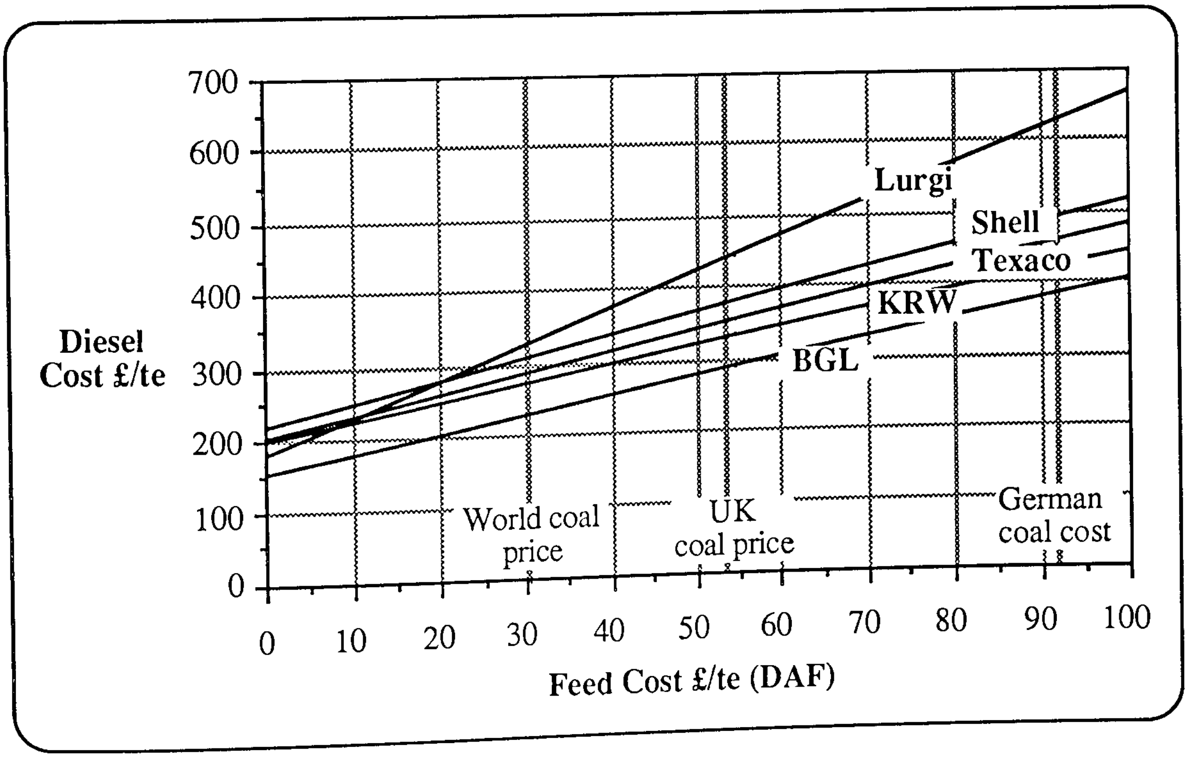

Figure 7.41 Diesel Costs, MOGD process, Alternative Gasifiers

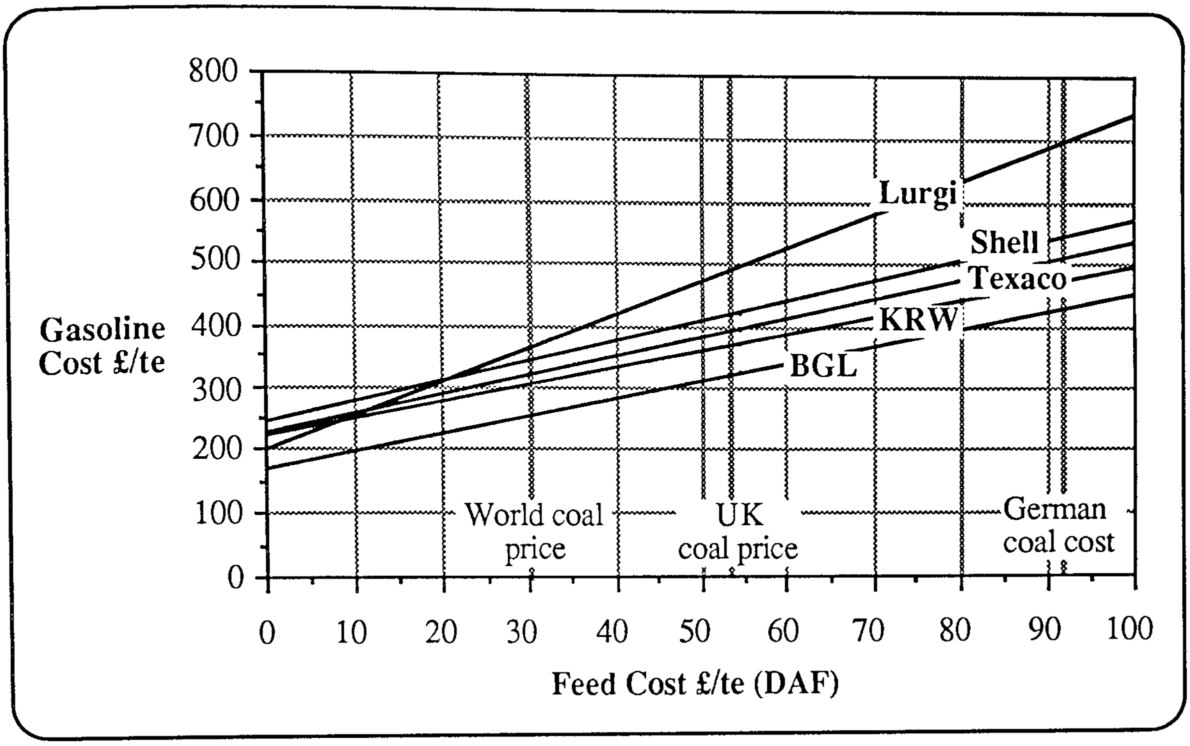

Figure 7.42 Gasoline Costs, MOGD process, Alternative Gasifiers

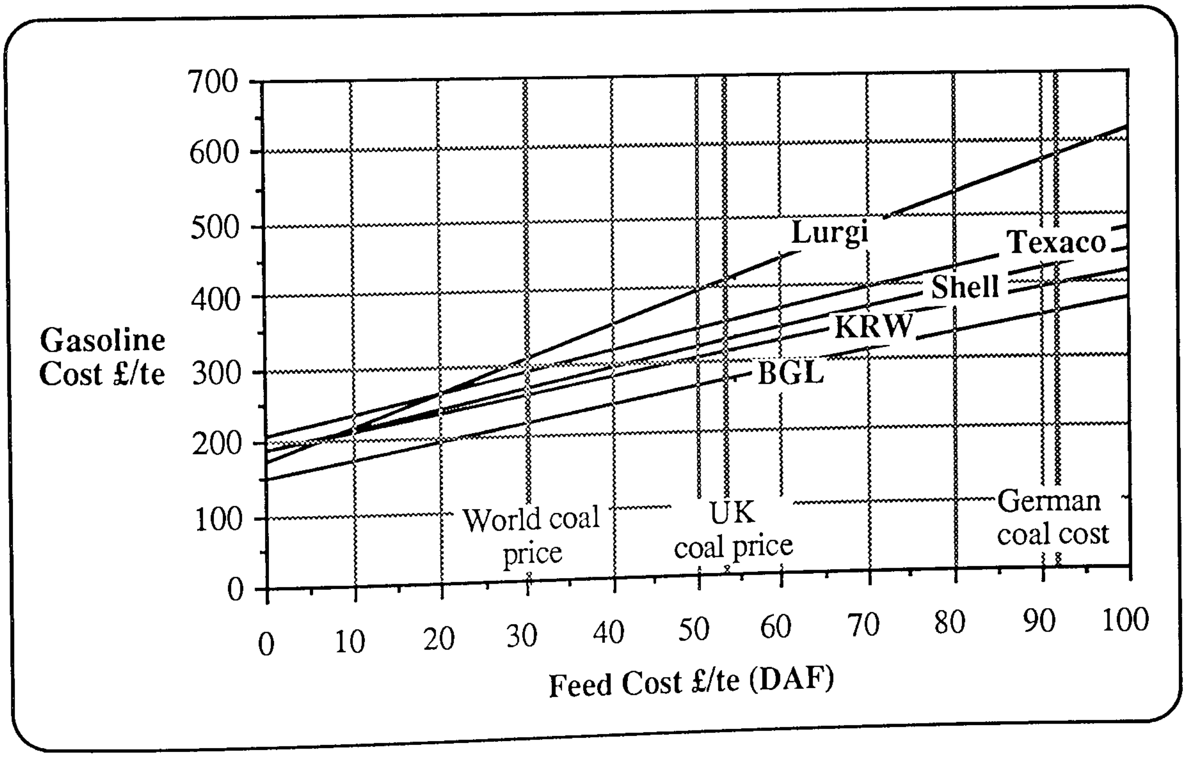

Figure 7.43 Gasoline Costs, MTG process, Alternative Gasifiers

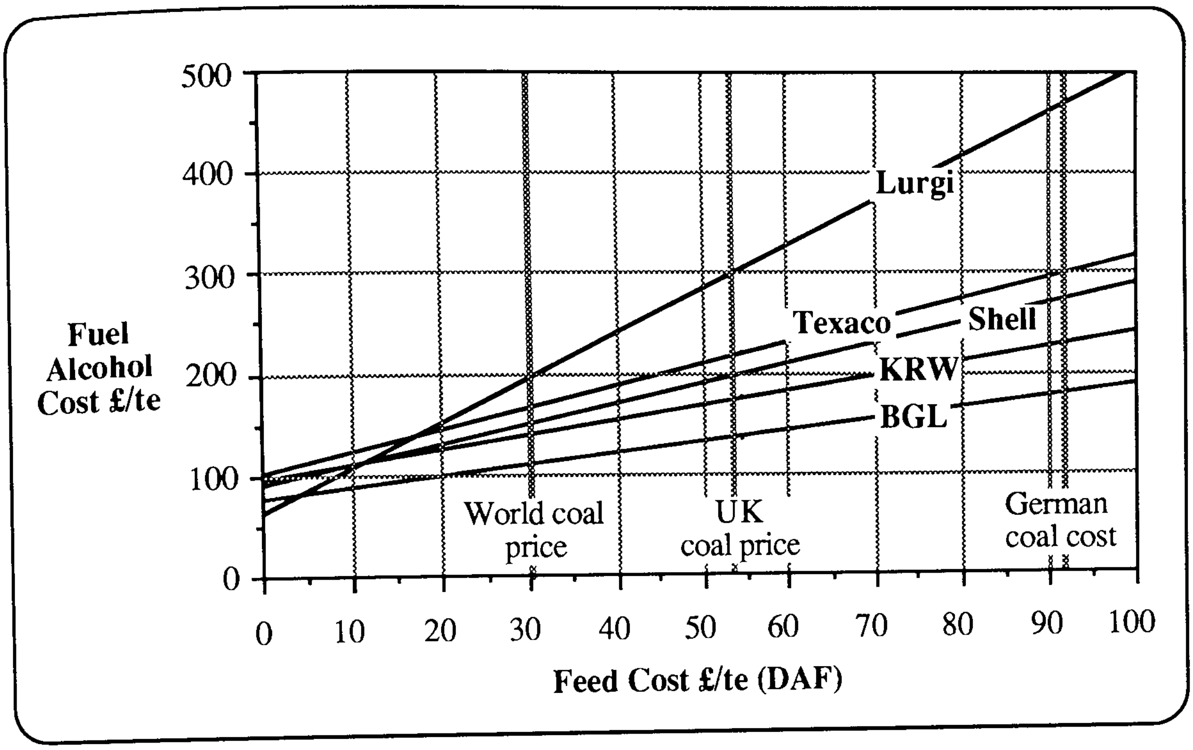

Figure 7.44 Fuel Alcohol Costs, Alternative Gasifiers

7.12 Economic and Utility Sensitivity Analysis

The base case values used in the results presented previously for the utility costs have been taken from a variety of sources and have been chosen to represent as realistically as possible the actual cost of these utilities in industry at the present time. The sources and explantions where required are discussed below.

The utilities are:

5 bar steam £/t	5.0
50 bar steam £/t	10.0
Process water £/t	1.0
Cooling water £/t	0.040
Fuel gas £/GJ	3.0
Hydrogen £/t	1500
Oxygen £/t	40.0
Power £/MW	30.0

The cost of steam is dependant on the cost of the energy used to produce it and the quantity used, Lurgi[1] recommended a cost of £5 / te for low pressure steam and £10 / te for high pressure steam as being reasonable, high pressure steam is normally assumed by them to be twice the cost of low pressure steam. The cost of process and cooling water depends upon the cost of the cost of make-up water and chemical treatment required. Power cost can be obtained from the local power company. Fuel gas can be costed on an energy equivalent basis to other fuels, a value of £3 / GJ was taken as typical. Hydrogen production cost depends upon the the method of production and the quantity of production. A value of 1500 £/te was taken as the cost of production as this represents the middle to higher production cost of hydrogen[129]. The cost of oxygen was taken as 40 £/te although the actual cost again depends on the quantity required, however at the quantities used for this study any economies of scale will be comparatively small. The figure was based on the cost of oxygen at atmospheric pressure and increased to assume a supply pressure of 35 bar[130].

From the above it can be seen that the values used for the utility costs, although close to the actual costs may be assumed to be approximate values only. It is therefore necessary to analyse the sensitivity of the model results to these parameters.

The economic parameters were chosen to be equivalent to the parameters used by British Coal and Ulster University in their respective studies of direct coal liquefaction. This was to enable the results of the indirect coal liquefaction model to be compared sensibly to the results of the direct coal liquefaction models. As the values chosen may not represent the real situation at any given time, eg inflation and interest rates which vary periodically, the effect of variations in these values should also be studied.

The sensitivity of the production cost of methanol, with variations of up to ±10% in the base case parameters as defined in Table 7.2, is shown in Figures 7.46 to 7.49. Figures 7.46 and 7.47 shows that the methanol production cost is most sensitive to the cost of the feed coal and the second most sensitive parameter is the availability of the plant. Figure 7.48 shows that of the utility costs the production cost of the methanol is most sensitive to the cost of the oxygen with the other utility costs having a comparatively insignificant affect on the product cost. Figure 7.47 shows the effect of utility costs on methanol production cost in greater detail, the effect of oxygen is not included to simplify the graph. In Figure 7.48 an increase in the cost of fuel gas is shown as having a negative affect on the product cost, this is due to the net production of fuel gas in the base case plant configuration and therefore an increase in the value of fuel gas lowers the overall utility costs.

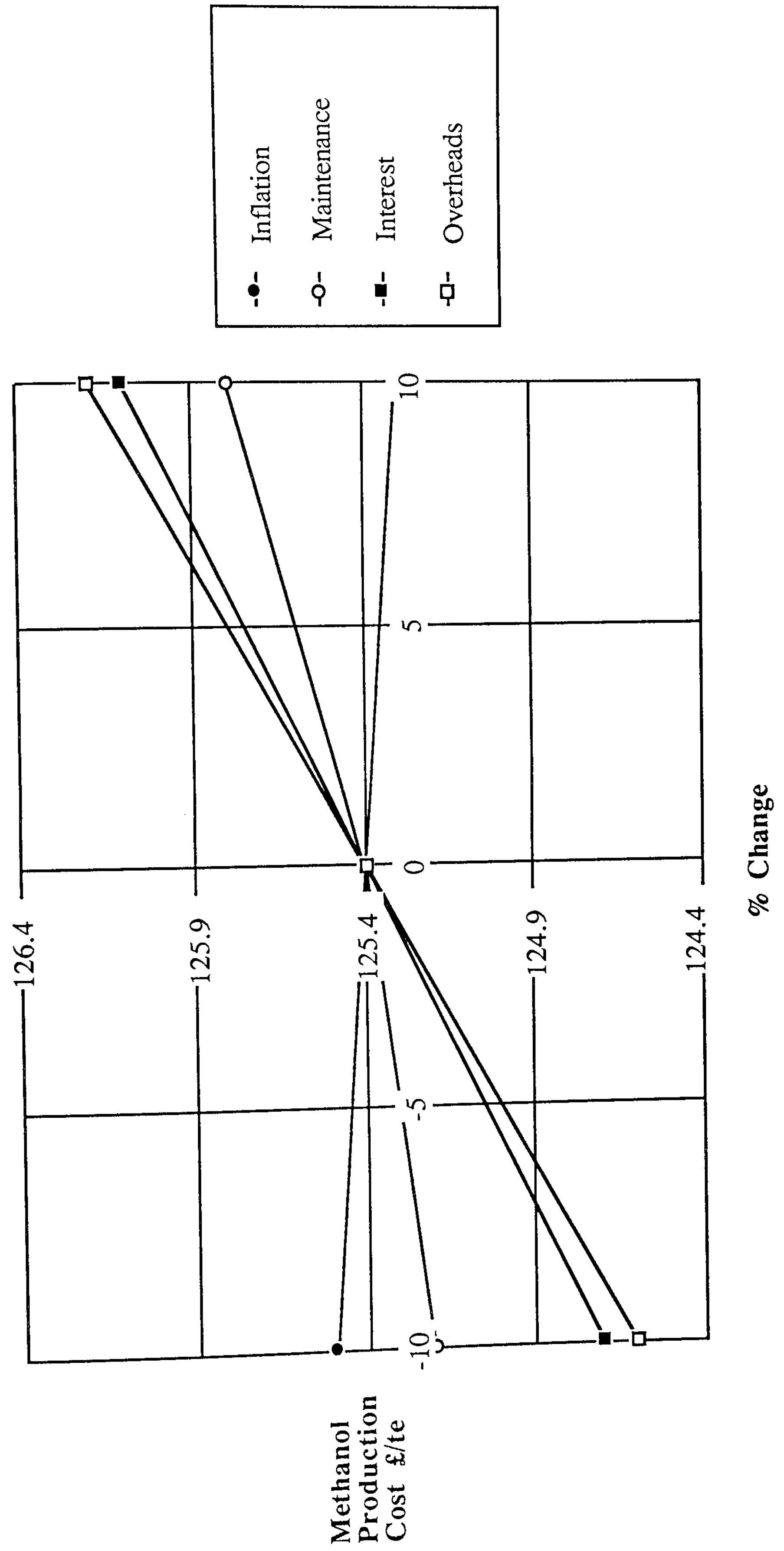

Figure 7.45 Effect of Economic Factors on Methanol Production Cost for Base Case

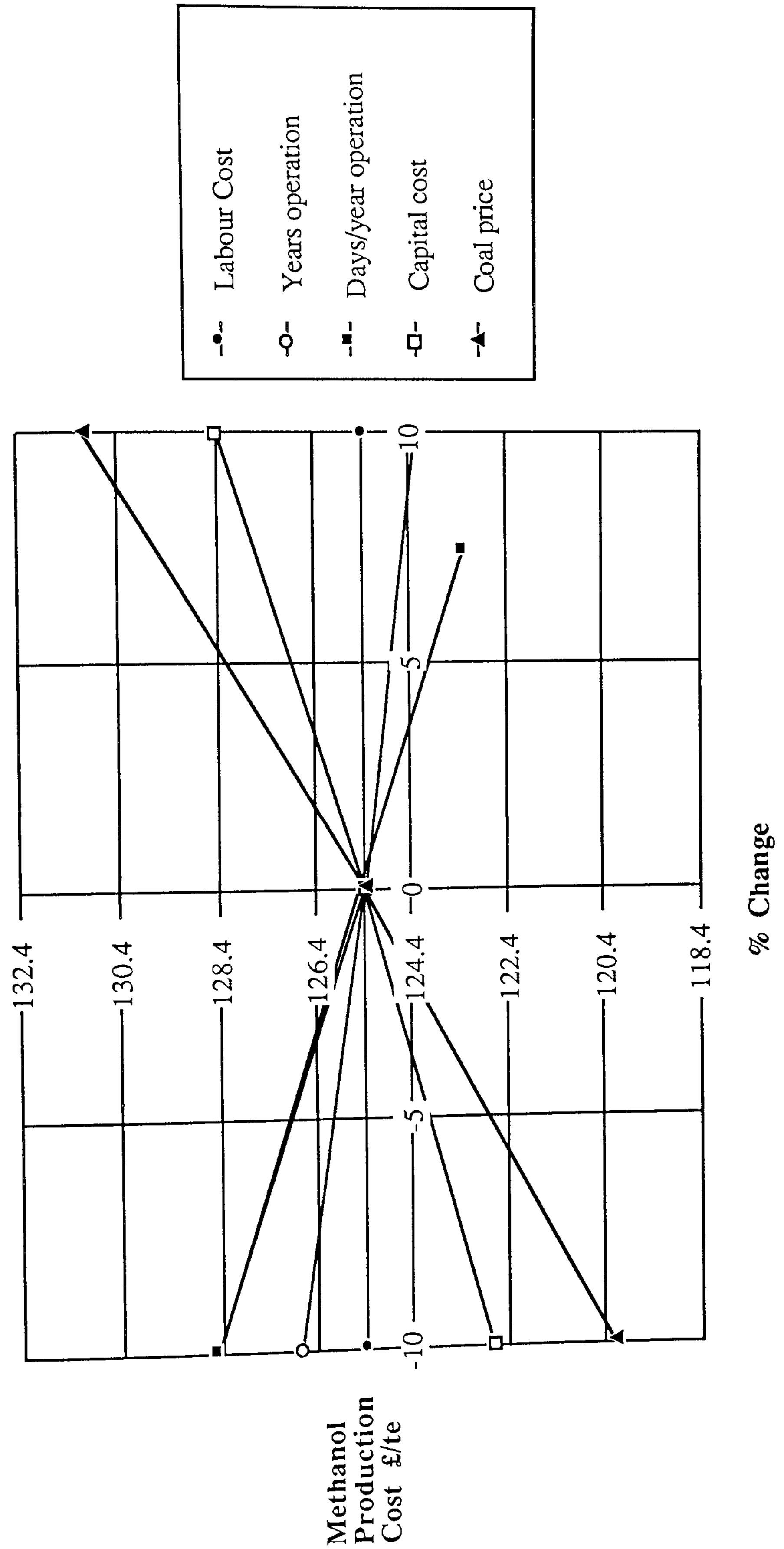

Figure 7.46 Effect of Economic Factors on Methanol Production Cost, for Base Case, Cont.

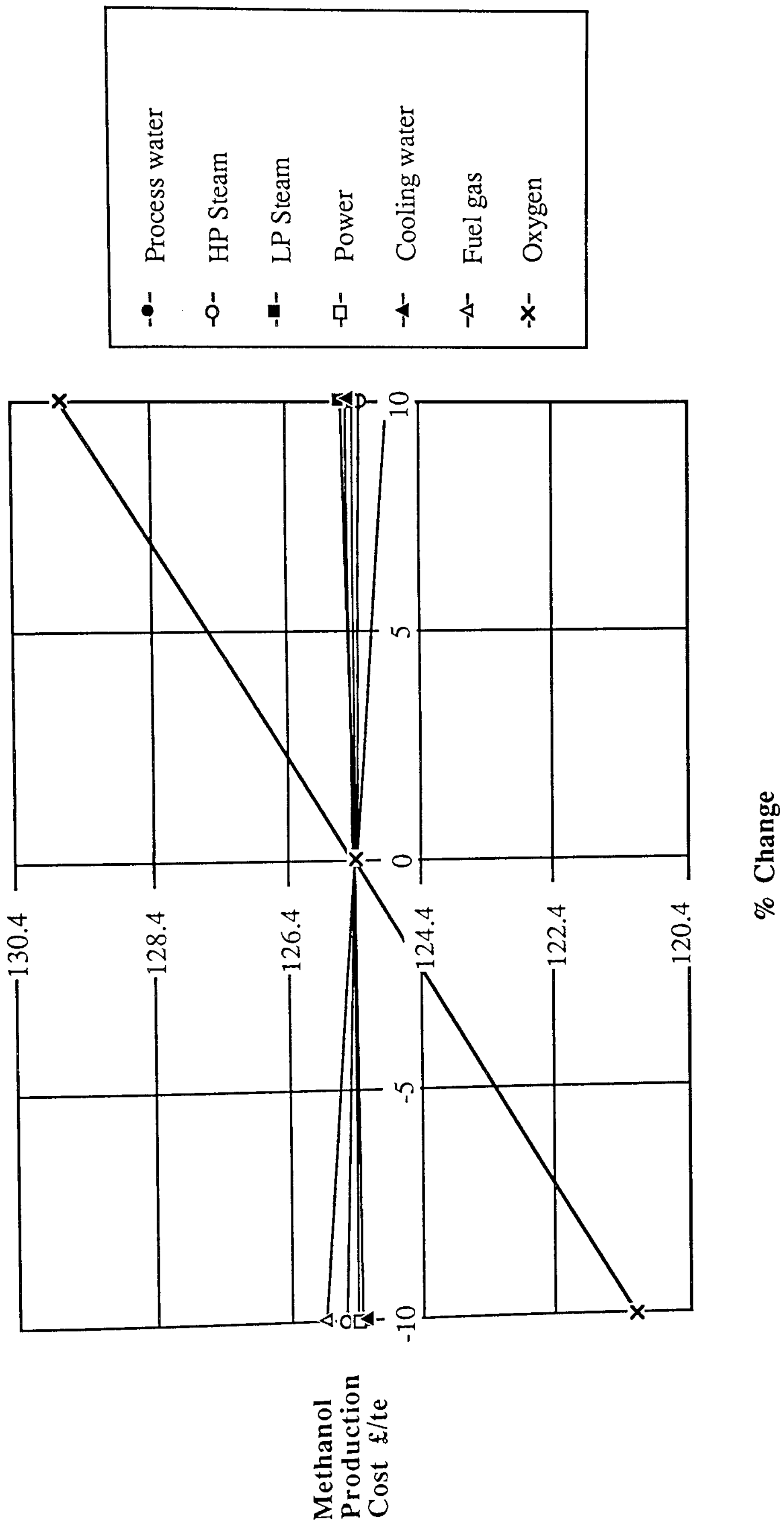

Figure 7.47 Effect of Utility Costs on Methanol Production Cost: Oxygen Effect

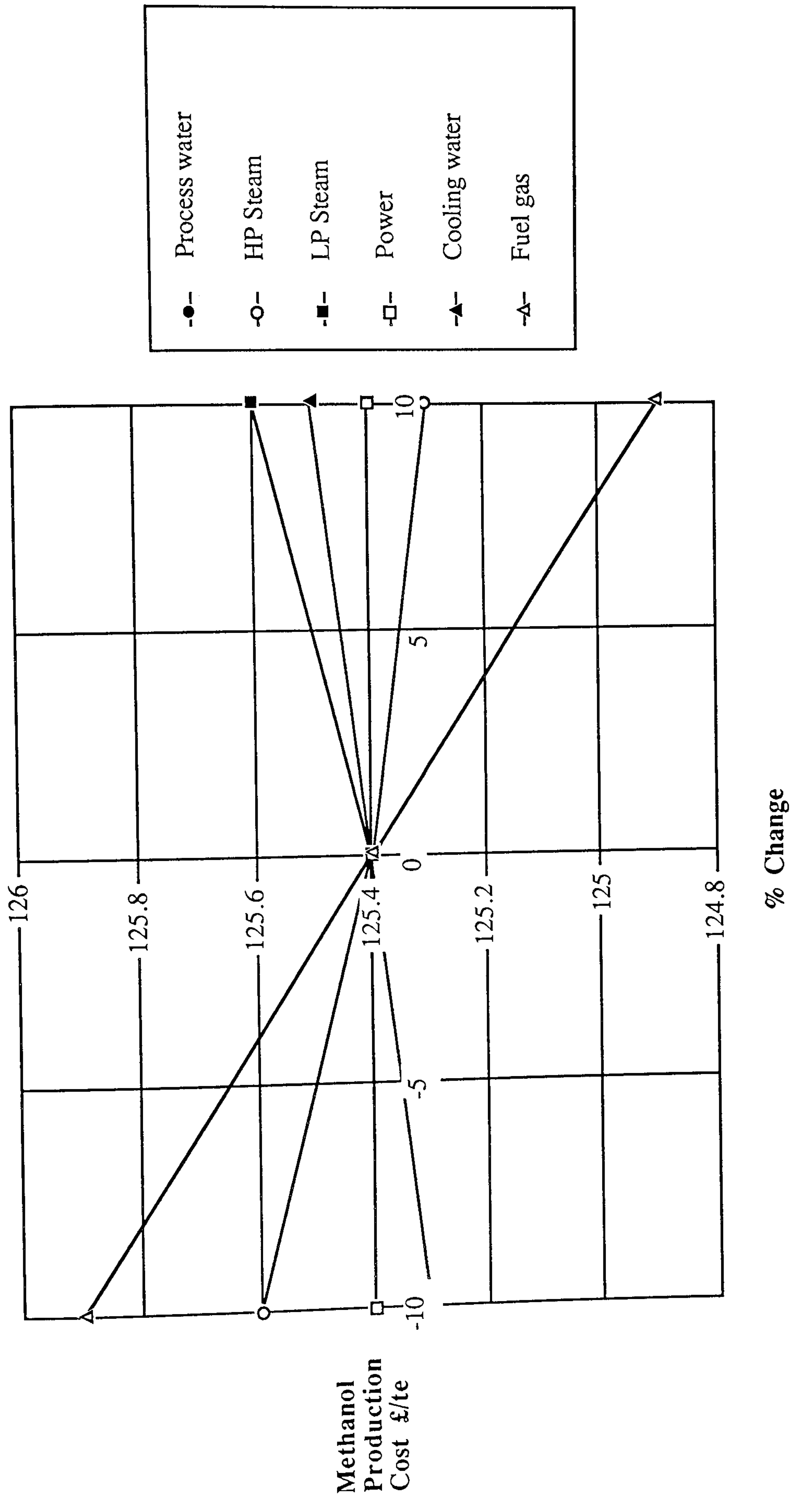

Figure 7.48 Effect of Utility Costs on Methanol Production Cost

7.13 Ideal Gasifier Case

The concept of an ideal gasifier can be proposed as that which produces the optimum or best attainable gas composition, for conversion to the desired product, at the lowest cost (minimum utility requirements). As this is a conceptual case it is assumed that for comparison purposes with other results that the capital cost of such a gasifier is taken as an average of the capital costs of all the gasifiers included in the model. This is assumed as the capital costs of the various gasifiers, included in this thesis, have been shown not to vary widely regardless of technology or design, as shown in section 5.7.

Depending on the particular end use of the gas a specific H_2 : CO ratio is desirable and minimum amounts of other compounds such as carbon dioxide and methane. If substitute natural gas where required as the end product, then methane would be desirable as the major constituent of the product gas, however this is not within the scope of this thesis. The ideal gasifier is therefore one which produces only CO and H_2 and uses a minimum amount of steam and oxygen to be thermally neutral.

As the product gas can never contain more hydrogen than carbon monoxide without shifting the carbon monoxide to carbon dioxide, then an ideal gasifier for the processes under consideration can assumed to be one which produces the maximum H_2 : CO ratio and converts all the carbon in the feed to carbon monoxide. This does not allow for equilibrium of the gases to occur and is therefore a practically unobtainable ideal, but represents the best possible case to which all gasifiers may be compared.

For the processes included in the modelling a H_2 : CO ratio of between 1.5 (fuel alcohol) and 2.1 (methanol) is required as defined by the process requirements described in sections 3.2 to 3.5. It can be shown that for a coal composition which contains C : H of 1 : 1 (Point of Ayr is 1 : 0.81) which is approximately true for many bituminous coals, the maximum H_2 : CO ratio obtainable, producing only CO and H_2 in the product gas, from a feed of H,C,O,O2 and H_2O is less than unity. Higher H_2:CO ratios are obtained if part of the CO is shifted to CO_2 in the gasifier but this requires the use of either additional oxygen, steam or both and is economically and thermally less efficient than the ideal case defined above.

Sulphur in the feed is assumed to go to hydrogen sulphide similar to the real gasifiers included in the model.

The gas produced from the gasifier is calculated based on the following assumptions:

- All sulphur is converted to hydrogen sulphide;
- All carbon is converted to carbon monoxide;
- All hydrogen is converted either to hydrogen gas, or hydrogen sulphide;
- All the oxygen is utilized in producing carbon monoxide;
- Only steam and oxygen are available as gasifying agents, (CO_2 could also be used);
- A minimum amount of oxygen and steam is used to gasify the coal;

- The exothermic and endothermic reactions must balance.

The last assumption of thermal neutrality is unobtainable in practice as the the rate of reaction of the gasification reactions becomes too slow at lower temperatures for a practical gasifier, it does however represent the highest efficiency possible for this system.

The following reactions represent those used in the calculation for the combustion and steam gasification of carbon respectively:

$C + 1/2\, O_2 <=> CO$	$\Delta H = -26.4$	eq 7.1
$C + H_2O <=> CO + H_2$	$\Delta H = 32.2$	eq 7.2

Although both reactions are equilibrium reactions, for the purposes of the present discussion the equilibrium position of the reactions is such that complete conversion of the carbon to carbon monoxide may be assumed. If the fractional conversion of carbon to carbon monoxide by equation 7.1 is represented by X and that by eq 7.2 by Y then thermal neutrality is represented by:

$$-26.4 * X + 32.2 * Y = 0$$

where $X = 1-Y$

therefore $Y = 0.82\, X$

Hence overall the reaction with carbon as the feed is:

$$1.82\, C + 1/2\, O_2 + 0.82\, H_2O \text{ --> } 1.82\, CO + 0.82\, H_2$$

With coal as the feed with composition CH the reaction is:

$$1.82\, CH + 1/2\, O_2 + 0.82\, H_2O \text{ --> } 1.82\, CO + 1.73\, H_2$$

This analysis neglects the heat required to dissociate the hydrogen from the coal and is therefore approximate.

- The H_2 : CO ratio in the product gas is 0.95 : 1.
- Oxygen required for gasification is 0.275 te / te dry ash free coal.
- Steam required for gasification is 0.45 te / te dry ash free coal.

Figure 7.49 show a comparison of methanol production costs for several gasifiers and the Ideal gasifier model. The Ideal gasifier model gives the lowest methanol production cost which is explained by the higher carbon conversion efficiency obtained with the improved gas composition of the gasifier. As shown in Figure 7.49 the carbon conversion efficiency is much higher than that of the other gasifiers, giving a greater conversion of feed coal to product methanol.

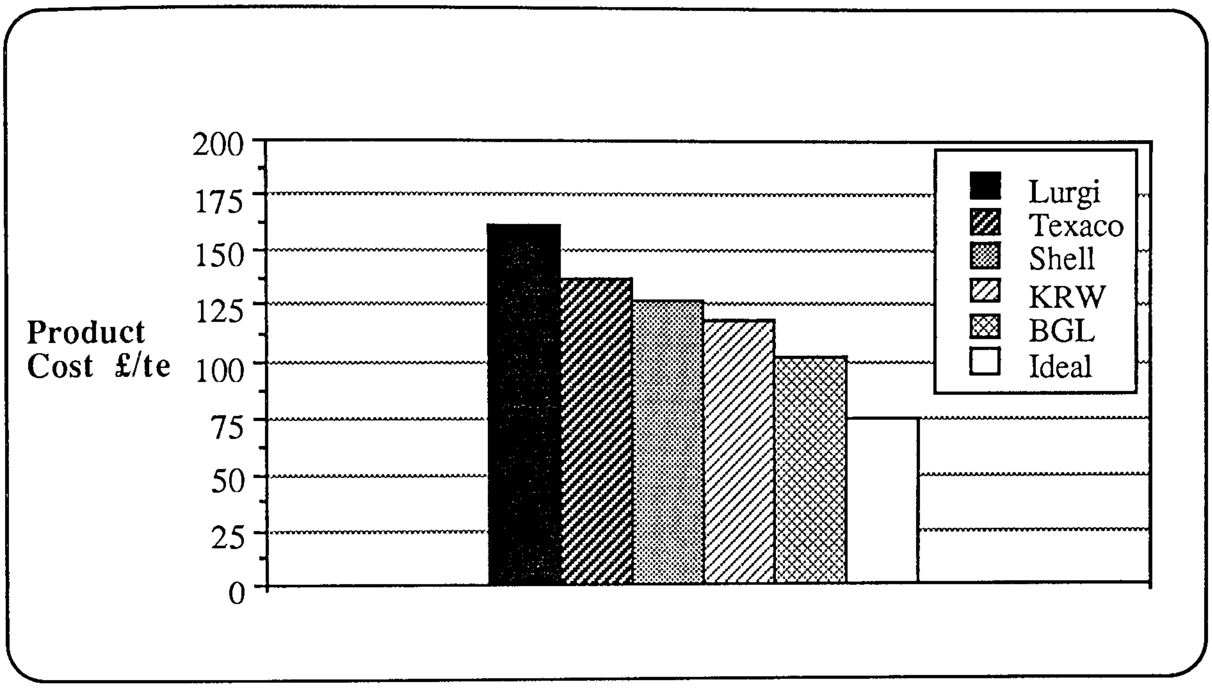

Figure 7.49 Product Cost of Methanol with Ideal Gasifier Compared to Other Gasifiers

The lower conversions obtained for the other gasifiers are due to the poorer composition of the gas for feed to the methanol plant. The reasons for the poorer gas quality vary according to the gasifier technology as follows:

- The Lurgi gasifier produces a gas composition of too high a H_2 : CO (>2:1) because of the large steam requirement in the gasifier for temperature control. An excess of H_2 is produced by the gasifier by shifting the CO to CO_2 and therefore part of the feed carbon is lost as CO_2. It is possible that CO_2 could be fed back to the gasifier, however this is beyond the scope of this thesis. Tars and oils are produced and sold as by-products hence some feed carbon is also converted to by-products and lost.

- The Texaco gasifier produces mostly CO, H_2 and CO_2, oxygen is used as the gasifying agent and the large water content of the slurry provides steam for gasification and equilibrium reactions. Due to the low residence time of the coal in the gasifier the gasifier operates at high temperatures and therefore excess oxygen (compared to the ideal gasifier) is used and less steam or moisture. Therefore, although hydrogen is produced by the steam/carbon reaction it is a comparatively small amount compared to the ideal case and the rest of the hydrogen required for methanol synthesis is produced by the water gas shift reaction, either in the gasifier or in the shift unit. This produces CO_2 and therefore part of the feed carbon is lost as CO_2.

- The Shell gasifier produces mostly CO and H_2 with small amounts of CO_2, however essentially only oxygen is used as the gasifying agent with very little if any steam (some residual moisture is in the feed). Very little hydrogen is produced by therefore by reaction of steam with carbon and the excess energy produced by gasifying with large amounts of oxygen is lost as hot product gas. The gasifier is marginally more efficient than the Texaco gasifier because less heat is lost in the product gas due to its lower steam content, therefore more of the energy produced leaves the gasifier as chemical energy rather than thermal energy.

- The KRW has a lower product cost and higher carbon conversion than the previous gasifiers as more steam is used in the gasification reactions to reduce the temperature and in the gasification reactions, producing more hydrogen as a result. The exit temperature of the gas is lower than the previous gasifiers and therefore more energy is utilized in gasification of the coal by the action of the steam.

- The BGL gasifier has the lowest production cost of the real gasifiers considered due to its lower oxygen consumption and countercurrent operation which allows a large portion of the heat in the product gas to be reclaimed by the incoming cold feed. Therefore, more energy leaves the gasifier as chemical energy rather than in the enthalpy of the gases. Also the gasifier produces methane and higher hydrocarbons which are converted to synthesis gas by steam reforming which produces a gas with a high hydrogen content. Methane production (5% of the product gas) in the gasifier followed by steam reforming of the recycle stream from the methanol plant is shown in the next section to lower the methanol production cost. The carbon conversion efficiency is slightly reduced compared to the KRW gasifier due to the production of by-product tars and additional losses in the steam reforming section of the plant.

The ideal gasifier therefore gives an ideal to which practical gasifiers producing gas for methanol production should aim for. The criteria for gasification technology improvement are as follows:

- The oxygen consumption should be as low as possible to reduce costs;
- As much as possible of the gasification reactions should be performed by steam, however large amounts of excess steam may produce too much hydrogen by the water gas shift reaction;
- The gas exit temperature should be low, with the heat being used inside the reactor for gasification;
- Methane appears to be advantageous in the gas as it produces a gas of high hydrogen concentration when steam reformed, this appears to offset the cost of steam reforming.

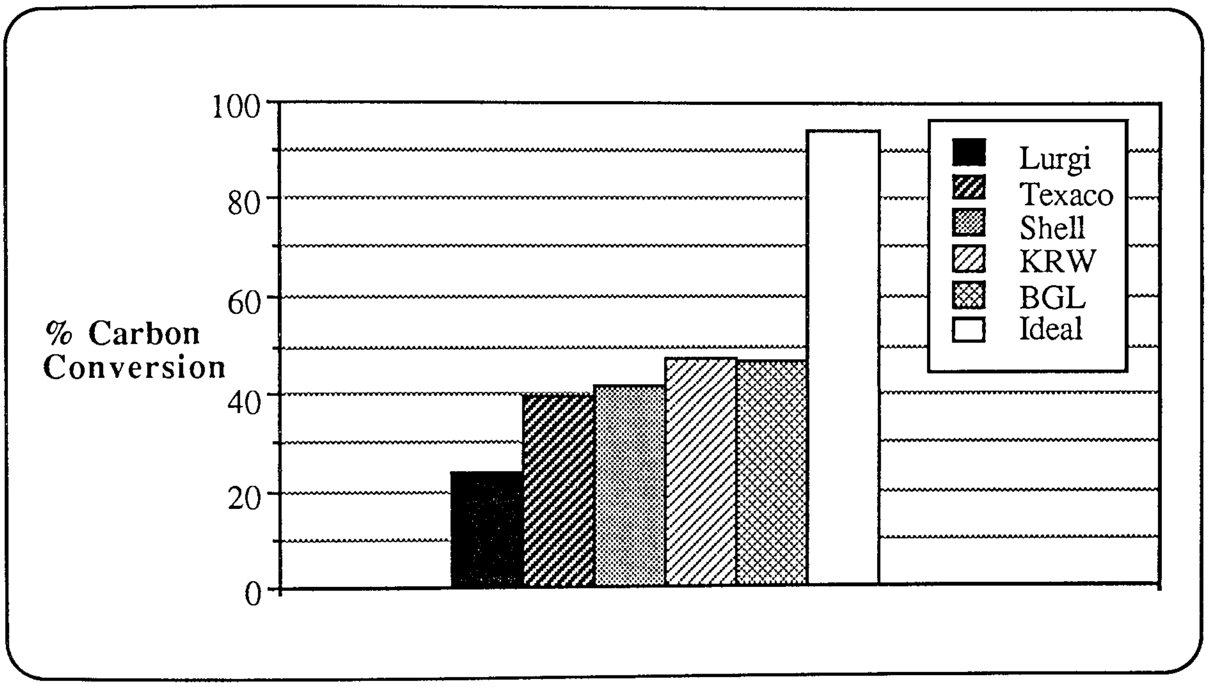

Figure 7.50 **Carbon Conversion to Methanol with Ideal Gasifier Compared to Other Gasifiers for Base Case**

7.14 Methane Effect On Product Cost

In order to assess the effect of increasing methane concentration on product cost the base case of shell gasifier and methanol synthesis plant was modified by adding 5 % methane to the product gas from the gasifier (and adjusting proportionally the other gases). Two cases were studied, firstly the methane was allowed to escape in the purge gas stream and sold as fuel gas and secondly the methane was steam reformed in the recycle stream and fed back to the CO_2 section of the plant. The results are shown in Figure 7.51 where it can be seen that allowing the gas to be credited as fuel gas marginally increased the cost of production of the methanol compared to the base case of no methane production, due to a lower conversion to methanol. Steam reforming the methane decreased the methanol production price by 3 £/te. Therefore it can be seen that the added cost of the steam reforming plant is more than offset by increased methanol production. The increase in methanol production is attributable to the increase in hydrogen production by steam reforming the methane.

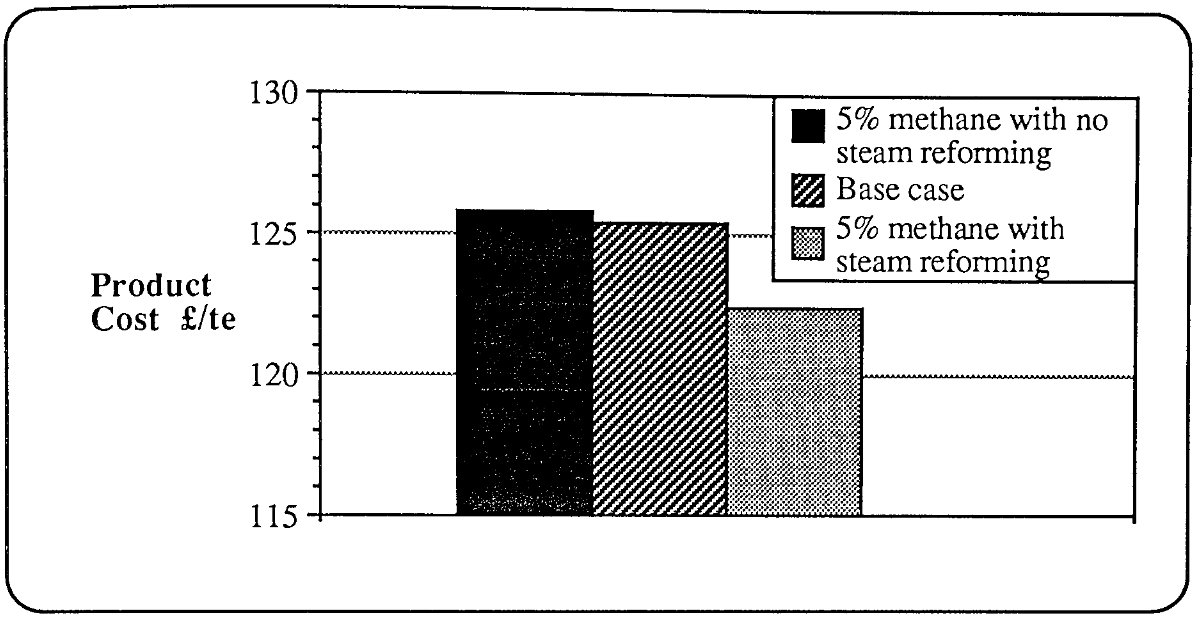

Figure 7.51 Effect of Methane Concentration On Base Case Product Cost

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CHAPTER 8
CONCLUSIONS

A computer model has been developed which has the ability to model a wide range of gasification processes, gas conditioning steps and synthesis gas conversion processes. The results of the model have been verified by comparison with published information and consultation with relevant authorities in the gasification and synthesis gas conversion industries. The hydrocarbon producing processes (SMDS, MTG and MOGD) were found to be uneconomic under current conditions in Europe with coal as the feedstock. The oxygenated hydrocarbon processes (methanol and fuel alcohol) however could be competitive provided that these products could be marketed effectively, and that traditional hydrocarbon based transport fuels can be displaced.

The basic parameters of coal type, throughput, choice of gasifier and choice of synthesis process, has the following effects on the overall conversion of feed to liquid product:

8.1 Coal type

The choice of coal type (bituminous, sub-bituminous or lignite) has considerable effect on product cost. This is in part due to the lower energy content of the lower rank coals per dry ash free tonne, which gives a lower conversion to product per tonne of feed. Also the lower rank feeds in general contain more ash and water than higher rank feeds which gives a lower efficiency in the gasifiers due to the loss of energy required to evaporate the water content of the feed and the heat lost with the removal of the hot ash. This is true also of gasifiers fed with a slurry as in general lower rank coals require a higher percentage of total water in the slurry.

8.2 Throughput

For the base case, economies of scale are significant up to a throughput of about 5000 te/day of feed, with the product price dropping by approximately 10 %, from 138 to 126 £/te. Between 5000 te/day of feed and 30000 te/day of feed the product price drops by only about 2 %. This is due to the use of multiple trains of both gasifiers and methanol synthesis process at throughputs of more than 2000 te/day of feed for the gasifier and 3000 te/day of methanol product for the methanol synthesis process.

8.3 Gasifier

The Shell gasifier was chosen as the base case due to its ability to handle virtually any coal. It was found not to give the lowest cost of production due to relatively high oxygen requirement and lower cold gas thermal efficiency than the most efficient fixed or fluidised bed gasifiers. The British Gas / Lurgi gasifier was found to give the lowest production cost for all cases, due to high thermal efficiency of the gasifier and low oxygen requirement per tonne of feed coal.

This comparison is not directly applicable to power generation using Integrated Gasification Combined Cycle (IGCC) plants as the High pressure steam produced by entrained flow gasifiers when the gas is cooled is of relatively higher value and usefulness than in a liquid fuels synthesis plant.

For the production of liquid fuels from coal the British Gas / Lurgi gasifier appears to give the most economical option, due to the lower oxygen and steam requirements for gasification and high cold gas efficiency due to the countercurrent nature of operation which recovers sensible heat form the output gas by heating the incoming coal. However this needs to be offset against a process which is more complex than other types of gasifiers that do not produce tars, oils or phenols as by-products. The gasifier can only handle large amounts of coal fines provided additional processing to produce briquettes or to agglomerate the fines is included. Also entrained gasifiers can be made larger in a single train than can a fixed bed gasifier and entrained flow gasifiers can in principle accept virtually any type of coal or lignite whereas some coals may present problems in fixed bed gasifiers[117].

8.4 Synthesis Process

The methanol synthesis process gave the lowest production cost per tonne and per GJ of product. The process has several advantages when compared to the other processes included in the model. The process has high conversion to product with very high selectivity and in one stage. The other processes are either in more than one stage, giving a higher capital cost (MTG and MOGD processes) or produce other products or by-products (Fuel Alcohol and SMDS) such as methane and higher hydrocarbons which have a lower value per GJ than liquid fuels, and recycling of these gases requires additional plant items and reduces the overall energy conversion of the processes. This does not take into account the relative usefulness of the products and assumes that a GJ of energy in methanol is equally as useful as a GJ of energy in gasoline for example.

Although alcohols are the most attractive fuels to produce in terms of cost of production and potential efficiency gains in use in engines, they are not an established transport fuel in Europe and would require a new marketing infrastructure. Countries such as Brazil, however, have successfully switched part of their transport fuel needs to alcohol (ethanol) through political and fiscal incentives. It is likely that the most immediate use of alcohols, as fuels, would be as gasoline / alcohol mixtures.

8.5 Economics

For the traditional hydrocarbon fuels, it appears from the results presented in Chapter 7, section 7.8 that production from cheap imported coal would not be economically viable unless Brent crude prices were consistently, significantly over 30 $/bbl or higher.

For oxygenated fuels the economics are more favourable, with methanol and fuel alcohol production from coal comparing favourably with traditional transport fuels. However, considerable changes in the energy distribution and usage patterns would be necessary before alcohols could provide a significant percentage of Europe's transport fuel usage. If alcohols produced from coal provided significant amounts of Europe's transport energy requirements then far reaching effects would be felt in the traditional oil industry. These would be due to a reduction in the value of gasoline and gasoil due to excess capacity. The price paid for crude oil would then have to drop significantly to sustain refining margins or significant amounts of the Naphtha/Gasoil fractions would have to be converted to alternative products such as kerosine or aromatic chemicals. Whatever the actual scenario the effect of large scale methanol fuel production would be far reaching and difficult to predict.

CHAPTER 9
RECOMMENDATIONS

9.1 Future Work

The recommendations are divided into two categories, those dealing with the computational aspect of the thesis and those dealing with the modelling of the processes.

9.1.1. Computational Recommendations

Any further developments of the computer model should be made on a selected computer and operating system. It is recommended that an IBM PC is used for this purpose for the following reasons:

- Specific features of a particular operating system can be used by the program to provide better interfacing of the program with the user.

- The use of main-frame computers for program development is unlikely to provide benefits, either in terms of programming effort, program portability or ease of use of the program.

- The original idea of producing a program that can be transferred between different operating systems without modification is not practical as compilers for personal computers rarely conform completely to a particular standard.

- The coal conversion modelling source code was adapted to work with an Object Oriented Compiler on the IBM PC and Apple Macintosh Computers. There are computational advantages in maintaining the source code as an object oriented program as discussed in Chapter 4.

Further modifications to the model should include:

- Modification of the main executive program to handle recycle loops, this should not be computationally difficult to perform although achieving a rapid rate of conversion for the recycle streams may be mathematically complex. This should be performed to enable the main synthesis gas conversion steps to be broken down into smaller sections, providing more flexibility in process configurations, and simplifying the possible addition of additional process units.

- The main program should include a routine to explain and modify the input datafiles when and if required.

- In the current version of the model the cost of the utilities are included as a unit cost, for example £ / KWh for power or £ / te for steam. The costs chosen for these values are intended to include all the production costs associated with the particular utility used. The costs of the utilities which require a significant amount of energy in their production are therefore based on current energy costs. The model should be made more consistent by including the capital costs of the plant items required for the utility production and taking a percentage of the feed coal as the feed for the utility production. This would allow the cost of the utilities to vary with the cost of the feed coal and make the model internally more consistent.

- The input of process steps could be performed more ergonomically on a graphical basis by using Icons and the mouse pointer to select options, as opposed to the use of menu driven inputs.

9.1.2. Modelling Recommendations

9.1.2.1 Gasifier models

Improvement of the gasifier model predictions for gas composition are unlikely to improve in a significant manner for the majority of the gasifiers. However some significant improvement is possible for the fixed bed gasifiers, where prediction of the composition and quantity of tars and methane produced is difficult and subject to uncertainty. This would require understanding of the detailed mechanisms involved in the breakdown of the chemical components of the coal under gasifier conditions and is likely to be beyond the scope of any gasifer model aimed at economic modelling. It is recommended that further detailed gasifier model development (with the possible exception of slight modifications) is not performed for the present economic modelling package. However, a detailed mathematical model could be developed to examine the non-steady state behaviour and also to predict gasification rates of specific gasifiers with different feedstocks. This would require well developed differential mathematical ability and would be costly in terms of time invested.

9.1.2.1 Fuel Alcohol Model

The fuel alcohol model is based on limited data which may be superseded by new developments in catalysts and the process generally. However it is unlikely to become as efficient as the methanol process as any Fischer-Tropsch process which produces products higher than C_1 is unlikely to have a product selectivity approaching 100 % which is possible with a process which produces only C_1 products such as methanol or methane. Therefore the by-products produced by the fuel alcohol process will always lower the thermal efficiency of the process, although it may approach that of the methanol synthesis process if by-products are reduced to a minimum and efficient uses found for the purged by-products (for example on site power generation). The fuel alcohol process should be studied in greater detail and with more information and compared in closer detail to the methanol process due to the similarity of the processes.

9.1.2.2 Assumed Product Value Ratios

When the product costs are calculated for processes producing multiple products, the values obtained are dependant upon the ratios of the relative values used in the program. As the relative value of products is not constant and changes dependently upon market forces a representative value must be used for the product value ratios. The values used in this thesis were provided by John Brown Engineers and Constructors Ltd and were based upon their in-house experience. A detailed examination of the relative value of different products within Europe, which will vary with market location, time of year and crude oil prices for example, was beyond the scope of this thesis. It is recommended that in future work careful consideration be given to the ratios used for the product prices as this affects significantly the calculated production costs of the products for the SMDS and the MOGD processes.

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Appendix A

Information Provided by John Brown Engineers and Constructors Ltd

STEP 401: GAS COMPRESSION

Purpose

To compress the raw syngas from the gasifiers to the pressure required for the downstream Shift, H_2S and CO_2 Removal steps.

Diagram

The following diagram is attached:
Figure 1 Process Flow Diagram (typical for a three stage compressor).

Previous Steps

Step 301: Oxygen Gasification
Step 302: Steam Gasification

Following Steps

Step 413: Shift Reaction

Description and Notes

The feed composition, temperature and pressure vary depending on the type of gasifier. The basis for the computer material balance, utilities and capital cost as outlined below takes account of these factors.

The material balance and utility usage are calculated specifically for each operating case. The capital cost data is calculated using a simplified approach to avoid calculating all the equipment sizes for each case. The cost data has been generated by estimating the cost for two different capacities for single stage, two stage and three stage machines. The costs for intermediate cases are calculated from the power consumed by the compressor using a scaling factor.

The raw syngas is cooled, where necessary, in the suction cooler and the condensed water removed in the suction KO drum. The syngas is compressed in a one, two or three stage machine, depending on the gasifier pressure. The equipment in each stage is identical and consists of a compressor casing (containing several wheels), a discharge cooler and KO drum to remove condensed water.

A cooler/KO drum is not provided on the outlet from the final stage. The gas is routed hot to the Shift Reaction step. Centrifugal compressors are used for all operating cases. A steam condensing turbine is used to drive the compressor using 100 bara steam.

MASS BALANCE

Main Input Stream

Flow	210	to	3,180 te/day syngas - biomass
Flow	2,420	to	46,150 te/day syngas - coal

Input Components

1	H_2	2	CO	3	CO_2	4	CH_4
5	C_2H_6	6	N_2	7	H_2S	8	H_2O

Auxiliary Input Stream

None

Main Output Stream

Output components - as input components. Flow rate and composition is calculated by John Brown algorithms.

By-product Stream

Condensate flow rate is calculated by John Brown algorithms to suit the saturated vapour pressure of water at 38°C. It is assumed that this water contains zero carbon dioxide etc.

Parameters for Program

Compressor adiabatic efficiency, %	
- 200 to 800 actual m3/hr	65
- 800 to 12,000 actual m3/hr	73
- 12,000 to 350,000 actual m3/hr	77
Minimum number of trains	2
Maximum inlet temperature to stage, °C	38
Maximum discharge temperature from stage, °C	190
Maximum compression ratio per stage	3.2
Discharge pressure from step, bara	28
Cooler pressure drop, bar	
- at 1 bara pressure	0.05
- above 1 bara pressure	0.2
Compressibility factor	1.0
Turbine Steam consumption, kg/kW.hr	
- 45,000 kW	4.29
- 7,000 kW	4.62
- 2,500 kW	4.64

The algorithms for estimating the compressor head, number of stages, power and discharge temperature are the standard equations for adiabatic compression published in NGPSA. The specific heat and adiabatic exponent are calculated at suction and discharge conditions and averaged. The specific heat equations for the components are obtained from Perry Chemical Engineers Handbook or Carl Yaws - A Guide to the Physical, Thermodynamic and Transport Property Data of Industrially important Chemical Compounds.

UTILITIES USAGE

Steam, 100 bara	Calculated by John Brown Algorithm
Steam condensate	Calculated by John Brown Algorithm
Cooling water (15°C rise)	Calculated by John Brown Algorithm

MAXIMUM TRAIN SIZE

The maximum train size is selected to be below both the following limits:
- 350,000 actual cubic metre/hour of syngas to the first compressor stage.
- 50,000 kilowatt compressor power.

ONSTREAM FACTOR

0.95

CAPITAL COST

Basis: mid 1988, UK, £ Sterling. Total battery limits cost of step are as follows:

High Capacity	**One Stage**	**Two Stage**	**Three Stage**
Capacity range actual m3/hr	6,000-100,000	50,000-140,000	70,000-340,000
Base Capacity actual m3/hr	100,000	140,000	340,000*
Base power kw	43,200	46,600	47,100
Base Cost			
One Train £	8,946,000	13,873,000	22,831,000
Scaling Factor	0.5	0.5	0.50
(Power)	(To 6000)	(To 50000)	(To 70000)
Low Capacity	One Stage	Two Stage	Three Stage
Capacity range actual m3/hr	250-6,000	16,000-50,000	6,000-70,000
Base capacity actual m3/hr	6,000	16,000	70,000
Base power kw	2,630	5,690	9,530
Base cost £	3,676,320	4,689,000	9,250,000
Scaling factor (Power)	0.75	0.5	0.75

Compressor costs are scaled on power in kW.

MODEL CONSTRUCTED BY:

John Brown Engineers and Constructors.
Basic costs for each of the compressor cases stated are based on indicative budget costs provided by manufacturers who have the capability to provide the machines and drivers with the range of sizes specified. This information is supported by John Brown in house data in order to interpolate cost factors. To which have been added allowances for interstage cooling and knock out drums where applicable.

HIGH CAPACITY CASE

All costs are based on single train cases, as basis of developing multiple train costs, these will be evaluated at a straight pro-rata basis on a single train.

* In some instance such as the "Three Stage Case" the through put and compressing condition requires duplicate machines per train.

The break point at which single compressors are accepted is dictated by the duty, reference the pressure ratio and gas discharge temperature.Within the accuracy of the costs developed this may be in the region of throughputs of approx 80,000 to 100,000 m3/hr.

MINIMUM CAPACITY CASE

The evaluation of the minimum capacity cases have been approached along the same lines as those adopted by maximum capacity option. Though inclusive installed costs have been developed, manufacturers availability in standard frame sizes will have a major effect on final process at the detail design stage.

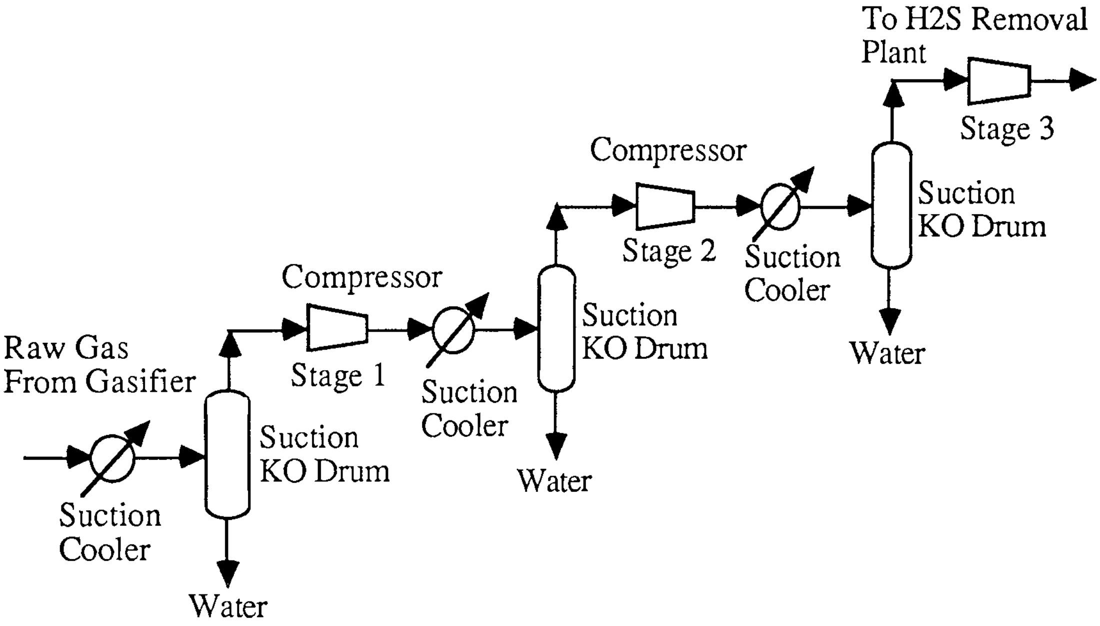


Figure 1 Gas Compression Flow Diagram

STEP 413: SHIFT REACTION

Purpose

To convert part of the carbon monoxide with steam to hydrogen and carbon dioxide to provide the required hydrogen to carbon monoxide molar ratio to the downstream syngas conversion unit.

Diagram

The following diagram is attached:
Figure 1 Process Flow Diagram

Previous Steps

Step 301: Oxygen Gasification
Step 302: Steam Gasification
Step 401: Gas Compression

Following Steps

Step 411: Sulphur Removal

Description and Notes

The feed/product composition and feed temperature and pressure vary depending on the type of gasifier. The amount of carbon monoxide to be Shifted depends on the type of gasifier and the type of downstream conversion unit which requires different hydrogen to carbon monoxide ratios.

The basis for the computer model material balance, utilities and capital cost as outlined below takes account of these factors. The material balance is calculated specifically for each operating case. The utilities and capital cost data are calculated using a simplified approach to avoid calculating all the equipment sizes for each case. This latter data has been generated by simulating the Shift unit for all feedstock conversion cases to methanol. The base data relates to a feed pressure of 31 bara and a feed carbon monoxide concentration of 25 to 40 mol%. Correction factors are applied to data generated for the base case to relate to different feed pressure and compositions. The shift reaction is assumed to be stoichiometric.

$$CO + H_2O = CO_2 + H_2$$

In most cases, only a small proportion of the carbon monoxide in the feed is required to be Shifted. Therefore, part of the syngas from the gasifier by-passes this process step.

MASS BALANCE

Main Input Stream

Flow	200	to	6,110 te/day syngas - biomass
Flow	2,360	to	73,930 te/day syngas - coal

Input Components

1	H_2	2	CO	3	CO_2	4	CH_4
5	C_2H_6	6	N_2	7	H_2S	8	H_2O

Auxiliary Input Stream

Steam, 50 bara

Input flow calculated to meet the specified mole steam per mole of feed to the Shift reactor (dry basis).

Main Output Stream

Output components as input components. Flow rate and composition is calculated by John Brown algorithms.

By-product Stream

Condensate flow rate is calculated by John Brown algorithms to suit the saturated vapour pressure of water at 38°C. It is assumed that this water contains zero carbon dioxide etc.

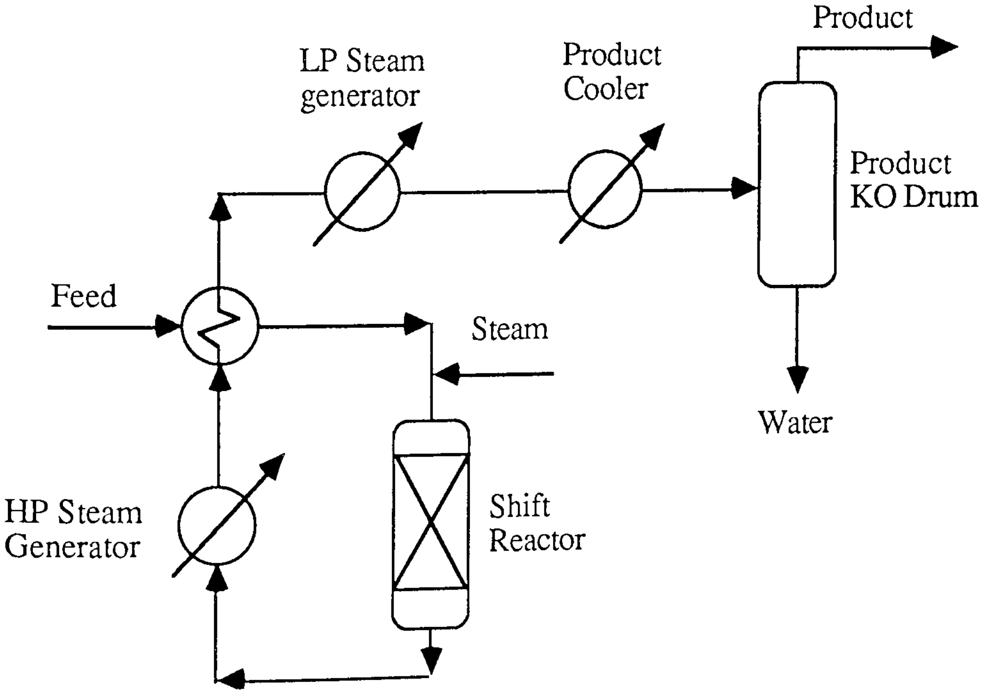


Figure 1 Shift Reaction Flow Diagram

STEP 411 A: SULPHUR REMOVAL - H_2S REMOVAL

Purpose

To remove the hydrogen sulphide and other sulphur compounds from the syngas stream.

Diagram

The following diagram is attached:

Figure 1 Process Flow diagram

Previous Steps

Step 413: Shift Reaction

Following Steps

Step 414:	Carbon Dioxide Removal
Step 411 B:	Sulphur Recovery
Step 411 C:	Tail Gas Treating

Description and Notes

This section of the Sulphur Removal step outlines the removal of hydrogen sulphide from the syngas stream in the high sulphur coal cases and uses the Selexol process. These high sulphur coal cases also contain varying amounts of other sulphur compounds e.g. carbonyl sulphide, mercaptans. The facilities required to remove these contaminants have not been evaluated in this study as their impact on the material balance and capital cost is considered to be small. The level of these contaminants in the syngas feed will be substantially reduced by the Shift Reaction step and in the Selexol Plant, but a hydrolysis reaction step may be necessary to reduce these contaminants to acceptable levels.

For the low sulphur molten bath IPG coal case and the biomass cases, the Selexol step is not required as the hydrogen sulphide levels are very low. For these cases, and for the syngas product from the Selexol Plant, a zinc oxide bed is needed to reduce the final syngas product sulphur content to that required by the downstream syngas synthesis units (typically 0.1 ppm sulphur). As the impact of the zinc oxide bed system on the material balance and capital cost is small, these facilities have not been evaluated.

The syngas feed composition (including sulphur content), flow rate and pressure vary depending on the type of gasifier. The basis for the computer model material balance, utilities and capital costs takes account of these factors. The material balance is calculated specifically for each operating case. The utilities and capital cost data are calculated using a simplified approach to avoid calculating all the equipment sizes for each case. Correction factors are applied to data generated for the base case to relate to different feed pressures and amounts of hydrogen sulphide to be removed.

The cool syngas feed is routed to the base of the H_2S absorber where the H_2S is removed by countercurrent washing with lean Selexol solvent in a packed bed. The product syngas from the top of the H_2S a is routed to the CO_2 Removal step. The rich solvent from the absorber is routed to the flash drum, at low pressure a light end rich gas stream is produced. These light ends can be recompressed and routed back to the absorber or used as the hydrogen rich stream for the Tail Gas Treating step.

The rich solvent is heated against lean solvent and pumped to the top of the regenerator. The regenerator is reboiled by a steam supplied reboiler, which strips out the absorbed H_2S, COS, CO. The regenerator offgas is cooled in an overhead condenser, and separated from the condensed water in the regenerator overhead accumulator. The condensed water is returned to the regenerator as reflux. The regenerator offgas is routed to the Sulphur Recovery Plant. The lean solvent is cooled against feed and final coolers and pumped back to the top of the absorber.

MASS BALANCE

Main Input Stream

Flow	200	to	3,100	te/day syngas - biomass
Flow	2,330	to	5	te/day syngas - coal

Input components
(The composition varies with each case, but the following values are used for generating the base case utilities and capital cost data).

1	H_2	41.3
2	CO	24.6
3	CO_2	25.0
4	CH_4	6.9
5	C_2H_6	0.0
6	N_2	0.8
7	H_2S	1.4
8	H_2O	0.2
Feed pressure, bara		27.0

Auxiliary Input Stream

None

Main Output Stream
Output components as input components. Flow rate and composition calculated by John Brown algorithms. Required total sulphur concentration is 0.1 ppm.

By-Product Stream
H_2S rich off gas stream routed to Sulphur Recovery. The flow rate is calculated by John Brown algorithms.

Parameters for Program
Mol% of feed components absorbed in the Selexol solvent.

H_2	0.13	CO	0.21	CO_2	15.23	CH_4	0.48
C_2H_6	3.09	N_2	0.18	H_2O	68.87		

Pressure drop over plant, bar 0.5

MAXIMUM TRAIN SIZE

Not known.

ONSTREAM FACTOR

0.95

CAPITAL COST

Basis: Mid 1988, UK, £ Sterling
Total battery limits cost of step f the base case with a feed pressure of 27 bara is as follows:

Base Plant Range te/day Sulphur	Base Plant Size te/day Sulphur	Base Plant Cost Million £	Scaling Factor (Power)
N/A	6173	3,528,000	0.6

For the higher pressure feed cases, at same inlet

Case	Feed Pressure	Barrel Installed Cost
Texaco LP	40	£ 2,787,000
Texaco and Prenflo HP	59	£ 2,223,000

MODEL CONSTRUCTED BY:

John Brown Engineers and Constructors using inhouse data for the material balance calculations, and using data provided by Norton for utilities and capital cost.

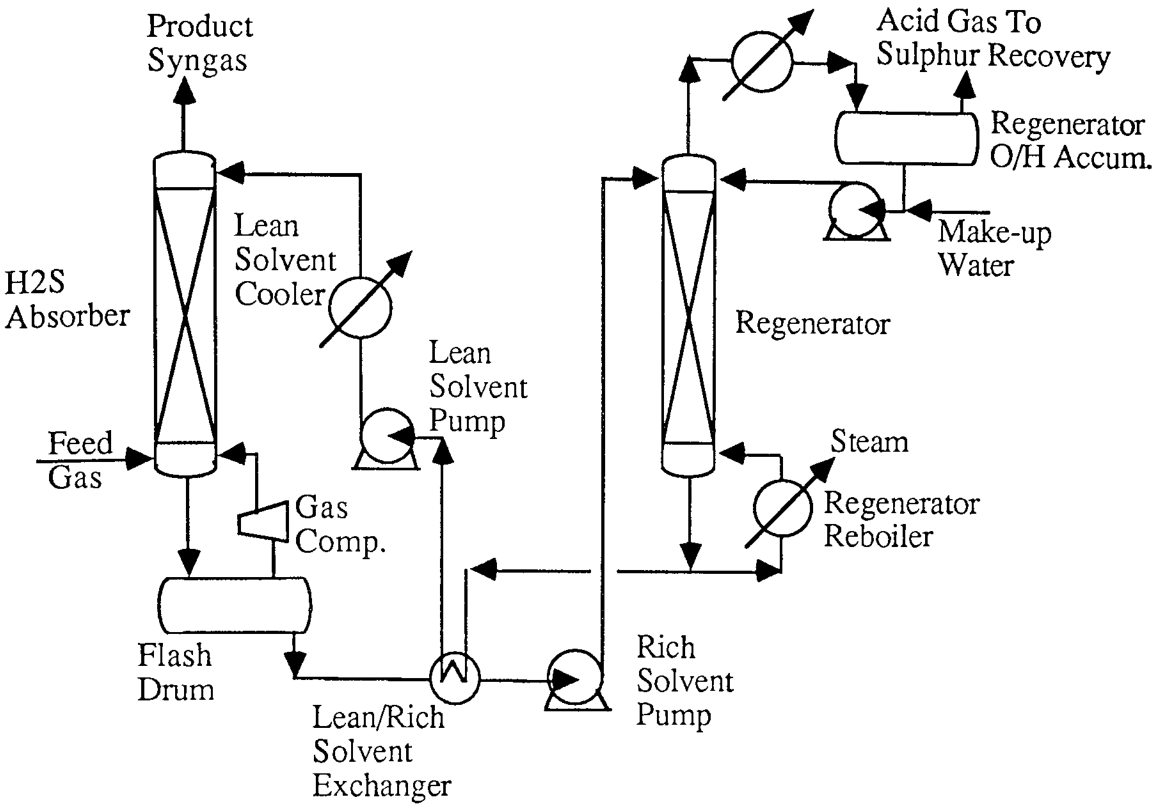


Figure 1 H_2S Removal Flow Diagram

STEP 411 B: SULPHUR REMOVAL - SULPHUR RECOVERY

Purpose

To recover sulphur from the H_2S rich stream from the H_2S Removal step.

Diagram

The following diagram is attached:
Figure 1 Process Flow Diagram

Previous Steps

Step 411 A: H_2S Removal

Following Steps

Step 411 C: Tail Gas Treating

Description and Notes

The Claus Sulphur Recovery plant removes typically 95% of the sulphur in the acid gas from the H_2S Removal plant. Part of the acid gas is burnt in the first stage of the sulphur furnace together with the recycle gas from the Tail Gas Treating unit to convert hydrogen sulphide to sulphur dioxide. The effluent from the first stage is then combined with the remaining part of the acid gas stream resulting in the reaction of hydrogen sulphide with sulphur dioxide to produce sulphur.

Effluent from the sulphur furnace is cooled in a waste heat boiler and sulphur removed in a condenser pass. Gas is reacted over catalyst in the catalytic reactors to produce additional sulphur by conversion of hydrogen sulphide, sulphur dioxide, carbonyl sulphide etc. The effluent gas is routed to the Tail Gas Treating Unit for further sulphur removal. Product sulphur is stored in a sulphur pit and pumped to offsites storage. A detailed material balance is not calculated for the Sulphur Recovery plant. The total amount of sulphur product from this plant and the Tail Gas Treating unit is calculated on removing 99.8 wt% of the sulphur in the feed from the H_2S Removal unit.

MASS BALANCE

Main Input Stream

Flow	48	to	1,024	te/day sulphur product - coal

Auxiliary Input Stream
Recycle gas from the Tail Gas Treating unit.

Main Output Stream
Sulphur product flow = 99.8 wt% of sulphur in the feed from the H_2S Removal unit.

By-product Stream
Effluent gas to the Tail Gas Treating unit.

UTILITIES USAGE		(Per te/day Sulphur Removed)
Steam, 5 bara	kg/hr	* 106
Steam, 20 bara	kg/hr	* 29
Boiler feed water	kg/hr	142
Blowdown	kg/hr	* 7
Fuel Gas (LHV)	MJ/hr	159
Electric power	kW	3.08

Note: * Indicates production

MAXIMUM TRAIN SIZE

The maximum train size is selected as 100 te/day of sulphur product. It is recommended that a spare train is provided.

ONSTREAM FACTOR

0.85

CAPITAL COST

Basis: Mid 1988, UK, £ Sterling
Total battery limits cost of step is as follows:

Range te/day Sulphur Removed	Base Plant te/day Sulphur Removed	Base Plant Cost Million £	Scaling Factor (Power)
50 - 500	50	3,000,000	0.62
501 - 800	500	12,500,000	0.72
801 - 1030	800	17,500,000	0.40

MODEL CONSTRUCTED BY:

John Brown Engineers & Constructors using inhouse data.
Cost data for the three base plants throughputs listed above is derived and checked against various sources of sulphur plant installed cost data. The wide range of the plant throughput, plus the limited data reference cost of plants above 500 te/day capacity precludes the use of a single scaling factor across the range of sizes. It is anticipated that plant in the larger group will tend to be multiple stream sizes of the smaller plants.

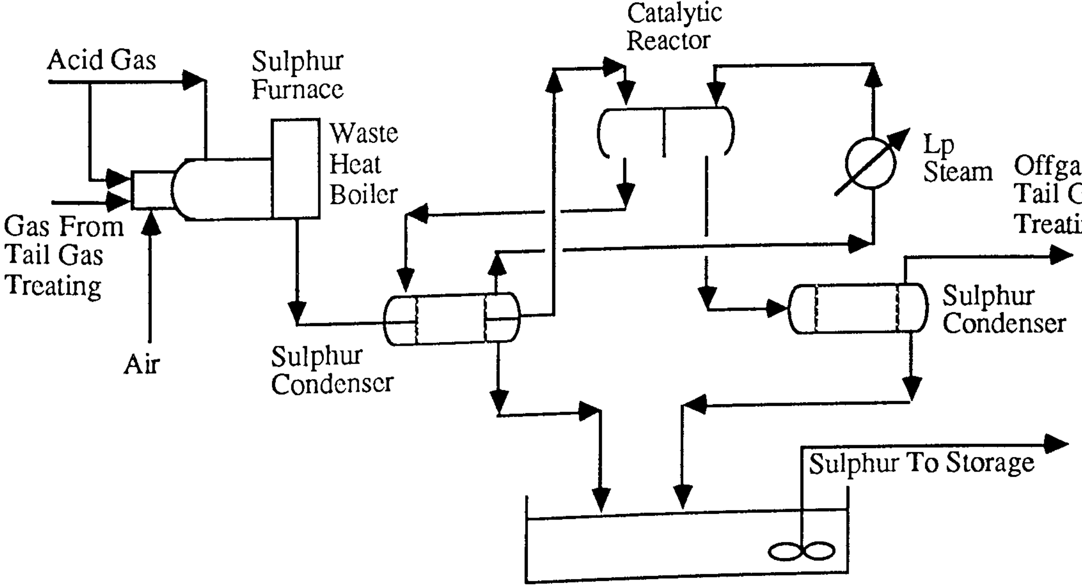


Figure 1 Sulphur Recovery Flow Diagram

STEP 411 C: SULPHUR REMOVAL - TAIL GAS TREATING

Purpose

To recover sulphur from the Sulphur Recovery plant tail gas to comply with air emission regulations.

Diagram

The following diagram is attached: Figure 1 Process Flow Diagram

Previous Steps

Step 411 B: Sulphur Recovery

Following Steps

None

Description and Notes

The tail gas from the Sulphur Recovery plant is mixed with a hydrogen rich stream and routed to the hydrogenation reactor, where sulphur compounds e.g. carbonyl sulphide, sulphur dioxide are hydrogenated to hydrogen sulphide. The gas stream is then cooled against low pressure steam generation and further cooled in the quench tower. The quench tower is served by a recirculating water stream with cooler.

The gas stream is routed to an absorber where the H_2S is absorbed in a recirculating amine stream, then processed in a thermal or catalytic incinerator and routed to atmosphere via a stack.

The rich amine is pumped from the absorber, heated against feed and passed to the top for the regenerator. The regenerator is provided with a steam reboiler and strips out hydrogen sulphide from the amine solution. The regenerator offgas is cooled in an overhead condenser, and separated from the condensed water in the regenerator overhead accumulator. The condensed water is returned to the regenerator as reflux. The regenerator offgas is recycled to the Sulphur Recovery plant.

The lean solvent is cooled against feed and final cooler and pumped back to the top of the absorber. A detailed material balance is not calculated for the Tail Gas Treating unit. The total amount of sulphur product from this plant and the Sulphur Recovery plant is calculated on removing 99.8 wt% of the sulphur in the feed from the H_2S removal plant.

MASS BALANCE

Main Input Stream

Flow 48 to 1,024 te/day sulphur product - coal

Auxiliary Input Stream

Hydrogen rich stream from H_2S Removal Unit

Main Output Stream

Treated tail gas.

By-product Stream

Recycle gas to sulphur furnace.

UTILITIES USAGE (Per te/day Sulphur Removed)

Steam, 5 bara kg/hr	16.7
Steam condensate kg/hr	*16.7
Electric power kW	1.17

Note:* indicates production

MAXIMUM TRAIN SIZE

The maximum train size is selected as 100 te/day sulphur product from the Sulphur Recovery plant.

ONSTREAM FACTOR 0.95

CAPITAL COST

Basis: Mid 1988, UK, £ Sterling

Total battery limits of step is as follows:

Range te/day Sulphur Removed	Base Plant te/day Sulphur Removed	Base Plant Cost Million £	Scaling Factor (Power)
50 - 500	50	900,000	0.62
501 - 800	500	3,125,000	0.72
801 - 1030	800	3,500,000	0.40

NOTES ON ESTIMATING

The statistics and cost data related to sulphur recovery tail gas treating facilities reflect the composition of the gas stream, costs detailed result from an analysis of this information. It is therefore assumed generally that scaling factors will reflect those specified for the sulphur recovery plant Step 411 B. In the analysis of available data the cost range indicated generally that tail gas treating facilities range from 30 % of the installed cost for the small plant to 20% of the larger plants.

MODEL CONSTRUCTED BY:

John Brown Engineers & Constructors using inhouse data.

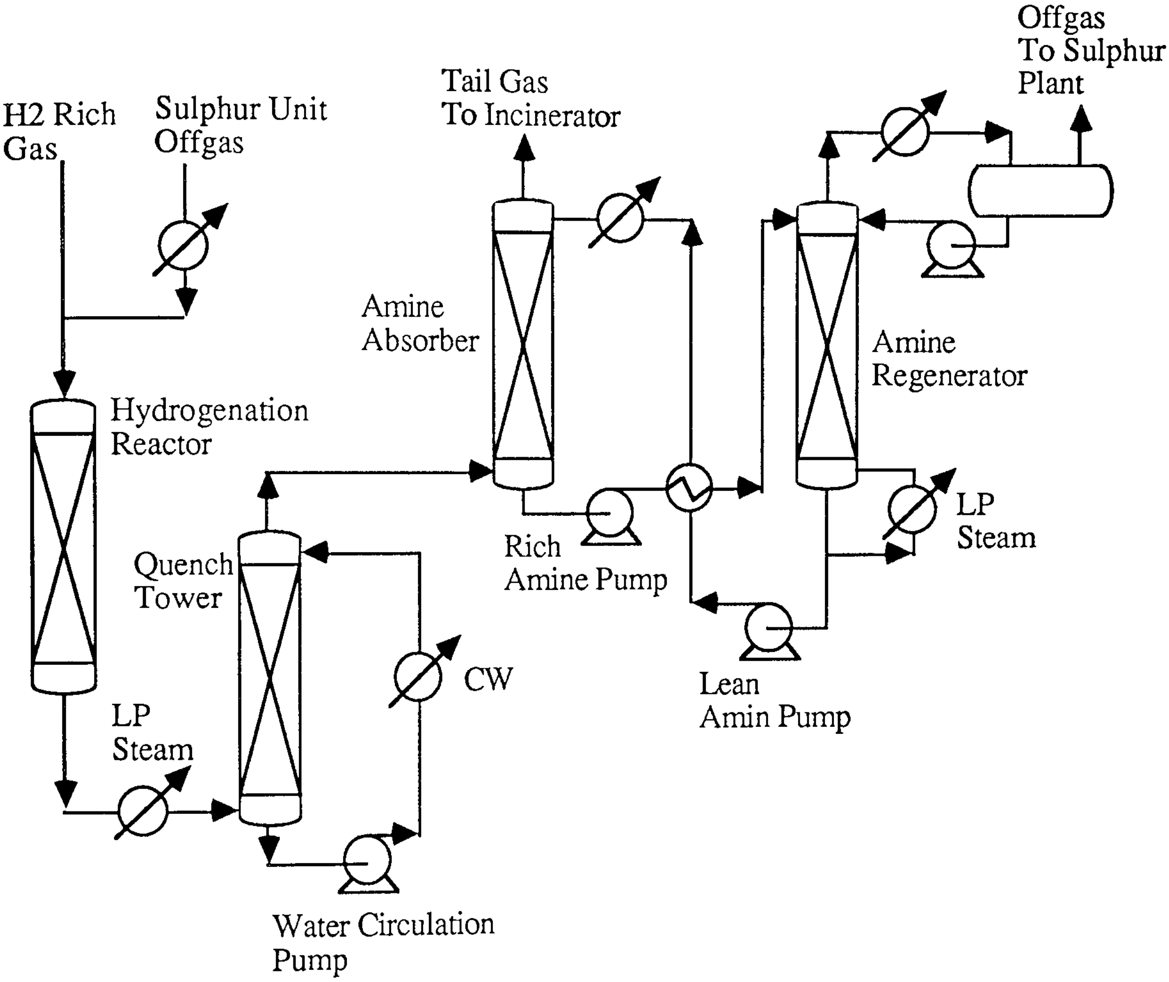


Figure 1 Tail Gas Treating Recovery Flow Diagram

STEP 414: CARBON DIOXIDE REMOVAL

Purpose

To remove the bulk of the carbon dioxide from the syngas stream.

Diagram

The following diagram is attached:
Figure 1 Process Flow Diagram

Previous Steps

Step 411 A: H_2S Removal

Following Steps

Step 421: Fischer Tropsch Synthesis and Refining
Step 431: Methanol Synthesis
Step 432: Fuel Alcohol Synthesis

Description and Notes

The syngas feed composition (including carbon dioxide content), flow rate and pressure vary depending on the type of gasifier. The basis for the computer model material balance, utilities and capital costs takes account of these factors. The material balance is calculated specifically for each operating case. The utilities and capital cost data are calculated using a simplified approach to avoid calculating all the equipment sizes for each case. Correction factors are applied to data generated for the base case to relate to different feed pressures and amounts of carbon dioxide to be removed. The cool syngas feed is routed to the base of the CO_2 absorber where the CO_2 is removed by countercurrent washing with lean Selexol solvent in a packed bed. The product syngas from the top of the CO_2 absorber is routed to the downstream syngas synthesis unit. The rich solvent from the absorber is routed to the flash drum, where at reduced pressure a light end rich gas stream is produced, compressed and routed back to the absorber. The rich solvent is routed to the top of the regenerator. The solvent is regenerated with air. The regenerator offgas is routed to a stack. The lean solvent is pumped back to the top of the absorber.

MASS BALANCE

Main Input Stream

Flow	260	to	4,990	te/day syngas - biomass
Flow	2,230	to	63,260	te/day syngas - coal

Input components

(The composition varies with each case, but the following values are used for generating the base case utilities and capital cost data).

1	H_2	48.3	2	CO	22.4	3	CO_2	18.6	4	CH_4	6.3
5	C_2H_6	0.0	6	N_2	4.3	7	H_2O	0.1			

Feed pressure, bara 26.5

Auxiliary Input Stream

None

Main Output Stream

Output components as input components. Flow rate and composition calculated by John Brown algorithms. Required total carbon dioxide concentration is 2 mol % (dry basis).

By-product Stream

CO_2 rich off gas stream routed to a stack. The flow rate is calculated by John Brown algorithms.

Parameters for Program

Mol% of feed components absorbed in the Selexol solvent.

H_2	0.13	CO	0.21	CH_4	0.48
C_2H_6	3.09	N_2	0.18	H_2O	68.87

Pressure drop over plant, bar 0.5
Mol% CO_2 in product syngas 2.0

UTILITIES USAGE

(Per te/day Carbon Dioxide Removed)

MAXIMUM TRAIN SIZE

Not known.

ONSTREAM FACTOR

0.95

CAPITAL COST

Basis: Mid 1988, UK, £ Sterling
Total battery limits cost of step for the base case with a feed pressure of 26.5 bara is as follows:

Base Plant Range te/day CO_2	Base Plant Size te/day CO_2	Base Plant Cost Million £	Scaling Factor (Power)
N/A	5,284	6,106,000	0.6

For the higher pressure feed cases, multiply the cost by the following factors:

Case	**Feed Pressure, bara**	**Multiplying Factor**
Texaco LP	39.5	0.79
Texaco and Prenflo HP	58.5	0.63

MODEL CONSTRUCTED BY:
John Brown Engineers and Constructors using inhouse data for the material balance calculations, and using data provided by Norton for utilities and capital cost.

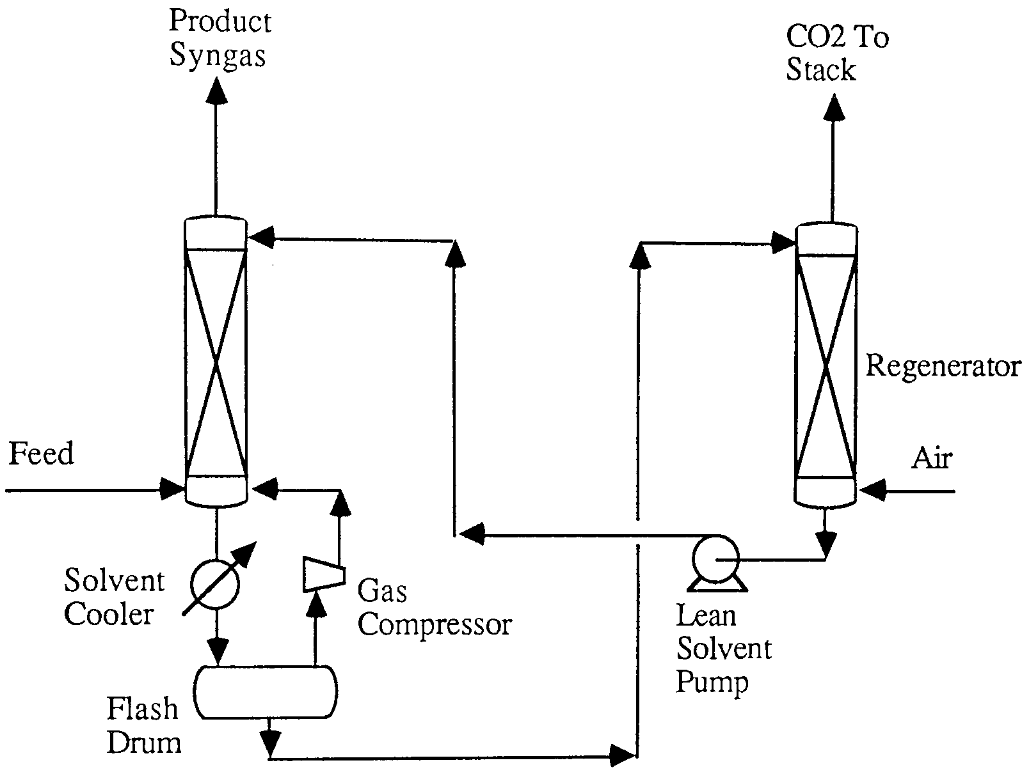


Figure 1 CO_2 Removal Flow Diagram

STEP 412: STEAM REFORMING

Purpose
To convert hydrocarbons to hydrogen and carbon monoxide to increase the amount of feedstock to downstream synthesis units and increase the total feed hydrogen to carbon dioxide molar ratio.

Diagram
The following diagram is attached:
Figure 1 Process Flow Diagram

Previous Steps
Step 421: Fischer Tropsch Synthesis and Refining
Step 431: Methanol Synthesis
Step 432: Fuel Alcohol Synthesis

Following Steps
Step 414: Carbon Dioxide Removal

Description and Notes
The feed composition is very dependent on the following parameters:

- amount of hydrocarbons in the syngas from the gasifier.
- amount of synthesis unit purge gas recycled to the reformer compared to the amount purged to fuel.
- The amount of hydrocarbons produced in the synthesis unit.

The basis for the computer model material balance takes account of these factors. The material balance is calculated specifically for each operating case. The utilities and capital cost data are calculated using a simplified approach to avoid calculating all the equipment sizes for each case. This latter data has been generated by simulating the Steam Reformer for all feedstock conversion cases to methanol. The base data refers to a hydrocarbon concentration in the feed of 25-30 mol%. Correction factors are applied to the data generated for the base case to relate to different feed hydrocarbon contents. The reforming reactions and Shift side reactions are assumed to be stoichiometric.

$$C_nH_{(2n+2)} + n\,H_2O = n\,CO + (2n+1)H_2$$
$$CO + H_2O = CO_2 + H_2$$

The feed gas is heated against the reaction products and in the reformer furnace convection bank to about 500°C and fed to the reformer furnace radiant coil. Steam is added to the feed to suit the required steam/hydro molar ratios. This coil contains the reforming catalyst. The reaction products leave the furnace at 850°C and are cooled against medium and low pressure steam generation, feed and finally the product cooler. The water condensed in the product cooler is removed in the product KO drum and routed to waste water treatment. The product gas is compressed, where necessary, and recycled to the main syngas feed upstream of the CO_2 Removal Plant.

MASS BALANCE

Main Input Stream

Flow	25	to	2,600	te/day feed - biomass
Flow	270	to	26,800	te/day feed - coal

Input Components

1	H_2	2	CO	3	CO_2	4	CH_4	5	C_2H_6
6	C_3H_8	7	C_4H_{10}	8	C_5H_{12}	9	N_2	10	H_2O

Auxiliary Input Stream

Steam, 50 bara. Input flow calculated to meet the specified steam to hydrocarbon molar ratio.

Main Output Stream

Output components as input components. Flow rate and composition is calculated by John Brown algorithms.

By-Product Stream

Condensate flow rate is calculated by John Brown algorithms to suit the saturated vapour pressure of water at 38°C. It is assumed that this water contains zero carbon dioxide etc.

Parameters for Program

Feed pressure	32 bara
Feed temperature	38°C
Mol% of hydrocarbons converted to carbon monoxide	60
Mol% of methane in reformer product (dry basis)	4
Steam to hydrocarbon molar	3

UTILITIES USAGE

(Per kg mol/hr hydrocarbons reformed)

		Base Case	Multiplying Factor (From Base Case)	
Feed mol% hydrocarbons (dry)		25 - 30	30 - 50	50 - 70
Steam, 5 bara	kg/hr	*37.3	0.832	0.753
Steam, 50 bara				
- Generated	kg/hr	*192	0.904	0.854
- added to feed	calculated by John Brown algorithms			
Process condensate	calculated by John Brown algorithms			
Cooling water (15°C rise)	te/hr	2.41	0.8	0.73
Boiler feed water	kg/hr	240.8	0.892	0.837
Blowdown	kg/hr	*11.5	0.892	0.837
Fuel gas (LHV)	MJ/hr	809	0.927	0.901
Electric power	kW	1.38	0.922	0.891

Note: * indicates production

MAXIMUM TRAIN SIZE

The maximum train size is selected as 930 kg.mol/hr of hydrocarbons reformed. This corresponds to a maximum of 280 tubes in the reforming furnace radiant section.

ONSTREAM FACTOR

0.95

CAPITAL COST

Basis: mid 1988, UK, £ Sterling

Total battery limits costs of step for base case of 25-30 mol% hydrocarbons in the feed is as follows:

Range kg.mol/hr Hydrocarbons Reformed	**Base Plant kg.mol/hr Hydrocarbons Reformed**	**Base Plant Cost Million £**	**Scaling Factor (Power)**
930 - 401	795	15,545,000	0.95
400 - 100	166	3,598,000	0.9

For feeds with higher hydrocarbons content, multiply the base costs, by the following factors:

Feed hydrocarbon Mol %	30-50	50-70
Multiplying factor	Plant Cost x 0.91	Plant Cost x 0.875

MODEL CONSTRUCTED BY:

John Brown Engineers and Constructors using inhouse data plus:

- o ICI Billingham, UK.
- o Foster Wheeler Fired Heater Division, Reading, UK who provided cost data for the reforming furnace to which have

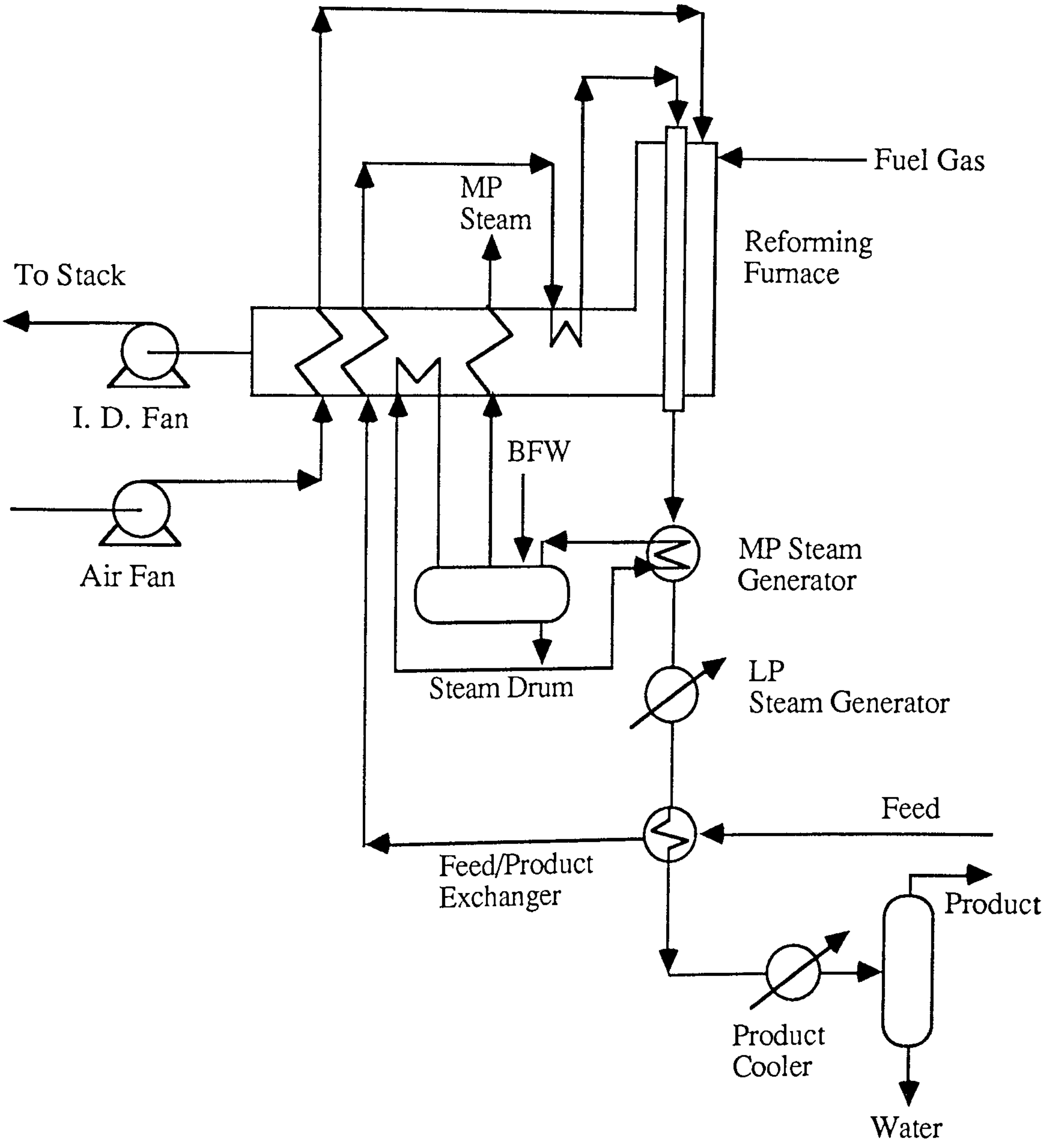


Figure 1 Steam Reforming Flow Diagram

STEP 491: HYDROGEN RECOVERY

Purpose

To recover hydrogen from the Methanol Synthesis unit purge stream and produce a high purity hydrogen stream for use in downstream MTG and MTO/MOGD hydrotreaters.

Diagram

The following diagram is attached:
Figure 1 Process Flow Diagram

Previous Steps

Step 431: Methanol Synthesis

Following Steps

Step 441: MTG Synthesis and Distillation
Step 442: MOGD Synthesis and Distillation

Description and Notes

The Methanol Synthesis purge gas stream containing about 55 mol% hydrogen is processed to recover a 99.5 mol% hydrogen rich stream which is used in the MTG and MTO/MOGD hydrotreaters.

The process is based on the Union Carbide Pressure Swing Adsorption unit (PSA). The feed gas is routed sequentially to one of the several parallel adsorbers, where the nitrogen, carbon dioxide, methane etc are captured by the adsorbent. The majority of the hydrogen passes through the bed. When the adsorbent is loaded with contaminants, the feed gas is switched to the next adsorber vessel.

The pressure is then reduced in the offline adsorber to just above atmospheric pressure to remove most of the contaminants from the adsorbent. This gas is routed to adjacent furnaces fitted with low pressure burners. The bed is then purged to remove remaining impurities, then repressurised again.

The purge gas feed composition varies with the operating case, particularly in the amounts of nitrogen and methane which are present in the syngas feedstocks. The computer model for the PSA unit assumes that the purge gas is of a fixed composition. This will lead to minor errors in the capital cost determination, but this impact on the overall project cost will be small.

MASS BALANCE

Main Input Stream

Flow	2	to	110	kg/hr H_2 product - biomass
Flow	16	to	1,330	kg/hr H_2 product - coal

Input Components, Mol%

1	H_2	55
2	CO	20
3	CO_2	9
4	CH_4	5
5	N_2	11
Feed pressure, bara		43

Auxiliary Input Stream

None

Main Output Stream

Output Components,

1	H_2	99.5
2	N_2/CH_4	0.5

Flow rate calculated on the basis of 90 mol% hydrogen recovery over the unit.

By-product Stream

Fuel gas flow rate and composition calculated by John Brown algorithms.

UTILITIES USAGE

No major utility usages.

MAXIMUM TRAIN SIZE

Not known.

ONSTREAM FACTOR
0.95

CAPITAL COST
Basis: mid 1988, UK, £ Sterling
Total battery limits cost of step is as follows:

Base Plant Range Nm3/d H_2 Product	Base Plant Size Nm3/d H_2 Product	Base Plant Cost £	Multi-plying Factor
401,000 - 1,800,000	1,600,000	3,553,000	0.85
1000 - 400,000	400,000	2,430,000	0.80

MODEL CONSTRUCTED BY:
John Brown Engineers and Constructors based on data provided by Union Carbide, Belgium.

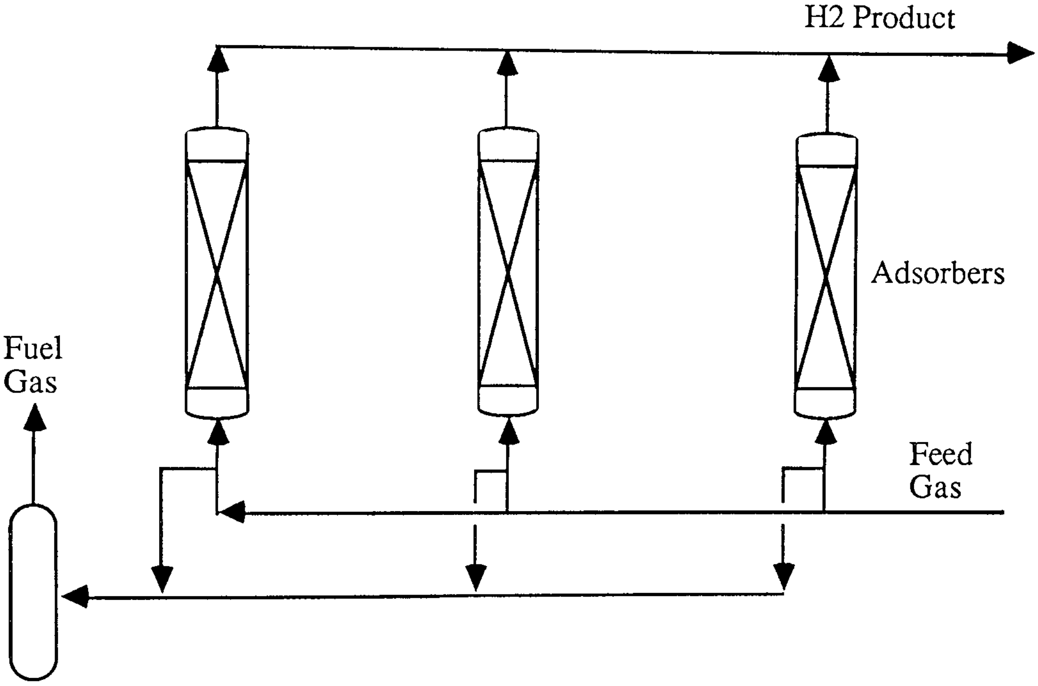


Figure 1 Hydrogen Recovery Flow Diagram

STEP 601: DISTILLATION OF CRUDE METHANOL
Purpose
To process the crude methanol from the Methanol Synthesis unit to produce a fuel grade methanol suitable for sale or MTO/MOGD Synthesis heating.

Diagram
The following diagram is attached:
Figure 1 Process Flow Diagram

Previous Steps
Step 431: Methanol Synthesis

Following Steps
Step 442: MOGD Synthesis and Distillation
Offsites: Storage and Facilities

Description and Notes
The methanol feed composition varies depending on the operating case. The material balance is calculated specifically for each feedstock, but utility and capital cost data are simply based on te/day of methanol product. The crude methanol is preheated and routed to the light ends column, which removes light ends from alcohol/water mixture. The overheads are cooled and condensate returned to the column as reflux. Light ends are routed to fuel gas. The light end column bottoms is routed to the refining column, which

fractionates the alcohol/water mixture. The methanol product is the overhead stream and higher alcohols are withdrawn from the column as a side-draw. The water is removed from the base of the column.

MASS BALANCE

Main Input Stream

Flow	80	to	1,950	te/day - biomass
Flow	920	to	24,100	te/day - coal

Input Components

1 H_2
2 CO
3 CO_2
4 CH_4
5 C_2H_6
6 N_2
7 H_2O
8 Dimethyl Ether
9 Butanol
10 Methanol

The crude methanol composition varies depending on the feedstock case. A typical quality is as follows:

Methanol	96 mol %
Water	3.7 mol %
Light Ends	0.1 mol %
Heavy Ends	0.2 mol %

Auxiliary Input Stream

None

Main Output Stream

Fuel grade methanol product.

Output Components, Mol%

1	Methanol	98.59
2	Dimethyl Ether	0.05
3	Butanol	0.05
4	Water	1.31

The methanol purity corresponds to 99 wt%. The flow rate is calculated by John Brown algorithms.

By-product streams

The flow of waste water, higher alcohols and off to fuel are calculated by John Brown algorithms.

UTILITIES USAGE

(Per te/day of Methanol Product)

Steam, 3.5 bara	kg/hr	2.51
Steam, 7 bara	kg/hr	17.88
Steam condensate	kg/hr	*20.39
Cooling Water	te/hr	0.093
Electric power	kW	0.174

Note: * indicates production

MAXIMUM TRAIN SIZE

The maximum train size of 3,000 te/day of methanol product is compatible with the Methanol Synthesis unit.limits cost of Step 601 is £ 25 million, for a plant to produce 3000 te/day of crude methanol product.

Scaling cost capacity factor: Exponent of 0.7 over 500 to 3000 te/day range.

MODEL CONSTRUCTED BY:

John Brown Engineers and Constructors using inhouse data and the following publications:

(a) EPRI Report AP-1592, Research Project 832-3. Lignite to Methanol - an Engineering Evaluation of Winkler Gasification and ICI Methanol Synthesis Route. By DM International 1980.

(b) EPRI Report AP-1962, Research Project 832-4. Coal to Methanol - an Engineering Evaluation of Texaco Gasification and ICI Methanol Synthesis Route. By Fluor 1981.

(c) Investigations on Catalysed Steam Gasification of Biomass, Appendix B, for US DOE. By Batelle 1981.

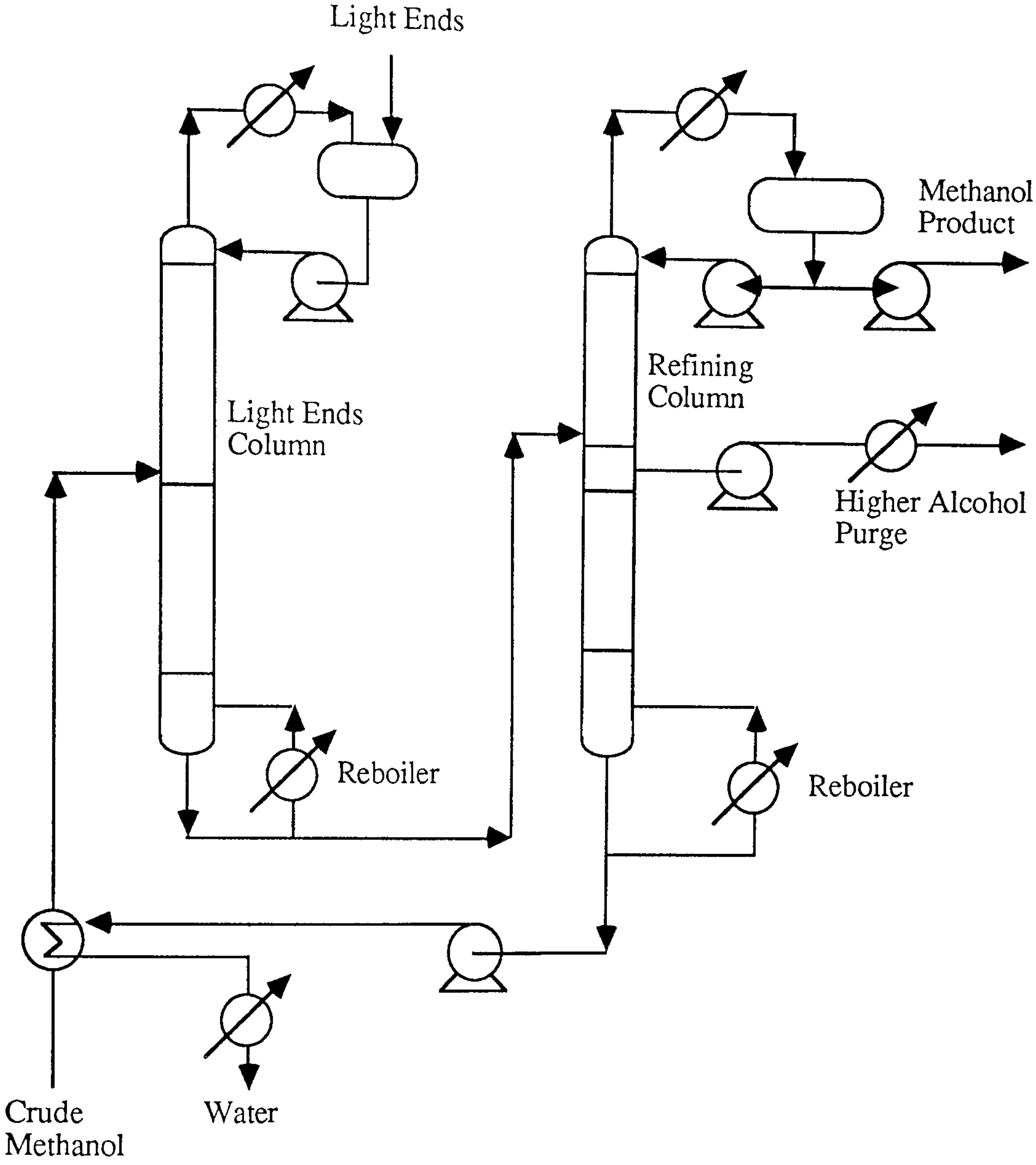


Figure 1 Methanol Distillation Flow Diagram

STEP 432: FUEL ALCOHOL SYNTHESIS AND DISTILLATION

Purpose

To convert syngas to a C_1 to C_6 alcohol mixture suitable for motor fuels blending, using the IFP process.

Diagram

The following diagrams are attached:
Figure 1 Block Flow Diagram
Figure 2 Reaction Unit Process Flow Diagram
Figure 3 Alcohol Distillation Process Flow Diagram

Previous Steps

Step 414: Carbon Dioxide Removal

Following Steps

Offsites: Storage and facilities

Description and Notes

(a) General

The composition of the syngas produced in the gasification steps is generally adjusted in the syngas treating/ conditioning units to meet a feed hydrogen to carbon mono molar ratio of 1.5. This is considered to be representative of the desired feed quality.

However, in several cases where the syngas feed from the Gasifier is high in hydrogen concentration, excess hydrogen is available which passes through the Alcohol unit unreacted. Also the amounts of inerts in the syngas feed varies depending on the type of gasifier and its feedstocks, and the amount of Alcohol purge gas recycled through the Steam Reformer. These significant differences in syngas feed composition are taken into account in the material balance model. Their effect on utilities and capital cost are assumed to be negligible.

The plant converts syngas to methanol and a higher alcohol mixture with by-products propane, butanes, pentanes, water and fuel gas. The facilities included in this plant are outlined on the Block Flow Diagram Figure 1, and are summarized:

- An Alcohol Synthesis Unit where syngas is converted to a C_1 to C_6 alcohol mixture.
- An Absorber which removes carbon dioxide from the recycle gas in the Synthesis Unit.
- An Alcohol Distillation Unit for separating the light ends and water from the alcohol mixture and splitting the alcohols in the light and heavy components.

(b) Reaction Unit

A simplified process flow diagram is shown in Figure 2. The consumptions of carbon monoxide and hydrogen, and production of alcohols, hydrocarbons and water are calculated from the following stoichiometric equations:

Alcohols: $n\,CO + 2n\,H_2 = CH(2n + 1)OH + (n - 1)H_2O$

Hydrocarbons: $CO + (2n + 1)H_2 = CnH(2n + 2) + n\,H_2O$

The syngas feed is compressed in the syngas compressor and routed to the first stage reactor system. Part of the compressed feed is heated to reactor temperature in a feed/ effluent exchanger. The reactions over a copper cobalt catalyst are exothermic, and the reactor is cooled by using a multibed system quenched with cold c feed gas. The reactor products are cooled against feed then in a product cooler and flashed in a separator. The liquid products from the separator are routed to the low pressure flash drum.

The unreacted syngas and vapour products from the first stage separator are routed to the second stage reactor system which is similar to the first stage. Part of the unreacted syngas and vapour products from the second stage separator are recycled back to the syngas feed compressor, via an absorber to remove the carbon dioxide produced in the side reactions. Purge gas is withdrawn from the reactor recycle circuit and recycled to the steam reformer or routed to fuel gas depending on the operating case. The combined liquid products ar flashed in a low pressure separator, the flash gases routed to fuel gas and the raw alcohols routed to the distillation plant. A side reaction of the low temperature alcohol synthesis catalyst is the Shift reaction. Though producing carbon dioxide which is an undesirable by-product, it offers the advantage of removing part of the water produced in the alcohol synthesis reactions, thus reducing the cost of the alcohol distillation section. The water content in the raw alcohol product from the section is typically 5 wt%.

(c) Distillation Unit

Among other technologies, the proven azeotropic distillation process is attractive for alcohol dehydration. Figure 3 presents the separation flowsheet. In the first column C_1, methanol is distiled off from the heavier alcohols water mixture. This mixture is dehydrated in azeotropic columns C_2 and C_3 which are operated with a water entrainer to deliver, as bottom products, the dehydrated heavier alcohols (from C_2) and the water (from C_3). Benzene has been used as a water entrainer at bench scale, in order to produce large samples of anhydrous alcohol mixtures (< 0.2 wt% of water). Other entrainers well known for ethanol azeotropic dehydration may be used as well. For the production of fuel alcohols, this scheme can be as it is not necessary to separate the alcohols into a methanol product and a higher alcohols product.

MASS BALANCES

Main Input Stream

Flow	90	to	3,060	te/day syngas - biomass
Flow	1,060	to	49,260	te/day syngas - coal

Input Components

1	H_2	2	CO	3	CO_2	4	CH_4
5	C_2H_6	6	N_2	7	H_2O		

Auxiliary Input Stream
None

Output Stream
Mixed alcohol components (wt%)

1	Methanol	60
2	Ethanol	19
3	Propanol	11
4	Butanol	5.5
5	Pentanol	2.5
6	Hexanol	2

The final fuel alcohol product contains 0.5 wt% water. The output flow rate is calculated by John Brown algorithms.

By-product Streams
Fuel gas and water flow rate and composition are calculated by John Brown algorithms.

Parameters for Program

Syngas feed hydrogen to carbon monoxide molar ratio	1.5
Syngas feed carbon dioxide content, mol%	2
Carbon monoxide in syngas feed converted in Shift reaction, mol%	28
Conversion of CO in syngas feed to alcohols plus hydrocarbons, mol%	90 Note (1)
Selectivity to alcohols, mol%	75
CO_2 content in syn. unit recycle gas downstream of CO_2 removal section, mol%	2
Operating pressures, bara	
- downstream feed compressor	85
- HP separator	80
Composition of hydrocarbons produced in the unit, wt%	
CH_4	74.3
C_2H_6	15.2
C_3H_8	7.9
C_4H_{10}	1.8
C_5H_{12}	0.8

Notes: (1) The conversion relates to the amount of carbon monoxide in the syngas feed minus the carbon monoxide converted in the Shift section downstream of the synthesis section.

UTILITIES USAGE

(Per te/day Alcohol Product)

Steam 3.5 bara	kg/hr	3.3
Steam 7 bara	kg/hr	23.2
Steam bara	kg/hr	13.6
Steam condensate	kg/hr	*40.1
Cooling water	te/hr	1.23
Electric power	kW	0.32

Notes:
(1) Usage assumed to be 30% higher than Methanol Synthesis and Distillation
(2)* indicates production

MAXIMUM TRAIN SIZE

The maximum train size is selected as 2,000 te/day of alcohol product.

ONSTREAM FACTOR

0.95

CAPITAL COST:

Mid 198 UK, £ Sterling. Total battery limits cost of step is summarized below.

RANGE te/day ALCOHOLS PRODUCT	BASE PLANT te/day ALCOHOLS PRODUCT	BASE PLANT £	SCALING FACTOR
2000 te/pd & BELOW	2000	250,000,000	£ 0.125 X 10^6
ABOVE 2000 te/pd			£ 0.108 X 10^6

MODEL CONSTRUCTED BY:

John Brown Engineers and Constructors based on the following articles published by IFP, France. It should be noted that these articles contain only general data which has been interpreted by John Brown to provide the basis for this model. Therefore it is suggested that this model should be further developed in future studies to reduce the level of uncertainties.

(a) Revue de L'IFP Production De Methanol et D'Alcools Superieurs a partir de Gaz via (CO + H_2). Editions Technip 1987 by P. Courty, D. Durand, J.C. Guibet (IFP) and N. Kawata, T. Yasuda, M. Yoshimoto (Idemitsu).

(b) Industrial Chemicals via C1 Processes. ACS Symposium Series 328, 1987. By P. Courty, A. Forestiere, C. Rainbault (IFP) and N. Kawata, T.Ohno, M. Yoshimoto (Idemitsu).

(c) Production of C1 - C6 Alcohols. AIChE Spring Meeting April 1986, New Orleans, USA. By L. Asselineau, P. Courty, P. Travers (IFP) and T. Ohno, M. Yoshimoto (Idemitsu).

(d) The IFP Process for Production of C1 - C6 Alcohols from Synthesis Gas. 11th World Petroleum Congress, London, September 1983. By P. Courty, J.P. Arlie, A. Convers, P. Mikitenko, A. Sugier (IFP).

(e) Aspects Economiques des Voies de Production des Carbutonts de Synthäse. Petrole & Techniques, No. 33, May 1987. By P. Roth, E. Matter, G. Bourbonneux. (Technip).

(f) C1 - C6 Alcohols from Syngas, Hydrocarbon Processing, November 1984. By P. Courty, J.P. Arlie, A. Convers, P. Mikitenko, A. Sugier (IFP).

(g) Precedes IFP de Synthese d'Alcools C1 - C6 et d Synthese du Methanol en Phase Liquide. By J.P. Arlie, J.P. Cariou, P. Courty (IFP).

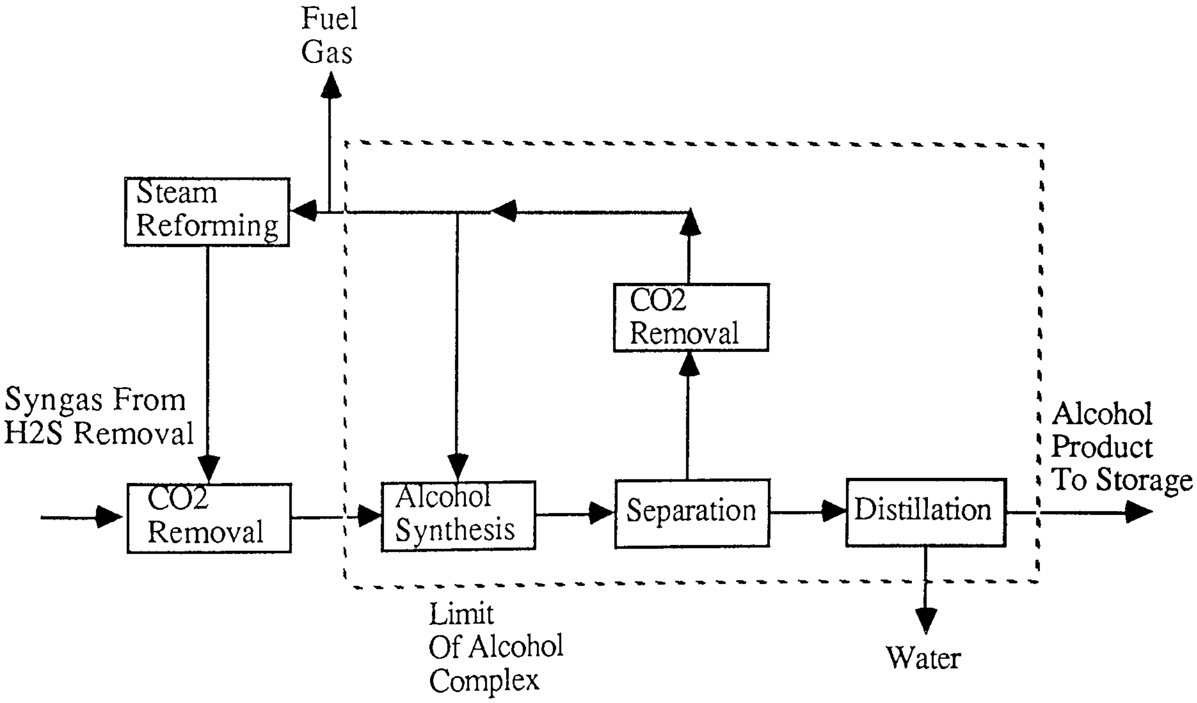


Figure 1 Fuel Alcohol Block Flow Diagram

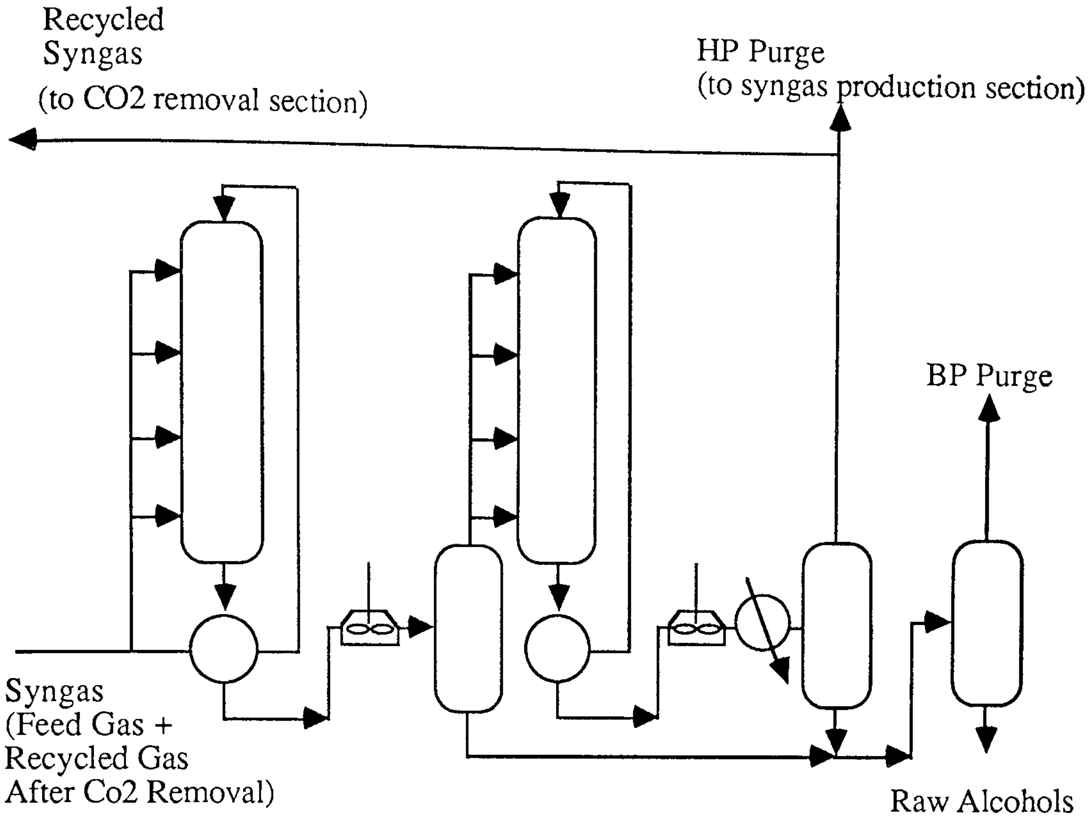


Figure 2 Fuel Alcohol Synthesis Flow Diagram

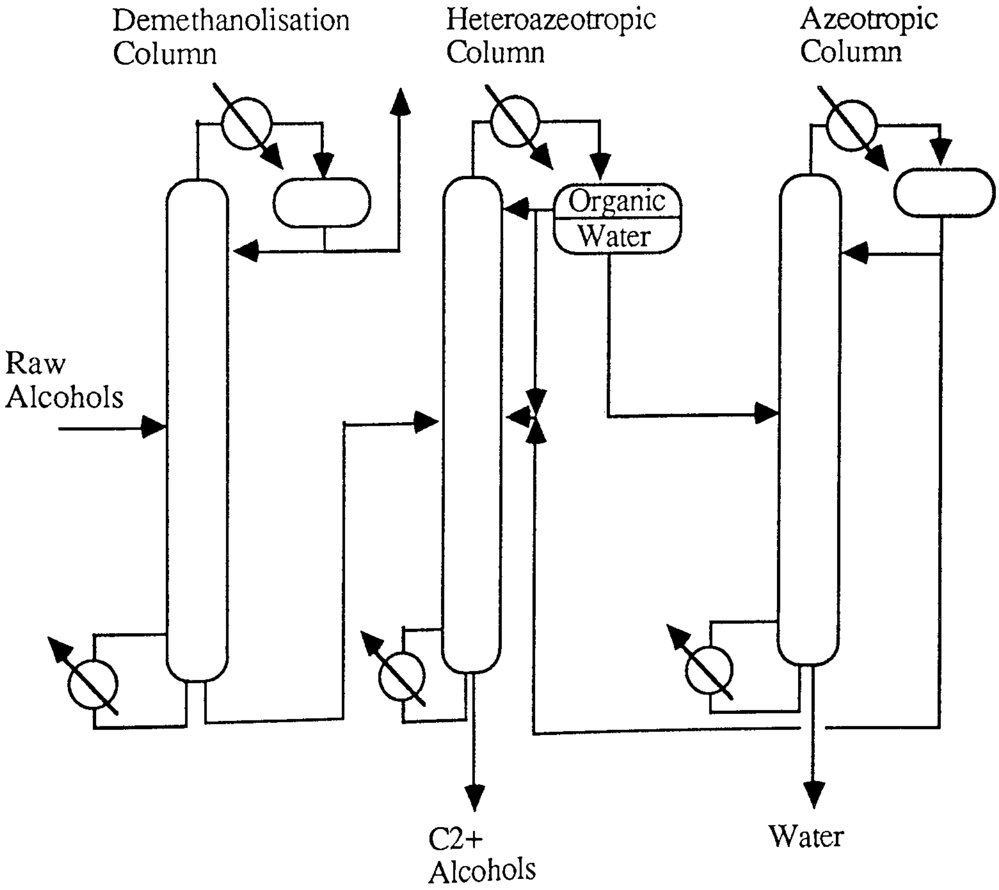


Figure 3 Fuel Alcohol Distillation Flow Diagram

STEP 431: METHANOL SYNTHESIS

Purpose

To convert synthesis gas to crude methanol

Diagram

The following diagram is attached:
Figure 1 Process Flow Diagram

Previous Steps

Step 401: Gas Compression
Step 411: Sulphur Removal
Step 412: Steam Reforming
Step 413: Shift Reaction
Step 414: Carbon Dioxide Removal

Following Steps

Step 412: Steam Reforming
Step 441: MTG Synthesis and Distillation
Step 601: Distillation of Crude Methanol

Description and Notes

The composition of the syngas produced in the gasification steps is generally adjusted in the syngas treating/conditioning units to meet the following approximate molar ratio, which is the optimum feed for methanol synthesis:

$$\frac{H_2 + CO_2}{CO + CO_2} = 2.1$$

However, in several cases where the syngas feed contains high hydrogen concentrations and Steam Reforming is used to convert part of the methane in the syngas feed, excess hydrogen is available. Also the amounts of inerts in the syngas feed varies depending on the type of gasifier and its feedstock, and the amount of methanol purge gas recycled thro the Steam Reformer. These significant differences in syngas feed composition are taken into account in the material balance computer model. Their effect on utilities and capital cost are assumed to be negligible.
The following reactions are assumed to be stoichiometric:

$$CO + 2\,H_2 = CH_3OH$$
$$CO_2 + 3\,H_2 = CH_3OH + H_2O$$

The gas feed is compressed in the syngas compressor, cooled in the feed gas cooler and water removed in the feed gas separator. The gas is combined with the recycle gas and further compressed to 100 bar in the recycle gas compressor.The gas is heated in the feed/effluent exchanger and passed to the methanol convertor. The copper oxide catalyst in the methanol convertor converts the H_2, CO, CO_2 to methanol with some dimethyl ether, higher alcohols and water produced from side reactions. The reactor products are cooled against reactor feed, then in the product cooler and flashed in the crude methanol separator. The conversion per pass through the reactor is low, thus high recycle ratios are used typically 5 The recycle gas is compressed in the recycle gas compressor and routed back to the reactor feed. Inert components e.g. nitrogen, methane and unreacted hydrogen are purged from the recycle gas stream, and recycled to Steam Reforming, Hydrogen Purification or fuel gas depending on the overall processing configuration. The crude methanol is finally flashed in the letdown vessel and pumped to the downstream gasoline synthesis units or methanol distillation.

MASS BALANCES

Main Input Stream

Flow	100	to	3,220	te/day syngas - biomass
Flow	1,060	to	40,740	te/day syngas - coal

Input components.

1	H_2	2	CO	3	CO_2	4	CH_4
5	C_2H_6	6	N_2	7	H_2O		

Main Output Stream

Crude methanol product components.

1 H_2 2 CO 3 CO_2 4 CH_4 5 C_2H_6
6 N_2 7 H_2O 8 Dimethyl ether 9 Butanol 10 Methanol

Output flow and quality is calculated by John Brown algorithm and varies depending on the feedstock case. However typical quality is as follows (mol%):

Methanol	96.0	Water	3.7
Light ends	0.1	Heavy ends	0.2

By-product Streams

(a) Purge gas to fuel flow calculated by John Brown algorithm

(b) Condensate flow rate calculated by program to suit the saturated vapour pressure of water at 38°C. It is assumed that this water contains zero carbon dioxide etc.

Parameters for Program

Feed sulphur content	< 0.1 ppm
Feed carbon dioxide content, mol% (dry basis)	2 Note (1)
Excess hydrogen in feed, mol% (dry basis)	7 Note (2)
Conversion of carbon monoxide in feed to methanol, mol%	95.1
Conversion of carbon dioxide in feed to methanol, mol%	49.9 Note (1)
Hydrogen conversion to methanol Stoichiometric from CO, CO_2 conversion	
Methanol yield	0.992 x mols CO, CO_2 converted to methanol
Operating pressures, bara	
- downstream feed compressor	85
- HP separator	80
- LP separator	4.8
Loss methanol in low pressure flash gas, mol methanol/100 mol flash gas	5.3

Levels of contaminants in crude met from separators, mol contaminants/100 mol pure methanol

	HP Separator	LP Separator
H_2O	433	0.03
CO	0.173	0.016
CO	21.098	0.44
CH_4	2.445	0.032
C_2H_6	1.044	0.052
N_2	0.093	0.016
Dimethyl ether	0.119	Note (3)
Butanol	0.133	Note (3)

Notes:

(1) Where excess hydrogen is available in the syngas feed, the amount of carbon dioxide entering the plant and conversion of carbon dioxide to methanol is increased to convert the excess hydrogen to methanol.

(2) For certain syngas feedstocks, the amount of hydrogen available in the purge gas stream is insufficient to supply the required flow of hydrogen to the MTG and MTO/MOGD complexes. In these cases, the excess hydrogen in the feed is increased from 7 mol%.

(3) All the dimethyl ether and butanol entering the LP separator is assumed to be routed to the final crude methanol

UTILITIES USAGE

	(Per te/day of methanol product)	
Steam 40 bara	kg/hr	10.46
Steam condensate	kg/hr	*10.46
Cooling water	te/hr	0.852
Electric power	kW	0.075

Notes: (1) HP Steam used to drive compressors.
(2) * indicates production

MAXIMUM TRAIN SIZE

Largest plant built to date is 2500 te/day methanol, with the current limit for a single train considered to be 3000 te/day.

ONSTREAM FACTOR

0.95

CAPITAL COST

Basis: mid 1988, UK, £ sterling. Total battery limits cost of Step 431 is £ 26,537,000 for a plant to produce 1800 te/day of crude methanol product.
Scaling cost capacity factor: Exponent of 0.65
Multiples of streams to be derived from the unit stream factor estimated to be approximately 0.85 x single base stream estimated cost.

MODEL CONSTRUCTED BY:

John Brown Engineers and Co using in-house data with assistance from:
o ICI, Billingham, UK
o Lurgi, Germany
o The following publications:-

(a) Methanol Fuel Economics, 1987 World Methanol Conference, San Fransisco. By D.B.Smith, Chevron USA.

(b) EPRI Report AP - 1592, Research Project 832 - 3. Lignite to Methanol - an Engineering Evaluation of Winkler Gasification and ICI Methanol Synthesis Route. By DM International 1980.

(c) EPRI Report AP - 1962, Research Project 832 - 4. Coal to Methanol - an engineering evaluation of Texaco Gasification and ICI Methanol Synthesis Route. By Fluor 1981.

(d) Investigations on Catalysed Steam Gasification of Biomass, Appendix B, for US DOE. By Batelle 1981.

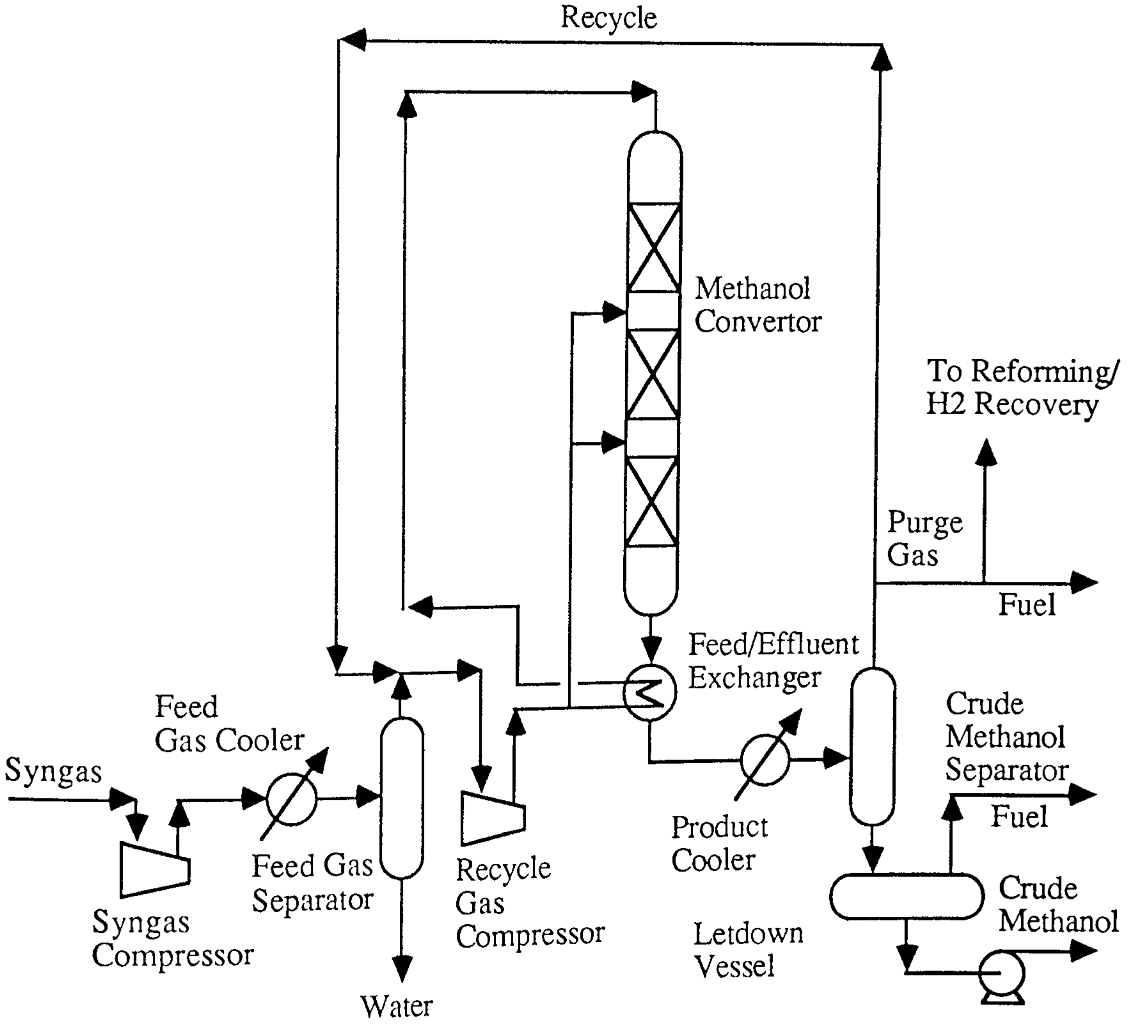


Figure 1 Methanol Synthesis Flow Diagram

STEP 441: MTG SYNTHESIS AND DISTILLATION

Purpose

To convert crude methanol to gasoline using the Mobil MTG (methanol to gasoline) process.

Diagram

The following diagrams are attached:
Figure 1 Overall Block Flow Diagram including Methanol Plant
Figure 2 MTG Reaction Unit
Figure 3 MTG Distillation Unit
Figure 4 Heavy Gasoline Treating Unit

Previous Steps

Step 431: Methanol Synthesis

Following Steps

Offsites: Storage and Facilities

Description and Notes

(a) General

The plant converts crude methanol to gasoline with by-products propane, butanes, water and fuel gas. The facilities included in this step are outlined on the Block Flow Diagram Figure 1, and are summarized below:

- MTG Reaction Unit where methanol is converted into hydrocarbons and water.
- A MTG Distillation Unit for separating the light ends from the gasoline range material and splitting the gasoline into light and heavy components.
- A Heavy Gasoline Treating Unit for reducing the durene content.

The crude methanol composition varies depending on the syngas feed case, which is taken into account in the overall material balance. However the c changes are assumed to have no impact on the utilities and capital cost.

(b) Reaction Unit

A simplified process flow diagram is shown in Figure 2. Methanol is essentially dehydrated into gasoline with water as a by-product of the conversion. The initial step in the transformation of methanol is the reversible catalytic dehydration of methanol to dimethyl ether. The equilibrium mixture dehydrates further over the ZSM-5 zeolite conversion catalyst to give light olefins which in turn react to heavier olefins. Finally, most of the olefins rearrange into paraffins, cycloparaffins and aromatics. Almost no hydrocarbons higher than C_{10} are f due to the shape selective nature of the conversion catalyst.

The reaction path is:

$$2(CH_3OH) \quad <=> \quad CH_3OCH_3 + H_2O$$

Light Olefins + H_2O<=>(C_5 + Olefins)<=>Paraffins,Cycloparafins,Aromatics

The MTG conversion reactor is operated in cyclic mode, alternating reaction and catalyst regeneration. The process operates at essentially 100% conversion of methanol to hydrocarbons and water until the ZSM-5 catalyst deactivates by carbon (coke) formation to an activity level such that only partial conversion of methanol occurs. When methanol breakdown occurs (approx. 0.1 wt% of methanol appearing in the aqueous phase product), the cycle is terminated. The reactor is then switched to the regeneration circuit for diluted air regeneration of the catalyst. The operating sequence is such that only one reactor is undergoing catalyst regeneration at any given time. Conversion is exothermic with the heat released in two steps; about 15% in the dehydration reactor and the remainder in the parallel conversion reactors. To control the conversion reactor temperature rise, effluent gases are recycled and mixed with the effluent from the dehydration reactor before being fed to the conversion reactors. The recycled effluent gases act as a heat sink to absorb the heat of reaction. The reactor effluent is used to heat the recycle gas stream, to vaporize the methanol feed, and to generate steam.

The dehydration reactor can operate for about a year before requiring catalyst regeneration. The conversion reactor regeneration system is used to burn off the coke from the dehydration catalyst. The feedstock to the MTG reaction system is crude methanol, which includes water and dissolved gases from the methanol production. It is preheated, vaporized and superheated in the methanol feed/reactor effluent exchangers. The heat is provided by cooling a portion of the hot conversion reactor effluent. The dehydration reactor is a downflow fixed bed adiabatic reactor in which the methanol feed is converted to an equilibrium mixture of methanol, dimethyl ether and water.

The effluent from the dehydration reactor is mixed with recycle gas from the recycle gas/reactor effluent exchangers and this feed mixture is distributed to the operating conversion reactors. The conversion reactor is a downflow fixed bed adiabatic reactor. The feed mixture is selectively converted by the ZSM-5 zeolite catalyst to gasoline components and water in this reactor.

The hot reactor effluent is split into two streams and later recombined for final cooling in the reactor effluent cooler. One stream is sent to the recycle gas/reactor effluent exchanger; the other is used to heat and vaporize methanol. The partially condensed reactor effluent flows to the product separator, in which the liquid stream separates into a liquid hydrocarbon phase and an aqueous phase. The liquid hydrocarbons are pumped to the Distillation Unit. The MTG water aqueous phase is transformed to the Process Water Treatment Unit or recycled to the gasification and syngas treating units. Part of the gas from the product separator is recycled and the remainder is sent to the Distillation Unit.

(c) MTG Distillation Unit

A simplified process flow diagram is shown in Figure 3. The Distillation Unit separates the light hydrocarbons from the gasoline range components and further separates the gasoline fraction into light gasoline and heavy gasoline. The heavy gasoline containing most of the durene (1,2,4,5 - tetramethylbenzene) formed in the reaction is fed to the HGT Unit.

The light components are separated into fuel gas, propane LPG and a mixed butanes stream. In addition, the hydrocarbon vapours from the MTG Reaction Unit are fed to an absorber in the Distillation Unit to maximize the gasoline recovery. Such a distillation unit consists of six distillation towers: deethanizer, stabilizer, depropanizer, gasoline splitter, lean oil stripper and absorber.

The liquid hydrocarbons are fed to the deethanizer to remove dissolved gases and a portion of the light hydrocarbons. These combined with the vapour hydrocarbons, are charged to the absorber to recover the heavier components. The absorber overhead is sent to the fuel gas system.

The deethanizer bottom is fed to the stabilizer to remove the light hydrocarbons up to butanes. This overhead product is sent to the depropanizer for separation into propane LPG and mixed butanes products. The stabilizer bottom is sent to the gasoline splitter to obtain light gasoline and heavy gasoline fractions. The heavy gasoline, containing the durene, is the feedstock to the HGT Unit. A side stream from the splitter is fed to the lean oil stripper, from where a lean cut is recovered and sent to the deethanizer.

(d) Heavy Gasoline Treating Unit

A simplified process flow diagram is shown in Figure 4. The gasoline produced in the methanol conversion reaction contains durene, a gasoline-range material with a 79°C freeze point. Durene (1,2,4,5 - tetramethylbenzene) is reduced in a Heavy Gasoline Treating Unit to meet finished gasoline quality requirements. Gases produced during heavy gasoline treating are stripped out of the gasoline and sent to the fuel gas system. The treated heavy gasoline is blended with light gasoline from the Distillation Unit to produce a finished gasoline with about 2 wt.% durene.

The HGT Unit is similar in principle to the mild catalytic hydrotreating processes used in petroleum refineries. The heavy gasoline from the Distillation Unit is combined with a hydrogen rich stream and preheated in the reactor effluent/feed exchanger before entering the reactor. The reactor effluent stream is cooled with process streams and cooling water or air before entering the separator. The treated heavy gasoline stream from the separator is stabilized in the product stripper and pumped to storage. The hydrogen rich vapour stream from the separator is recycled by the recycle compressor with a small purge to the fuel gas system.

Mass balance

Main Input Stream

Flow	80	to	1950	te/day crude methanol - biomass
Flow	920	to	24100	te/day crude methanol - coal

Input Components

1 H_2	2 CO	3 CO_2	4 CH_4	5 C_2H_6
6 N_2	7 H_2O	8 Dimethyl ether	9 Butanol	10 Methanol

The crude methanol composition varies depending on the feedstock case. A typical quality is as follows:

Methanol	96 mol %	Water	3.7	mol %
Light ends	0.1 mol %	Heavy ends	0.2	mol %

Auxiliary Input Stream

Hydrogen 99.9 mol/% purity.

Input flow = crude methanol flow * 0.000396 (wt)

Main Output Streams

Blended gasoline of the following quality:

Gravity, °API 64

Octane numbers;

Research, clear	93
Motor, clear	83
(R+M)/2	88
Reid vapour pressure, bar	0.69
Durene content, wt. %	2

No detectable sulphur, nitrogen, oxygenates

Output flow = input crude methanol flow * 0.35794 (wt) + heavy ends in the methanol feed.

By-Product Streams

(a) Fuel Gas

Calorific value = 5 540 kcal/kg

Output flow = input pure methanol flow * 0.00932 (wt) + light ends in the methanol feed

(b) Propane

Composition, vol.%

Ethane	4.0	Propylene	3.	Propane	90.5
Isobutane	1.	Butenes	0.1		

Output flow = input pure methanol flow * 0.02001 (wt)

(c) Butanes

Composition, vol.%

Propane	0.1	Isobutane	74.2	Butenes	8.1
N. Butane	17.4	Pentanes	0.2		

Output flow = input pure methanol flow * 0.04802 (wt)

(d) Water

BOD, mg/l	800	-	2 000
COD, mg/l	1 000	-	3 500

Output flow = input pure methanol flow * 0.56471 (wt) + water in the methanol feed

BATTERY LIMIT CONDITIONS

FEED	- methanol	38	25.5
	- hydrogen	38	43.8
Products	- light gasoline	38	5.9
	- heavy gasoline	38	9.0
	- fuel gas	38	6.9
	- propane	38	16.2
	- butanes	38	6.9
	- water	38	11.7

Utilities Usage

(per te/d of pure methanol feed)

Steam, 5 bar	kg/hr	* 1.402
Steam, 50 bar	kg/hr	6.35
Steam, 100 bar	kg/hr	20.49
Steam condensate	kg/hr	* 30.94
Cooling water (15°C rise)	kg/hr	2457
Boiler feed water	kg/hr	6.44
Fuel gas (LHV)	MJ/hr	0.835
Electric power	KW	1.763

Note: * Indicates production

MAXIMUM TRAIN SIZE

1950 te/day of blended gasoline

ONSTREAM FACTOR

0.937

CAPITAL COST

Total battery limits cost of step 441 is £ 70 million, for a plant to produce 1150 te/day of blended gasoline. Scaling cost capacity factor:

- Exponent of 0.6 for gasoline production range of 575 to 1150 te/day
- Exponent of 0.85 for gasoline production range of 1150 to 1955 te/day

MODEL CONSTRUCTED BY:
John Brown Engineers and Constructors based on data provided by Mobil Research and Development Corporation, Princeton, New Jersey, USA.

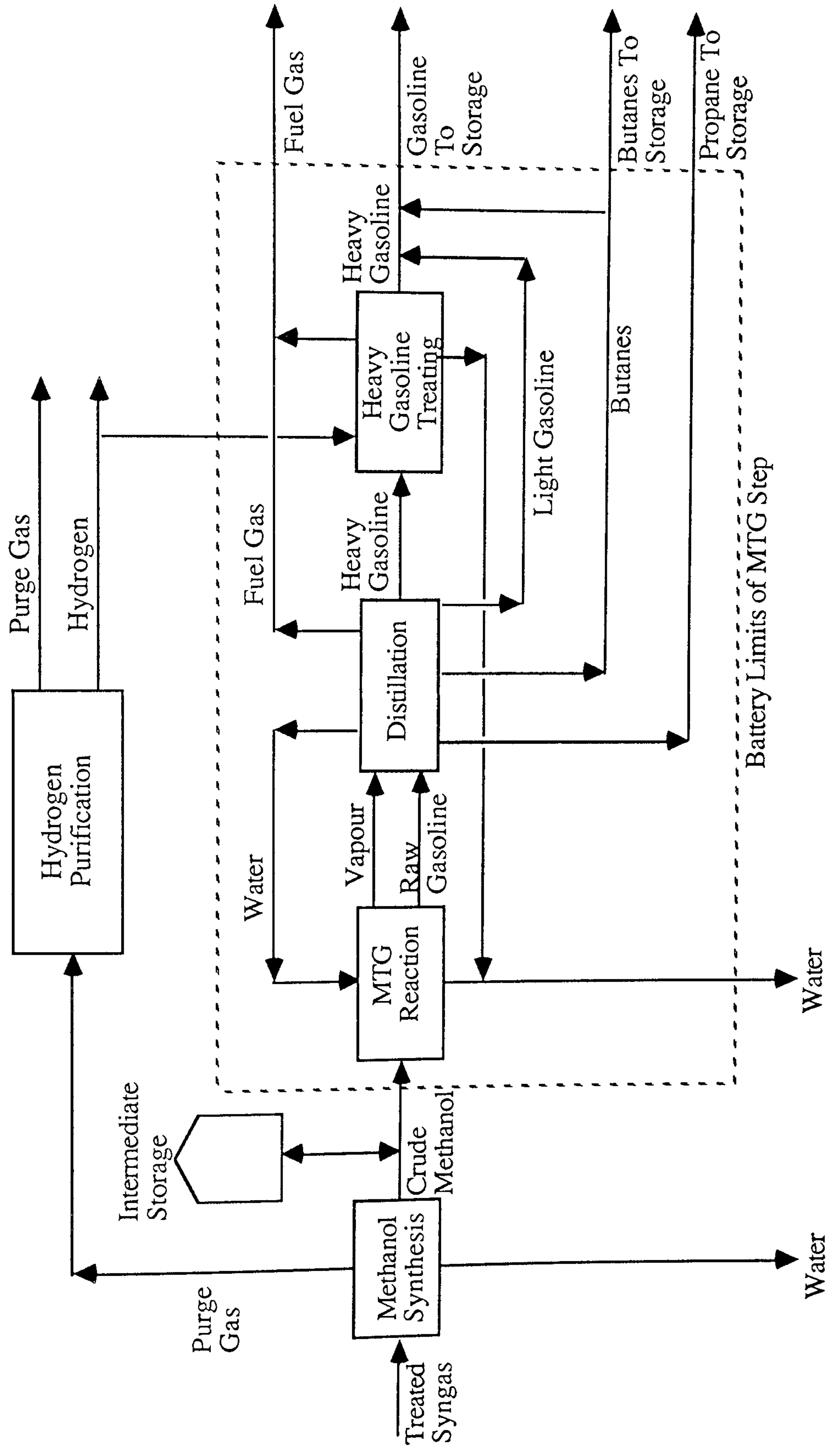


Figure 1 Methanol To Gasoline Block Flow Diagram

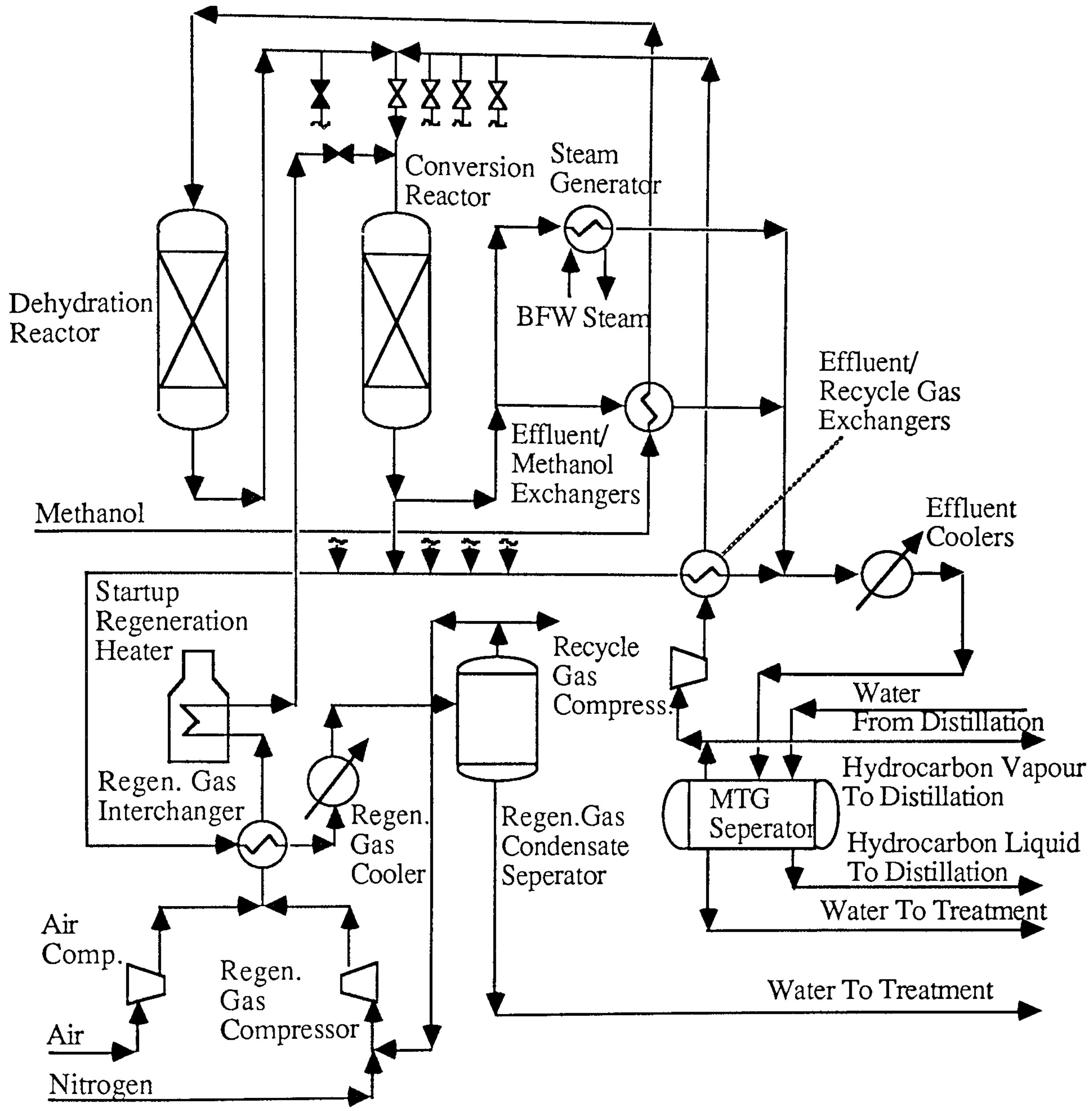


Figure 2 MTG Plant Reaction Unit Simplified Process Flow Diagram

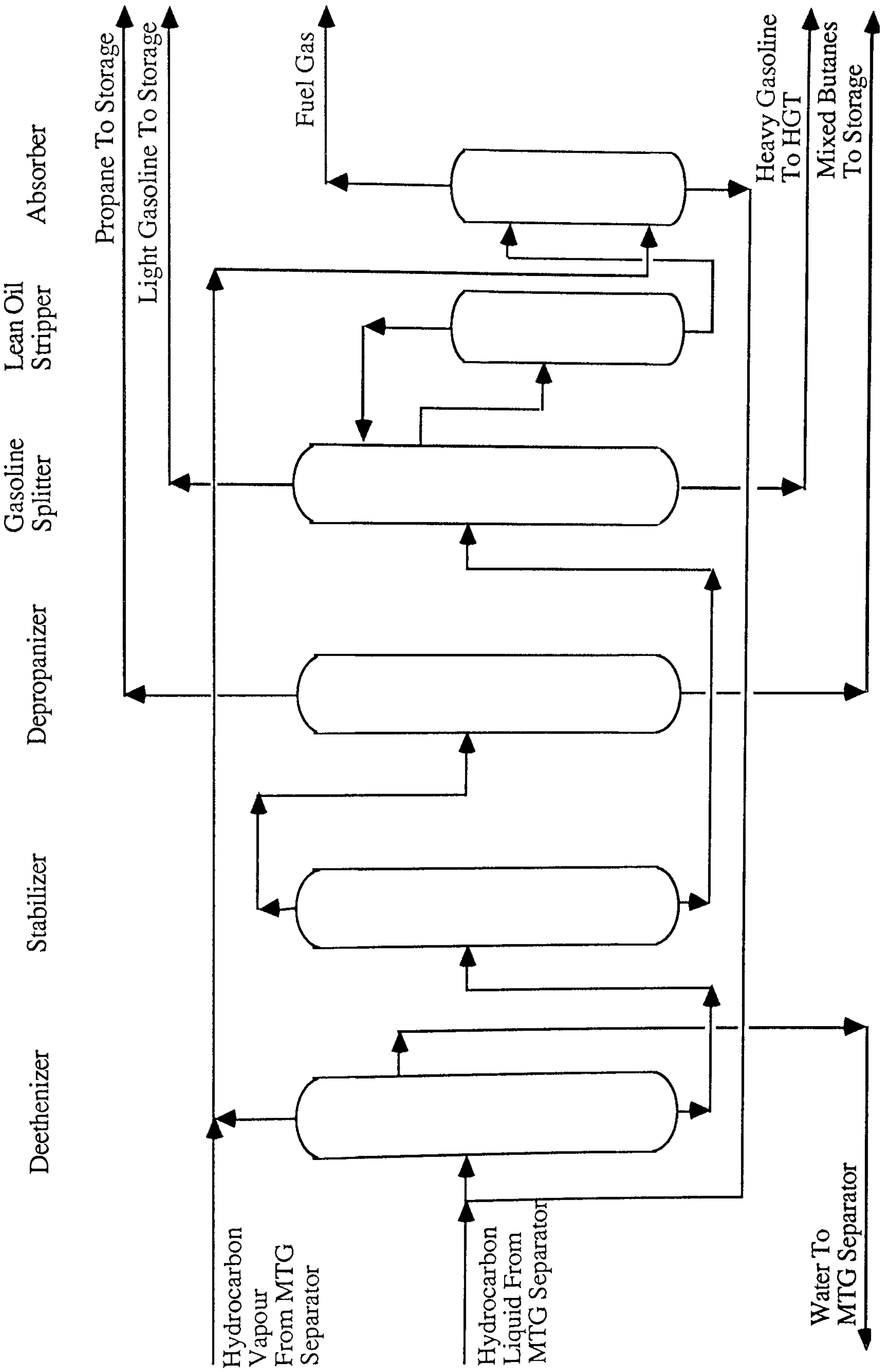


Figure 3 MTG Distillation Unit Simplified Process Flow Diagram

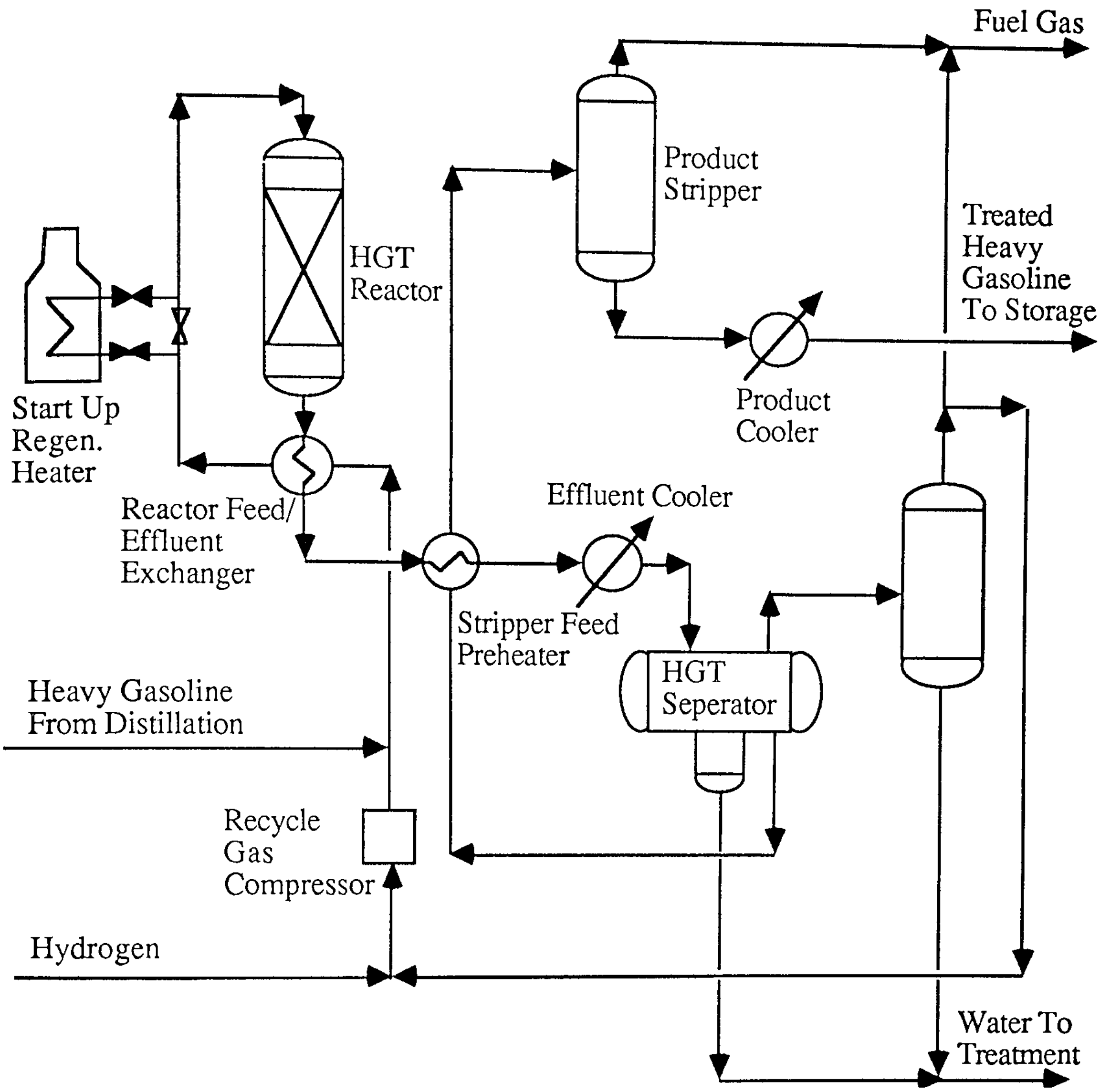


Figure 4 MTG - HGT Unit Simplified Process Flow Diagram

STEP 442: MOGD SYNTHESIS AND DISTILLATION

Purpose

To convert dewatered methanol to a gasoline, jet fuel and diesel using the Mobil MTO (methanol to olefines) and MOGD (Mobil olefins to gasoline/distillate) processes.

Diagram

The following diagrams are attached:
Figure 1 Overall Block Flow Diagram including Methanol Plant
Figure 2 MTO Unit
Figure 3 MTG Reaction Distillation Unit
Figure 4 HDT Unit
Figure 5 HF Alkylation Unit

Previous steps

Step 601: Methanol Distillation

Following steps

Offsites: Storage and Facilities

Description and notes

(a) General

The plant converts dewatered methanol to gasoline, jet fuel and diesel products. By-products include propane, water and fuel gas. The plant imports normal butane for finished gasoline RVP adjustment, and hydrogen for use in the HDT unit. The MTG/MOGD complex can, if required, be adjusted to give different yields of gasoline, jet fuel and diesel. The data presented corresponds to a distillate/gasoline (D/G) volume ratio of 1.28. The D/G ratio can be increased to 1.5 by routing the heavy aromatics stream to distillate, instead of gasoline. The D/G ratio can be reduced below 1.28 by routing the MTO C_5+ product around the MOGD Unit directly to gasoline blending. Still lower D/G ratios can be obtained by adjusting MTO and/or MOGD operations. The facilities included in this step are outlined on the Block Flow Diagram Figure 1 and are summarized below:

- A MTO Unit which converts methanol to light olefins with some paraffins, cycloparaffins and aromatics.
- A MOGD Feed Preparation Unit which receives the hydrocarbon streams from the MTO Unit and processes them to produce a MOGD Unit feedstock of light olefins, a heavy aromatics stream and an ethylene recycle stream for the MTO Unit.
- A MOGD Unit where light olefins are oligomerized into gasoline and distillate products.
- A distillate Hydrotreating (HDT) Unit where the olefinic MOGD distillate is saturated to improve the cetane number, and fractionated to jet fuel and diesel products.
- A HF Alkylation Unit which reacts propylene and butylenes with isobutane to produce alkylate which is routed to the gasoline product.
- Intermediate storage between the major process units, where considered necessary.
- Component storage for the various streams routed to gasoline with an automated gasoline blending unit.

(b) MTO Unit

A simplified process flow diagram is shown in Figure 2. During conversion methanol is essentially dehydrated into hydrocarbons with water as a by-product. The initial transformation step is the reversible catalytic dehydration of methanol to dimethyl ether. The equilibrium mixture dehydrates further to yield light olefins which in turn react to heavier olefins. Finally, the olefins rearrange into paraffins, cycloparaffins and aromatics. Almost no hydrocarbons higher than C10 are formed due to the shape selective nature of the catalyst. MTO and MTG operations differ from each other by the reactor operating conditions. In MTO, olefin formation is maximized, up to 75 wt.%, while in MTG paraffin/aromatic formation is maximized. Sufficient reactivity, however, is maintained in MTO operation for complete conversion of methanol and dimethyl ether.

The MTO reactor contains a fluidised bed of zeolite catalyst which is continuously regenerated. At a methanol charge rate of 5 000 metric tons/SD two reactor/regenerator trains are provided. Vaporized methanol and ethylene recycle from the MOGD Feed Preparation Unit are reacted by upward flow through the fluidized bed. The exothermic heat of reaction is removed by steam generation in internal coils. The raw methanol feed is preheated, vaporized and superheated by heat exchange with the reactor effluent. An additional steam vaporizer is required for start up and trim heating.

The elutriated catalyst particles in the reactor effluent are removed in a series of cyclones located within the reactor. Additional fines are recovered in an external separation unit and returned to the reactor. Three phases - a vapour and two immiscible liquids - are obtained in the product separator. The vapour overhead of light olefinic hydrocarbons is sent to the compression train area in the MOGD Feed Preparation Unit. The two liquid phases are separated by internal weirs into a hydrocarbon phase, consisting mainly of heavy paraffins and aromatics, and an aqueous phase. The water product is pumped to the wastewater treatment plant or can be returned to the coal slurry facility. The hydrocarbon product is sent to the fractionation area in the MOGD Feed Preparation Unit. The zeolite catalyst is deactivated by coke deposition. To restore activity catalyst is withdrawn continuously and regenerated by burning the coke. The coked catalyst flows down through a standpipe to a lift pipe. The catalyst is then lifted to the regenerator by a flue gas recycle stream. Flue gas recycle is used to control the oxygen concentration and, thus, the regeneration temperature. In a coal based synfuels plant nitrogen from the air separation plant may be substituted for the flue gas recycle system. Air is introduced into the dense bed for coke combustion. The elutriated catalyst is removed from the regenerator effluent in a series of internal cyclones and returned to the bed. The net combustion gases are sent to a catalytic converter, or to a furnace, for conversion to CO_2 before exhausting to the atmosphere.

(c) MOGD Feed Preparation Unit

The MOGD Feed preparation Unit receives the hydrocarbon streams from the MTO Unit and processes them to produce a MOGD Unit Feedstock, product blending stocks and an ethylene recycle stream for the MTO Unit. The MTO vapour product is recovered in a compression train followed by an absorption step. The raw MTO liquid product is stabilized and fractionated into blending stocks. Ethylene recycle is obtained from a cryogenic recovery unit.

(d) MOGD Reaction and Distillation Unit

A simplified process flow diagram is shown in Figure 3. The MOGD Unit oligomerizes light olefins into gasoline and distillate boiling range hydrocarbons over the ZSM-5 zeolite catalyst in a series of three fixed bed reactors. A fourth reactor is out of service at any given time for regeneration. Light olefin conversion is over 90 wt.%. The reaction is exothermic. A model reaction pathway is shown below:-

Light olefins <=> Gasoline <=> Distillate

The reaction is not true oligomerization in that there is both a forward and reverse reaction. For example, propylene, $C_3=$, will oligomerize forward to yield $C_6=$, $C_9=$, $C_{12}=$, etc. As it does, however, the above products will crack back to lower molecular weight olefins, which in turn will oligomerize forward. The net result is a product containing compounds with continuous carbon numbers, i.e., C_4, C_5, C_6, C_7, C_8, C_9 etc. The average product carbon number is a function of process conditions, i.e. temperature, pressure and contact time. In addition, the molecular weight of the liquid recycle used for reactor temperature control also affects the final product composition.

Because of the shape selectivity of the ZSM-5, a very well defined product structure is obtained. Generally, it is a long straight chain of carbon atoms with an attached methyl group about every four carbon atoms. Ethyl or longer side chains are also present in smaller amounts.

In combination with the MTO technology, the distillate mode of MOGD operation is used. A major factor in MOGD Unit Design is controlling the heat of reaction. The light olefin rich feed from the MOGD Feed Preparation Unit and the gasoline recycle are used to cool the effluents from the three reactors onstream. The feed temperature is then raised in a charge heater to the reaction temperature. By using three reactors with intercooling and liquid recycle the temperature rise in each reactor is held within the acceptable limit. With certain feedstocks a small hydrogen partial pressure is required to maintain acceptable catalyst ageing cycle rates. The make-up hydrogen is obtained from the hydrogen plant. To maintain the desired hydrogen partial pressure, a small hydrogen recycle stream is obtained from the MOGD Unit separation section. The effluent from the third reactor after initial heat exchange with the feed is sent to the separation section where it is separated into debutanizer feed, liquid recycle and recycle hydrogen streams. The separation section consists of separators, heat exchangers and coolers.

The butane and lighter components in the debutanizer overhead are sent to the Alkylation Unit. The debutanizer tower bottoms is fed directly to the gasoline/distillate splitter. Its overhead goes to gasoline blending. The olefinic distillate bottoms is cooled and pumped to storage for the HDT unit.

Catalyst regeneration is required when the maximum design inlet reactor temperature is reached. The design cycle length between regenerations for each reactor is 12 days. Initial cycle length is estimated to exceed 50 days. Regeneration consists of in-situ burning of the coke by using controlled quantities of air in an inert atmosphere. Regeneration time is estimated to be about 3 days per reactor. The regeneration loop consists of air and recycle gas compressors, recycle gas driers, knockout pots, exchangers and air/recycle gas heater.

(e) HDT Unit

A simplified process flow diagram is shown in Figure 4. The purpose of the Hydrotreater is to saturate the olefinic MOGD distillate product in order to improve combustion quality and storage stability. Olefin saturation results in a slight increase in the distillate volume. In addition, a nominal amount of fuel gas and naptha are produced. A commercial hydrotreating catalyst is used.

The untreated MOGD distillate is combined with the make-up hydrogen from the hydrogen plant and recycle gas. This mixture is preheated by heat exchange with the reactor effluent and further heated to reaction temperature in the charge heater.

To control the temperature rise from the exothermic heat of reaction, the reactor consists of multi-catalyst beds with inter bed quenching by cold untreated distillate and/or recycle gas. Reactor effluent is then cooled and condensed by heat exchange and flashed in the product separator.

The separator vapour is the recycled gas. The unit pressure is controlled by a bleed stream from the separator. The separator liquid is stripped of light ends and gasoline in a tower. A small stripper is used to prepare specification jet fuel. The tower bottoms is the diesel fuel product. Both are pumped to storage. Sulphide addition is required to maintain a minimum H_2S concentration in the recycle gas for catalyst activity maintenance. Scrubbing the HDT unit fuel gas is expected not to be required because the total sulphur concentration is low.

Catalyst decoking is expected to be required only once every 1 to 2 years with the clean feed and close control of the bed temperature rise. There are no special requirements for the conventional steam/air regeneration to be used. Standard sulphiding chemical injection is required after regeneration.

During catalyst regeneration the sulphided catalyst will be oxidized forming sulphur dioxide. Caustic scrubbing is used to remove it from the regeneration off-gases. The discharge effluent is sent to waste water treating. After regeneration and during initial unit start up, the oxide form of the catalyst is pretreated to the sulphide form. Dimethyl sulphide addition is generally used in the sulphiding step.

Appropriate conventional procedures are used to control and limit H_2S emissions. The sulphiding system is also used during normal unit operation to maintain a minimum H_2 level in the recycle gas specified for the specific catalyst used.

(f) HF Alkylation Unit

A simplified process flow diagram is shown in Figure 27. Alkylation is the reaction of propylene and butylene with isobutane over an acid catalyst to form highly branched heptanes and octanes (alkylate). Alkylate is a high quality gasoline blending component. Alkylation is used in the MTO/MOGD plant to utilize isobutane in the gasoline product rather than in the less economical C_4 LPG product. With the conventional Alkylation Unit tower system, a N-butane product for gasoline pressuring and a C_3 LPG product are also produced. The C_3 and C_4 hydrocarbons from the MOGD Unit debutanizer are compressed and charged to a high pressure deethanizer. The overhead product, C_2 and lighter components, is sent to the MOGD Feed Preparation Unit for maximum olefin recovery and utilization. The deethanizer bottoms are sent to the conventional commercial HF Alkylation Unit.

The C_3 and C_4's from the deethanizer are dried, mixed with recycle isobutane and contacted with HF acid, with the heat of reaction removed in the acid cooler. The reactor products are separated in the settler, and routed to the main fractionator. The alkylate product from the bottom of the main fractionator is cooled and routed to gasoline blending. Normal butane is withdrawn as a side draw, routed through a KOH treater to remove traces of HF and routed to gasoline blending. The main fractionator overheads are fractionated in the depropaniser and propane stripper to remove HF from the propane. The traces of HF are removed in the defluorinator and KOH treater, and the propane routed to storage.

Mass balance

Main Input Stream

Flow	80	to	1860	te/day syngas - biomass
Flow	900	to	23090	te/day syngas - coal

Input Components, wt.%

1	Methanol	98.59
2	Dimethyl Ether	0.05
3	Butanol	0.05
4	Water	1.31

Auxiliary Input Stream

I. Hydrogen

99.5 mol/% purity.

Input flow = pure methanol flow * 0.0014 (wt)

II. Normal butane

Input flow = pure methanol flow * 0.0153 (wt)

Main Output Streams

I. Gasoline

Blended gasoline of the following quality:

Gravity, °API	61.3
Octane numbers;	
Research, clear	93.9
Motor, clear	86.2
(R+M)/2	90.1
Reid vapour pressure, bar	0.76
Sulphur ppm	< 5

No detectable nitrogen, oxygenates.

Output flow = input crude methanol flow * 0.2503 (wt) + heavy ends in methanol feed

II. Jet Fuel

Gravity, °API	47.4	Sulphur wt %	< 0.04
Freeze point, °C	< -60	Flash point, °C	50
Smoke point, mm	>30	Aromatics, vol %	< 5
Olefins, vol %	< 2		
JFTOT Breakpoint, °C	343	Deposit Code	< 3
Pressure Drop, mm Hg	0		

Output flow = input pure methanol flow * 0.1190 (wt).

III. Diesel Fuel

Gravity, °API	40.5	Sulphur wt %	< 0.04
CFPP, °C	<-30	Flash point, °C	100
Cetane number	58	Smoke point, mm	<-30
Aromatics, vol %	< 5	Olefins, vol %	<2

Output flow = input pure methanol flow * 0.0360 (wt)

By-Product Streams

I. Fuel Gas

Calorific value = 9 400 kcal/kg

Output flow = input pure methanol flow * 0.0484 (wt) + light ends in methanol feed

II. Water

BOD, mg/l	3 000 - 3 600
COD, mg/l	5 700 - 6 000

Output flow = input pure methanol flow * 0.5630 (wt) + water in methanol feed

BATTERY LIMIT CONDITIONS

		°C	Bar
FEED	- methanol	38	25.5
	- hydrogen	66	42.1
	- import nC4	30	6.9
Products	- gasoline	43	5.5
	- jet fuel	43	5.5
	- diesel	43	5.5
	- water	43	1.7
	- fuel gas	43	10.3

Utilities Usage

(per te/d of crude methanol feed)

Steam, 3.5 bar	kg/hr	*3.094
Steam, 11 bar	kg/hr	1.61
Steam, 41.4 bar	kg/hr	*0.78
Steam condensate	kg/hr	*9.934
Cooling water (15°C rise)	te/hr	0.4792
Boiler feed water	kg/hr	13.02
Fuel gas (LHV)	MJ/hr	16.52
Electric power	KW	1.14

Note * indicates production

MAXIMUM TRAIN SIZE

MTO	25000	te/day methanol feed
MOGD	5000	te/day methanol feed

ONSTREAM FACTOR

0.9

CAPITAL COST

Basis: Mid 1988, UK, £ Sterling. Total battery limits cost of step is as follows:-

Methanol feed range te/day	Feed Base plant te/day	No. Trains MTO	No. Trains MOGD	Base plant Installed Cost £	Scaling Factor (power)
2 000 to 4 000	2 500	1	1	89.7	0.7
4 000 to 6 000	5 000	2	1	150.4	0.7
6 000 to 9 000	7 500	3	2	220.8	0.75

MODEL CONSTRUCTED BY:

John Brown Engineers and Constructors based on data provided by Mobil Research and Development Corporation, Princeton, New Jersey, USA.

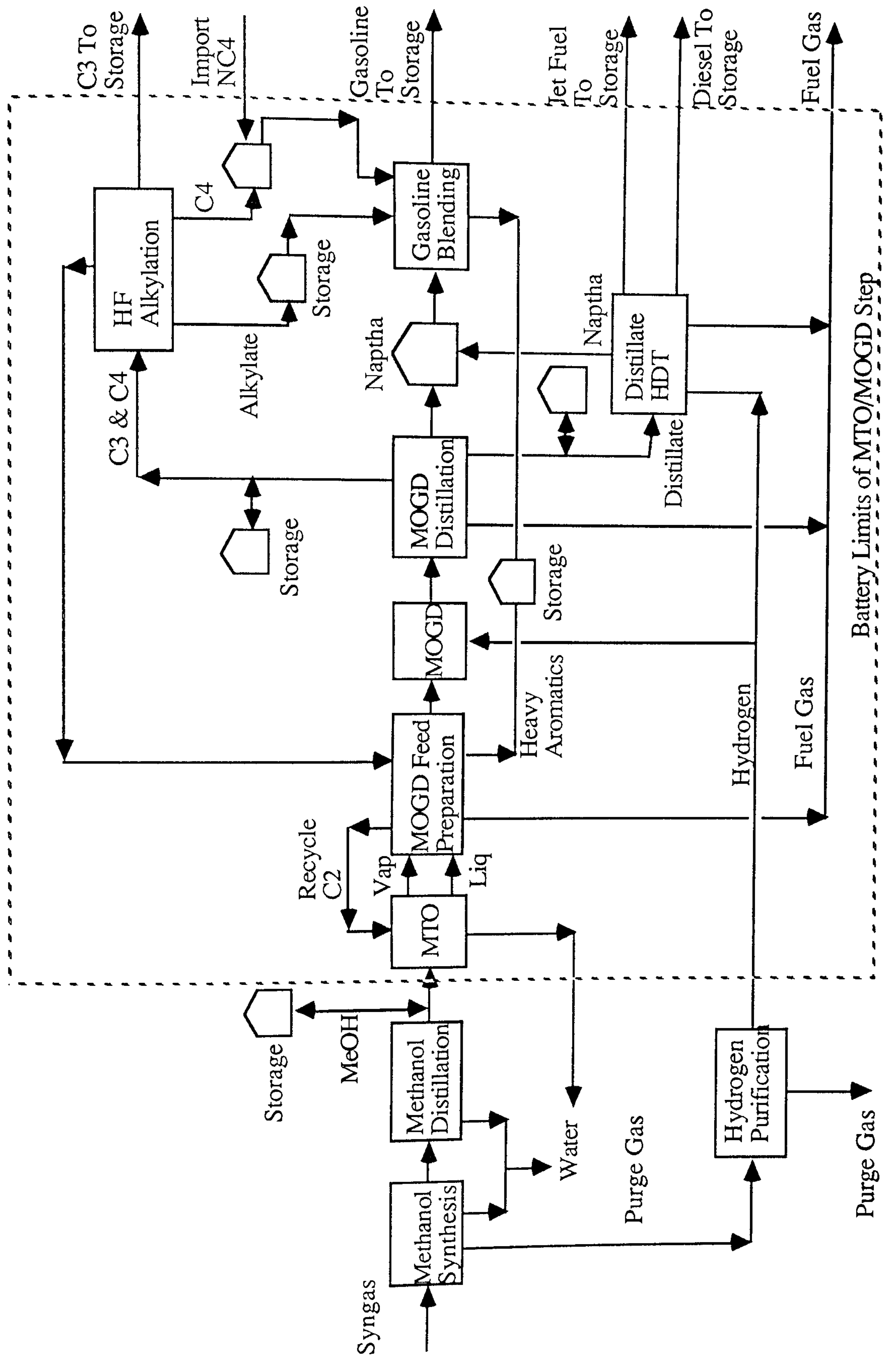


Figure 1 MTO/MOGD Block Flow Diagram

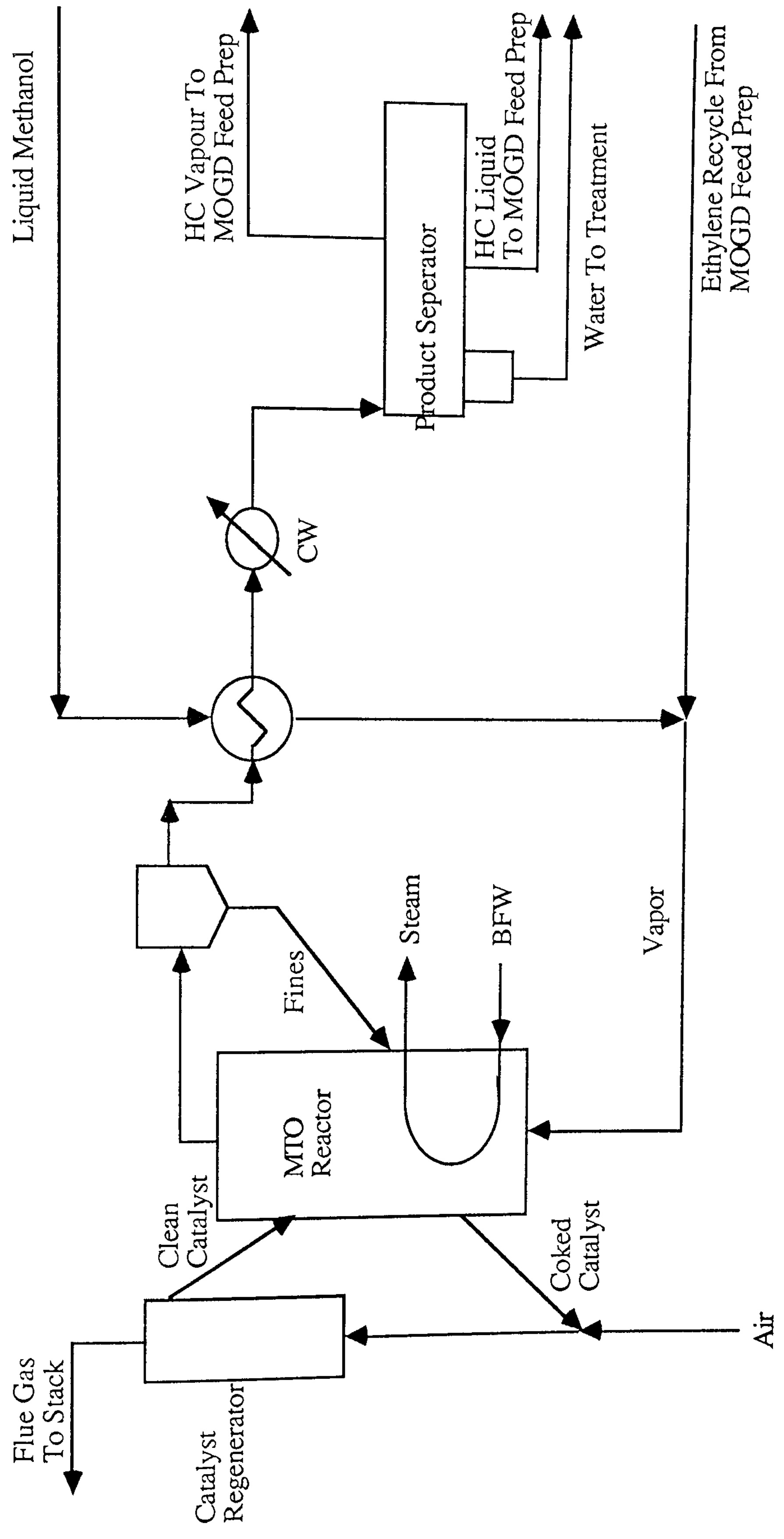


Figure 2 MTO Unit -One Train Simplified Process Flow Diagram

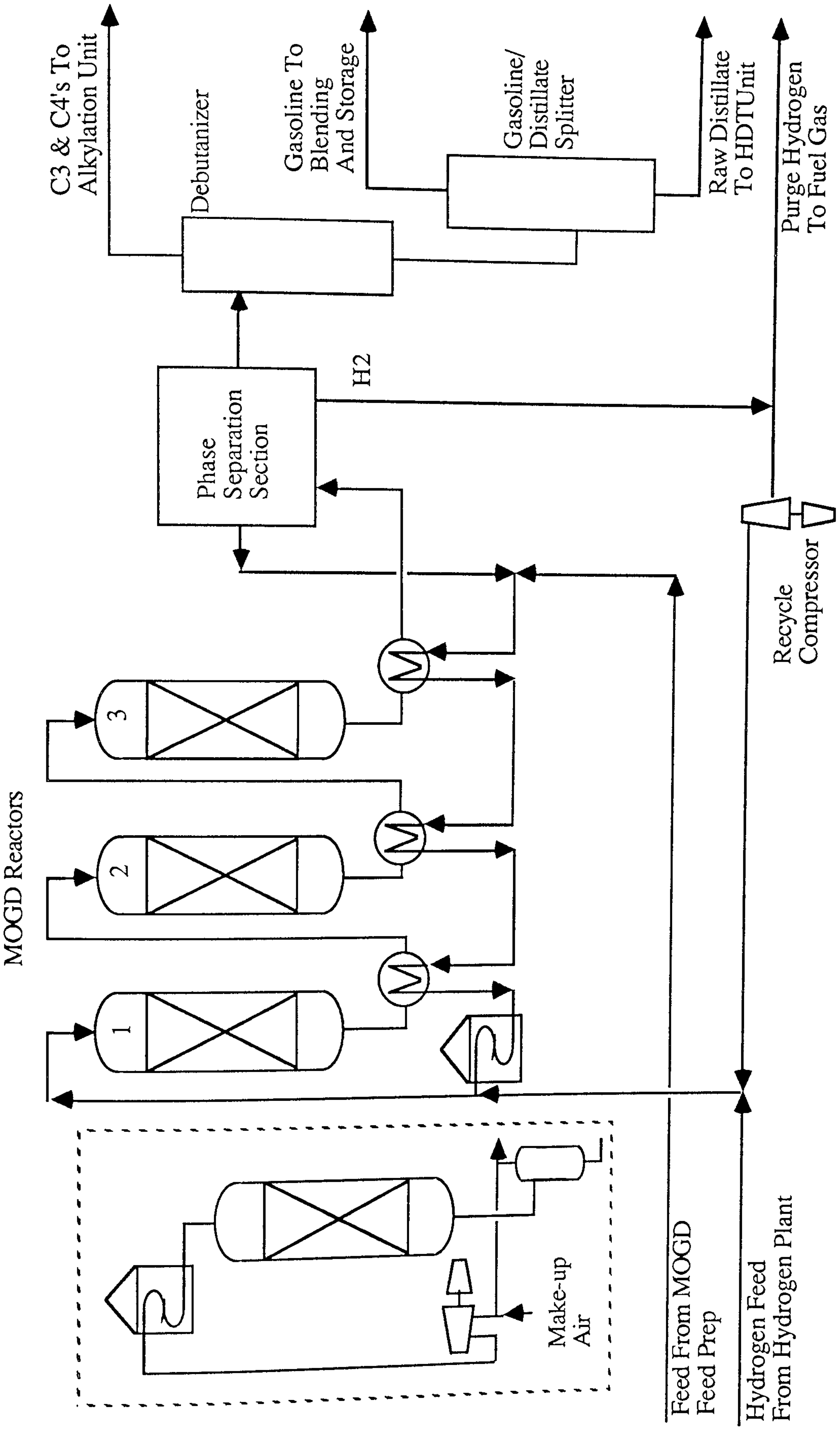


Figure 3 MOGD Reaction Unit Simplified Process Flow Diagram

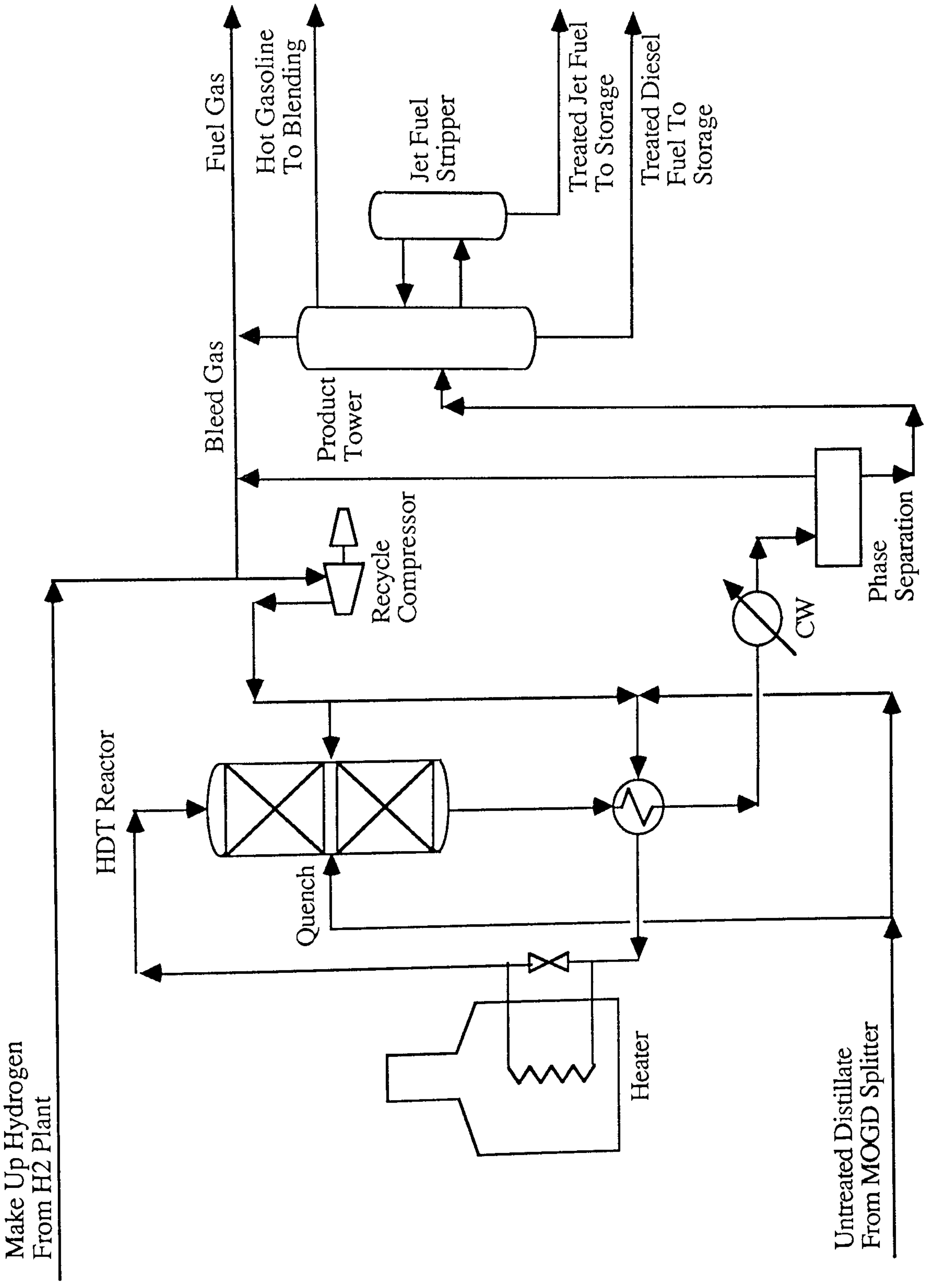


Figure 4 HDT Unit Simplified Process Flow Diagram

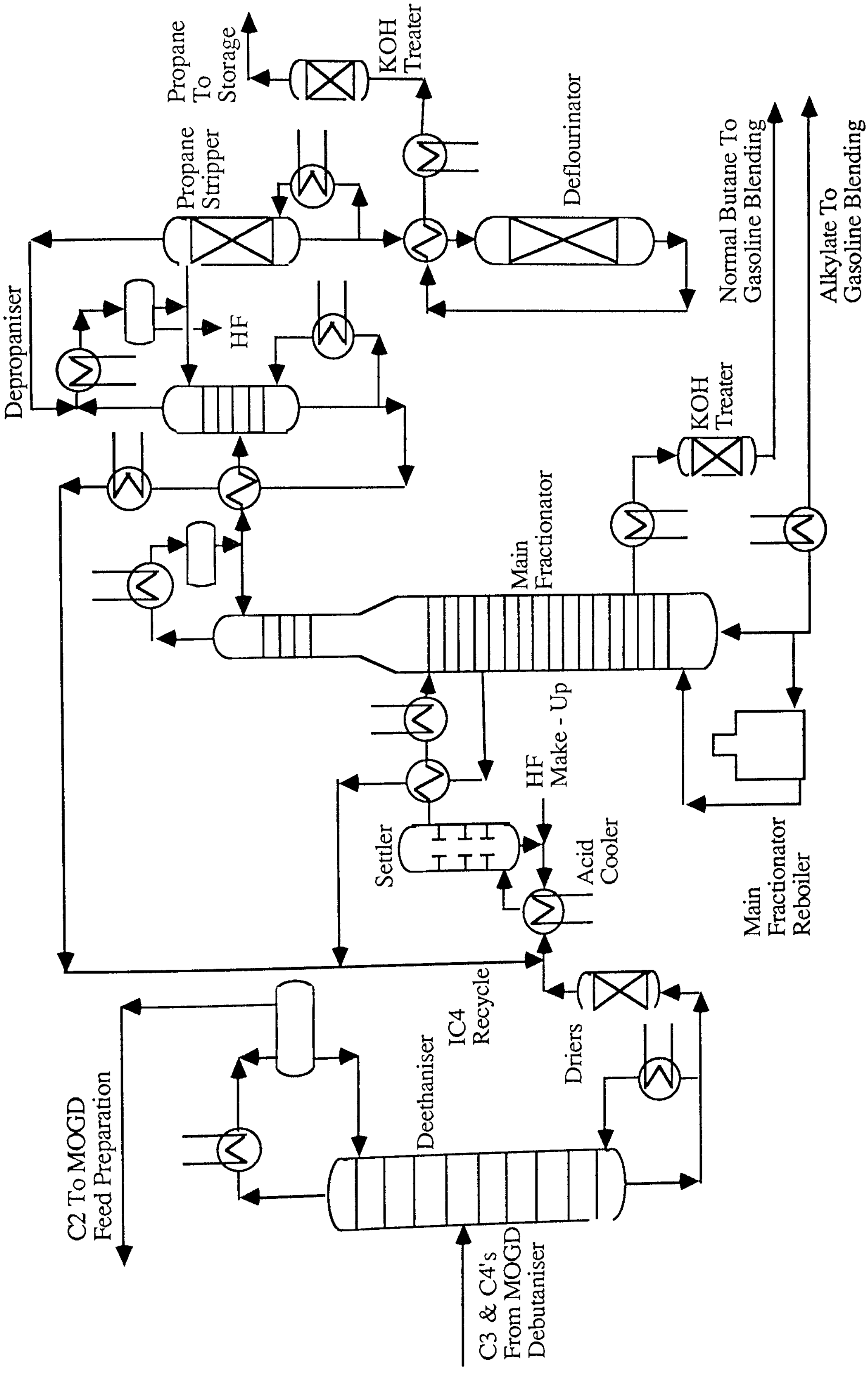


Figure 5 HF Alkylation Unit Simplified Process Flow Diagram

STEP 421: FISCHER TROPSCH SYNTHESIS AND DISTILLATION

Purpose

To convert syngas to naphtha, kerosine and gas oil using the Shell Middle Distillate Synthesis process (SMDS).

Diagram

The following diagram is attached:
Figure 1 Block Flow Diagram

Previous Steps

Offsites: Storage and Facilities

Description and Notes

(a) General

Fischer Tropsch type catalysts are currently only commercially used in the Arge and Synthol processes in operation at Sasol in South Africa. A number of current development programs are aimed at improved performance targets for Fischer Tropsch synthesis. It appears that Shell are at an advanced stage in the development of more productive catalysts and to produce a range of conventional hydrocarbon products to match those currently produced from crude oil. Thus the Shell Middle Distillate Synthesis (SMDS) route is elected for this step. The SMDS complex converts syngas to naphtha, kerosine and gas oil with by-products fuel gas and water. The facilities included in this complex are outlined on the block flow Diagram, Figure 1, and are summarized below:

- A Heavy Paraffin Synthesis Unit (HPS) where hydrogen and carbon monoxide are converted to a waxy product using Fischer Tropsch catalysts.
- A Heavy Paraffin Conversion Unit (HPC) which cracks the wax into middle distillate fractions.
- A distillation unit to separate the HPC products into light ends, Naptha, Kerosine and Diesel products.
- A steam Reforming Unit which converts part of the light ends by-product from the Fischer Tropsch reactions to provide feed to the Hydrogen recovery unit.
- A Hydrogen Recovery unit to recover hydrogen from the Steam Reformer product. The high purity hydrogen stream is routed to the HPC and the syngas hydrogen to carbon monoxide molar ratio.

The amounts of nitrogen and hydrocarbons in the syngas feed vary depending on the type of gasifier, which are taken into account in the computer model material balance. It is assumed however that the level of inerts have no effect on utilities and capital cost.

(b) Heavy Paraffin Synthesis (HPS)

The Heavy Paraffin Synthesis Unit is the heart of the SMDS process in which mainly normal paraffins are formed by means of Fischer Tropsch synthesis. The reaction mechanism follows the well known Schulz/Flory polymerization kinetics, which is characterized by the probability of chain growth, (SC) vs. chain termination. There is always a regular molecular weight distribution in the total product and a high SC corresponds with a high average molecular weight of the paraffinic product. The reaction takes place in a fixed bed multi-tubular reactor in which a proprietary Shell catalyst is used.

$$CO + 2\,H_2 = (-CH_2-) + H_2O$$

During the reaction a considerable amount of heat is released. The heat generated in the catalyst filled tubes is recovered, using boiling water, to produce steam. The catalyst has a life of several years, including infrequent in-situ regeneration. Spent catalyst, the only solid waste, can conceivably be returned to the manufacturer for metals recovery.

(C) Heavy Paraffin Conversion Unit (HPC)

One of the prerequisites for attaining a high selectivity towards middle distillates is a sufficiently high average molecular weight of the raw product. This product, which is predominantly waxy but contains small amounts of olefins and oxygenates, has to be isomerized and cleaned up, while little hydrocracking should take place cocurrently. A commercial Shell catalyst is used in a trickle-flow reactor as is employed in refinery hydrocracking operations, but under rather mild conditions. The HPC is operated in a recycle mode, conversion per pass is kept low to optimise retention of the heavier fractions. By adjusting cut-points and recycle rates, the composition of the product package can, within a certain margin, be adjusted to local requirements.

(d) Distillation

The distillation unit is designed to distil the HPC product stream into the following products:

- fuel gas
- naphtha
- kerosine
- gas oil.

MASS BALANCE

Main Input Stream

Flow	100	to	3200	te/day syngas - biomass
Flow	1000	to	40700	te/day syngas - coal

Input components

1. H_2
2. CO
3. CO_2
4. CH_4
5. C_2H_6
6. N_2
7. H_2O

Sulphur content < 0.02 ppm volume.

Auxiliary Input Stream

None

Main Output Streams

The SMDS complex can be operated in a variety of modes to suit the final desired product slate. Two typical modes of operation yield the following products (wt%):

	Gas Oil Mode	Kerosine Mode
Fuel Gas	5.4	5.5
Naptha	5.9	5.2
Kerosine	9.6	18.3
Gasoil	23.5	15.5
Water	55.6	55.5

It is "assumed" that one ton of the above products are produced from one ton of hydrogen and carbon monoxide in the main syngas feed.

(a) Naphtha

The naphtha quality is similar to that obtained from crude oils. It is highly paraffinic and free from nitrogen and sulphur and is therefore ideal as a petrochemical feedstock e.g. ethylene production. If required for use as a gasoline blending component, Catalytic Reforming would be needed.

(b) Kerosine

The kerosine quality is summarized below. It easily meets all jet fuel specifications (except density) and can be used as a blending stock to upgrade lower quality products from crude oil distillation.

Boiling range,	°C	150-250
Density at 15°,	kg/m3	750
Freezing point,	°C	-47
Smoke point, mm		> 50

(c) Gas Oil

The gas oil quality summarized below easily meets all diesel specifications. It can be used as blending stock to upgrade lower quality products from crude oil distillation.

Boiling range, °C	250 - 360
Density at 15°C, kg/m3	780
Pour point, °C	-10
Blending cetane number	75

Parameters for program

"Assumed" minimum feed pressure, bara	40
"Assumed" conversion of H_2, CO in HPS, mol%	98
"Assumed" main syngas feed hydrogen to carbon monoxide molar ratio	1.7

UTILITIES USAGE

(Per te/day of distillate products)
Utilities usage data are not available. However, it is "assumed" that the SMDS complex is self sufficient in fuel and steam. The following values are "assumed":

Process condensate kg/hr	20
Boiler feed water kg/hr	300
Blowdown kg/hr	15
Electric Power kW	6

MAXIMUM TRAIN SIZE

The maximum train size corresponds to 1,450 te/day of distillate products.

ONSTREAM FACTOR

"Assumed" 0.95

CAPITAL COST

Basis: Mid 1988, UK, £ Sterling
"Assumed" total battery limits costs of step are as follows:

Range te/day Distillate Products	Base Plant te/ day Distillate Products	Base Plant Cost, £	Scaling Factor (Power)
500 - 1800	1300	137 000 000	0.8
1900 - 3000	2020	198 000 000	0.7

MODEL CONSTRUCTED BY:

John Brown Engineers and Constructors using data supplied by Shell, The Hague, Holland and the following articles. The majority of the data necessary to build an accurate model of the SMDS complex is of a confidential nature, thus could not be released by Shell. Therefore much of the data listed above is generated by John Brown and can be therefore indicative only - this data is clearly identified above as "assumed".

(a) SMDS paper for ICE Conference, London, Dec. 1988 by M.J. Van der Burgt, C.J. Van Leeuwen, S.T.Sie, P.L Zuidevald, H.M.H Wechem.
(b) Shell Middle Distillate Synthesis Process by M.J. Van der Burgt, C./J Van Leeuwen, J.J del'Amico, S.T.Sie.
(c) Liquid Hydrocarbons from Natural Gas presented at Petro Pacific 1984, Melbourne, Australia by M.J. Van der Burgt, S.T. Sie.
(d) Shell's Middle Distillate Synthesis Process presented at AIChE spring Meeting 1988 by H. Voetter, M.J. Van der Burgt.

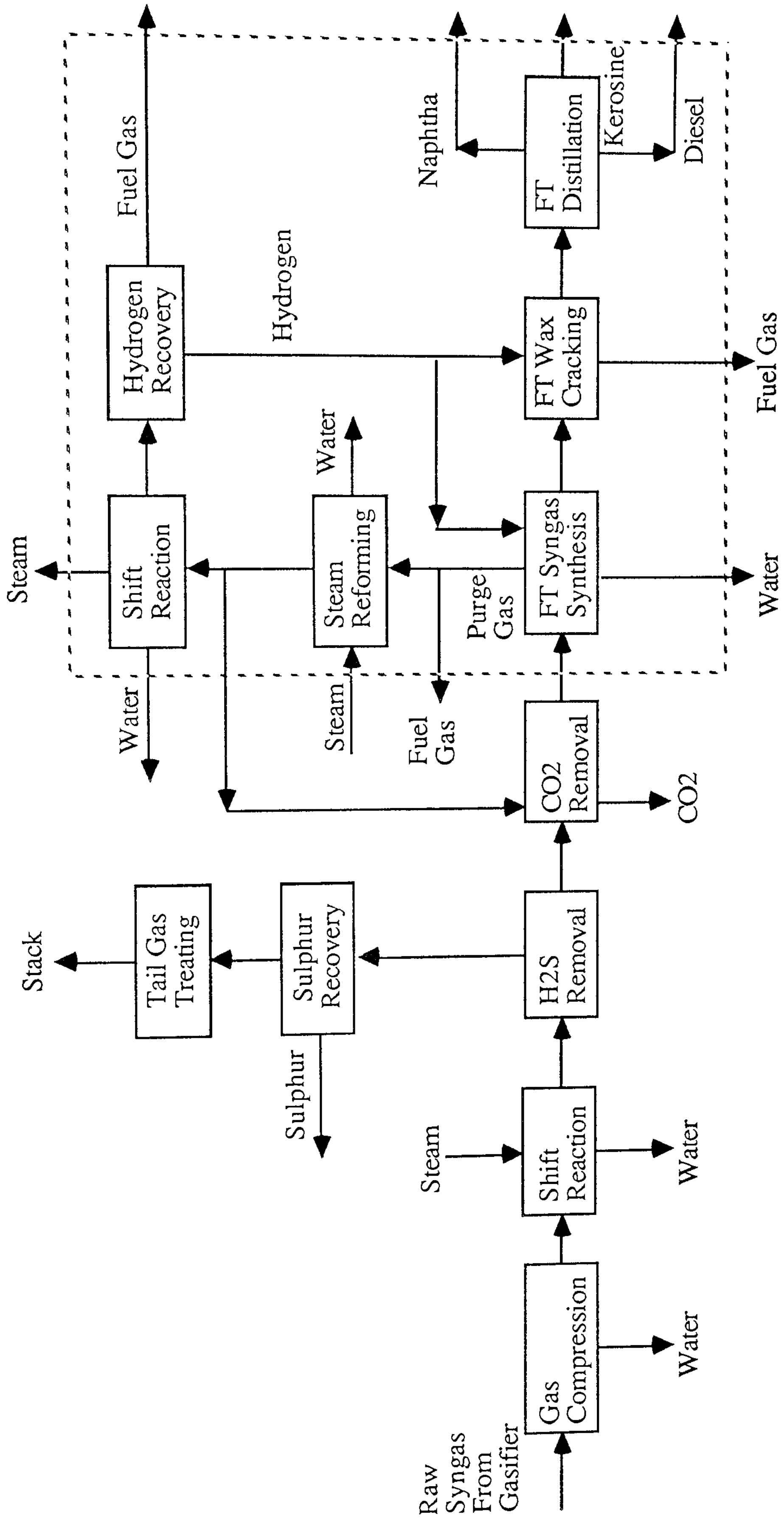


Figure 1 Shell SMDS Block Flow Diagram

STEP 500: OFFSITE STORAGE AND FACILITIES
CAPITAL COST BASIS
MID 1988 - U.K. STERLING

It is not feasible to develop all inclusive unit costs or factors for offsite storage and facilities based on logical assumptions. This is because storage requirements depend on the size of the process units being considered. To do so at this stage would requires a considerable amount of time and effort being spent on developing realistic project schemes. As a basis for costing the offsite storage complex within the accuracy specified at this point JBE&C would recommend a unit cost of £ 16.50 per barrel of storage, based on fixed roof tanks, inclusive of:-

- Tank supply & installation
- Product transfer equipment
- Civils works
- Piping, instrument & electrics
- Painting & insulation

No costs have been included in the above rate of £ 16.50 for the following facilities since these are specific to local requirements and product marketing policy referenced to specific process studies:-

- Jetties including piping & loading facilities
- Road & rail loading
- Power generation
- Steam generation
- Specific blending systems
- Single or small tank storage systems

Appendix B

Summary of program results output

B.1 Shell

B.1.1 Point of Ayr

B.1.1.1 Methanol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Shell Methanol             FINANCIAL CASE : 54.3 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow    % mass   % energy    % C.Conv.
                                 t/d     yield     yield        Effic.
Methanol                      9350.5      93.5      62.4         41.9
TOTAL ENERGY PRODUCTS         9350.5      93.5      62.4         41.9
PRODUCTION COSTS
                                 £/t     ECU/t
Methanol                       127.3     190.9

PLANT CAPITAL COST             509.9 M pounds,     764.9 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Shell Methanol             FINANCIAL CASE : 0 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow    % mass   % energy    % C.Conv.
                                 t/d     yield     yield        Effic.
Methanol                      9350.5      93.5      62.4         41.9
TOTAL ENERGY PRODUCTS         9350.5      93.5      62.4         41.9
PRODUCTION COSTS
                                 £/t     ECU/t
Methanol                        69.2     103.8

PLANT CAPITAL COST             509.9 M pounds,     764.9 M ECU
```

B.1.1.2 Fuel Alcohol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Shell F/A                  FINANCIAL CASE : 54.3 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow    % mass   % energy    % C.Conv.
                                 t/d     yield     yield        Effic.
Fuel alcohol                  4975.2      49.8      43.2         27.1
TOTAL ENERGY PRODUCTS         5000.2      50.0      43.2         27.1
PRODUCTION COSTS
                                 £/t     ECU/t
Fuel alcohol                   198.4     297.6

PLANT CAPITAL COST             497.7 M pounds,     746.6 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Shell F/A                FINANCIAL CASE : 0 £/te 0 ROI
FEEDSTOCK:
Point of Ayr              10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                     Flow    % mass  % energy    % C.Conv.
                               t/d     yield     yield       Effic.
Fuel alcohol                4975.2      49.8      43.2         27.1

TOTAL ENERGY PRODUCTS       5000.2      50.0      43.2         27.1
PRODUCTION COSTS
                               £/t     ECU/t
Fuel alcohol                  89.2     133.9

PLANT CAPITAL COST           497.7 M pounds,     746.6 M ECU
```

B.1.1.3 MTG

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Shell MTG                FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Point of Ayr              10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                     Flow    % mass  % energy    % C.Conv.
                               t/d     yield     yield       Effic.
Gasoline                    3380.8      33.8      45.6         30.3
Propane LPG                  187.1       1.9       2.8          1.8
Butane LPG                   449.0       4.5       6.5          4.4

TOTAL ENERGY PRODUCTS       4016.9      40.2      54.9         36.6
PRODUCTION COSTS
                               £/t     ECU/t
Gasoline                     331.5     497.2
Propane LPG                  282.1     423.1
Butane LPG                   282.1     423.1

PLANT CAPITAL COST           600.7 M pounds,     901.0 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Shell MTG                FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Point of Ayr              10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                     Flow    % mass  % energy    % C.Conv.
                               t/d     yield     yield       Effic.
Gasoline                    3380.8      33.8      45.6         30.3
Propane LPG                  187.1       1.9       2.8          1.8
Butane LPG                   449.0       4.5       6.5          4.4

TOTAL ENERGY PRODUCTS       4016.9      40.2      54.9         36.6
PRODUCTION COSTS
                               £/t     ECU/t
Gasoline                     193.0     289.5
Propane LPG                  164.2     246.4
Butane LPG                   164.2     246.4

PLANT CAPITAL COST           600.7 M pounds,     901.0 M ECU
```

B.1.1.4 MOGD

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================
RUN: Shell MOGD                    FINANCIAL CASE : 54.3 £/te 0 ROI
FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow     % mass   % energy    % C.Conv.
                                  t/d      yield     yield        Effic.
Diesel                          336.6        3.4       4.5          3.0
Gasoline                       2340.4       23.4      31.6         21.0
Kerosine                       1112.7       11.1      14.3         10.0

TOTAL ENERGY PRODUCTS          3789.8       37.9      50.4         34.0
PRODUCTION COSTS
                                  £/t      ECU/t
Diesel                          355.5      533.2
Gasoline                        394.5      591.8
Kerosine                        212.7      319.0

PLANT CAPITAL COST              679.0 M pounds,    1018.4 M ECU
```

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================
RUN: Shell MOGD                    FINANCIAL CASE : 0 £/te 0 ROI
FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow     % mass   % energy    % C.Conv.
                                  t/d      yield     yield        Effic.
Diesel                          336.6        3.4       4.5          3.0
Gasoline                       2340.4       23.4      31.6         21.0
Kerosine                       1112.7       11.1      14.3         10.0

TOTAL ENERGY PRODUCTS          3789.8       37.9      50.4         34.0
PRODUCTION COSTS
                                  £/t      ECU/t
Diesel                          204.6      307.0
Gasoline                        227.1      340.7
Kerosine                        122.4      183.6

PLANT CAPITAL COST              679.0 M pounds,    1018.4 M ECU
```

B.1.1.5 SMDS

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================
RUN: Shell SMDS                    FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow     % mass   % energy    % C.Conv.
                                  t/d      yield     yield        Effic.
Diesel                         2578.4       25.8      34.6         26.4
Naphtha                         645.7        6.5       8.7          6.6
Kerosine                       1051.9       10.5      14.1         10.8

TOTAL ENERGY PRODUCTS          4276.0       42.8      57.4         43.8
PRODUCTION COSTS                  £/t      ECU/t
Diesel                          287.2      430.8
Naphtha                         285.3      427.9
Kerosine                        323.2      484.8

PLANT CAPITAL COST              634.1 M pounds,     951.2 M ECU
```

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: Shell SMDS                FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Point of Ayr              10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                    Flow    % mass  % energy    % C.Conv.
                              t/d     yield    yield       Effic.
Diesel                     2578.4      25.8     34.6        26.4
Naphtha                     645.7       6.5      8.7         6.6
Kerosine                   1051.9      10.5     14.1        10.8

TOTAL ENERGY PRODUCTS      4276.0      42.8     57.4        43.8
PRODUCTION COSTS              £/t     ECU/t
Diesel                      163.9     245.8
Naphtha                     162.8     244.2
Kerosine                    184.4     276.6

PLANT CAPITAL COST          634.1 M pounds,     951.2 M ECU
```

B.1.2 Sub-bituminous

B.1.2.1 Methanol

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: Shell Methanol            FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit     10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                    Flow    % mass  % energy    % C.Conv.
                              t/d     yield    yield       Effic.
Methanol                   8409.5      84.1     62.5        40.0

TOTAL ENERGY PRODUCTS      8409.5      84.1     62.5        40.0
PRODUCTION COSTS

                              £/t     ECU/t
Methanol                    134.9     202.4

PLANT CAPITAL COST          475.0 M pounds,     712.5 M ECU
```

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: Shell Methanol            FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit     10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                    Flow    % mass  % energy    % C.Conv.
                              t/d     yield    yield       Effic.
Methanol                   8409.5      84.1     62.5        40.0

TOTAL ENERGY PRODUCTS      8409.5      84.1     62.5        40.0
PRODUCTION COSTS

                              £/t     ECU/t
Methanol                     70.4     105.5

PLANT CAPITAL COST          475.0 M pounds,     712.5 M ECU
```

B.1.2.2 Fuel Alcohol

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Shell F/A                     FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Fuel alcohol                  4474.5      44.7     43.3         25.9

TOTAL ENERGY PRODUCTS         4497.0      45.0     43.3         25.9
PRODUCTION COSTS
                                 £/t     ECU/t
Fuel alcohol                   214.5     321.8

PLANT CAPITAL COST             481.6 M pounds,     722.5 M ECU
```

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Shell F/A                     FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Fuel alcohol                  4474.5      44.7     43.3         25.9

TOTAL ENERGY PRODUCTS         4497.0      45.0     43.3         25.9
PRODUCTION COSTS
                                 £/t     ECU/t
Fuel alcohol                    93.2     139.8

PLANT CAPITAL COST             481.6 M pounds,     722.5 M ECU
```

B.1.2.3 MTG

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Shell MTG                     FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Gasoline                      3040.6      30.4     45.7         28.9
Propane LPG                    168.3       1.7      2.8          1.7
Butane LPG                     403.8       4.0      6.5          4.2

TOTAL ENERGY PRODUCTS         3612.7      36.1     55.0         34.9
PRODUCTION COSTS
                                 £/t     ECU/t
Gasoline                       350.9     526.3
Propane LPG                    298.6     447.9
Butane LPG                     298.6     447.9

PLANT CAPITAL COST             564.4 M pounds,     846.6 M ECU
```

```
              ASTON LIQUID FUELS PRODUCTION MODEL
              ===================================

RUN: Shell MTG                FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit      10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                     Flow    % mass  % energy    % C.Conv.
                               t/d     yield    yield       Effic.
Gasoline                    3040.6      30.4     45.7        28.9
Propane LPG                  168.3       1.7      2.8         1.7
Butane LPG                   403.8       4.0      6.5         4.2

TOTAL ENERGY PRODUCTS       3612.7      36.1     55.0        34.9
PRODUCTION COSTS               £/t     ECU/t
Gasoline                     197.0     295.4
Propane LPG                  167.6     251.4
Butane LPG                   167.6     251.4

PLANT CAPITAL COST           564.4 M pounds,      846.6 M ECU
```

B.1.2.4 MOGD

```
              ASTON LIQUID FUELS PRODUCTION MODEL
              ===================================

RUN: Shell MOGD               FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit      10000.0 daf t/d,    13736.3 raw t/d
PRODUCTS:                     Flow    % mass  % energy    % C.Conv.
                               t/d     yield    yield       Effic.
Diesel                       302.7       3.0      4.5         2.9
Gasoline                    2104.9      21.0     31.6        20.0
Kerosine                    1000.7      10.0     14.3         9.5

TOTAL ENERGY PRODUCTS       3408.4      34.1     50.5        32.4
PRODUCTION COSTS               £/t     ECU/t
Diesel                       376.1     564.1
Gasoline                     417.4     626.1
Kerosine                     225.0     337.5

PLANT CAPITAL COST           631.4 M pounds,      947.0 M ECU
```

```
              ASTON LIQUID FUELS PRODUCTION MODEL
              ===================================

RUN: Shell MOGD               FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit      10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                     Flow    % mass  % energy    % C.Conv.
                               t/d     yield    yield       Effic.
Diesel                       302.7       3.0      4.5         2.9
Gasoline                    2104.9      21.0     31.6        20.0
Kerosine                    1000.7      10.0     14.3         9.5

TOTAL ENERGY PRODUCTS       3408.4      34.1     50.5        32.4
PRODUCTION COSTS               £/t     ECU/t
Diesel                       208.3     312.5
Gasoline                     231.2     346.9
Kerosine                     124.6     187.0

PLANT CAPITAL COST           631.4 M pounds,      947.0 M ECU
```

B.1.2.5 SMDS

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================

RUN: Shell SMDS                  FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield        Effic.
Diesel                        2307.6      23.1     34.5         25.1
Naphtha                        577.8       5.8      8.6          6.3
Kerosine                       941.4       9.4     14.1         10.2

TOTAL ENERGY PRODUCTS         3826.8      38.3     57.2         41.6
PRODUCTION COSTS
                                 £/t     ECU/t
Diesel                         307.2     460.7
Naphtha                        305.1     457.7
Kerosine                       345.7     518.5

PLANT CAPITAL COST             605.8 M pounds,     908.7 M ECU
```

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================

RUN: Shell SMDS                  FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield        Effic.
Diesel                        2307.6      23.1     34.5         25.1
Naphtha                        577.8       5.8      8.6          6.3
Kerosine                       941.4       9.4     14.1         10.2

TOTAL ENERGY PRODUCTS         3826.8      38.3     57.2         41.6
PRODUCTION COST                  £/t     ECU/t
Diesel                         169.4     254.1
Naphtha                        168.2     252.4
Kerosine                       190.6     285.9

PLANT CAPITAL COST             605.8 M pounds,     908.7 M ECU
```

B.1.3 Lignite

B.1.3.1 Methanol

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================

RUN:                             FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield        Effic.
Methanol                      6795.0      67.9     60.2         37.5

TOTAL ENERGY PRODUCTS         6795.0      67.9     60.2         37.5
PRODUCTION COSTS                 £/t     ECU/t
Methanol                       158.3     237.4

PLANT CAPITAL COST             473.1 M pounds,     709.6 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN:                            FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Methanol                      6795.0     67.9     60.2         37.5

TOTAL ENERGY PRODUCTS         6795.0     67.9     60.2         37.5

PRODUCTION COSTS
                                 £/t    ECU/t
Methanol                        78.4    117.6

PLANT CAPITAL COST             473.1 M pounds,     709.6 M ECU
```

B.1.3.2 Fuel Alcohol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Shell F/A                  FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Fuel alcohol                  3615.5     36.2     41.7         24.3

TOTAL ENERGY PRODUCTS         3633.6     36.3     41.7         24.3

PRODUCTION COSTS
                                 £/t    ECU/t
Fuel alcohol                   258.7    388.0

PLANT CAPITAL COST             479.5 M pounds,     719.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Shell F/A                  FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv
                                 t/d     yield    yield       Effic.
Fuel alcohol                  3615.5     36.2     41.7         24.3

TOTAL ENERGY PRODUCTS         3633.6     36.3     41.7         24.3

PRODUCTION COSTS
                                 £/t    ECU/t
Fuel alcohol                   108.5    162.7

PLANT CAPITAL COST             479.5 M pounds,     719.2 M ECU
```

B.1.3.3 MTG

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================
RUN: Shell MTG                    FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield    yield        Effic.
Gasoline                        2456.8      24.6     44.0         27.1
Propane LPG                      136.0       1.4      2.7          1.6
Butane LPG                       326.3       3.3      6.3          4.0

TOTAL ENERGY PRODUCTS           2919.1      29.2     52.9         32.7
PRODUCTION COSTS                   £/t     ECU/t
Gasoline                         406.6     609.9
Propane LPG                      346.0     519.1
Butane LPG                       346.0     519.1

PLANT CAPITAL COST               545.6 M pounds,      818.4 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================
RUN: Shell MTG                    FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield    yield        Effic.
Gasoline                        2456.8      24.6     44.0         27.1
Propane LPG                      136.0       1.4      2.7          1.6
Butane LPG                       326.3       3.3      6.3          4.0

TOTAL ENERGY PRODUCTS           2919.1      29.2     52.9         32.7
PRODUCTION COSTS                   £/t     ECU/t
Gasoline                         216.1     324.2
Propane LPG                      183.9     275.9
Butane LPG                       183.9     275.9

PLANT CAPITAL COST               545.6 M pounds,      818.4 M ECU
```

B.1.3.4 MOGD

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Shell MOGD                   FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield    yield        Effic.
Diesel                           244.6       2.4      4.4          2.7
Gasoline                        1700.8      17.0     30.5         18.8
Kerosine                         808.6       8.1     13.8          8.9

TOTAL ENERGY PRODUCTS           2754.0      27.5     48.6         30.4
PRODUCTION COSTS                   £/t     ECU/t
Diesel                           438.3     657.5
Gasoline                         486.5     729.7
Kerosine                         262.2     393.3

PLANT CAPITAL COST               606.8 M pounds,      910.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================
RUN: Shell MOGD                  FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,   24096.4 raw t/d
PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield        Effic.
Diesel                         244.6       2.4      4.4          2.7
Gasoline                      1700.8      17.0     30.5         18.8
Kerosine                       808.6       8.1     13.8          8.9

TOTAL ENERGY PRODUCTS         2754.0      27.5     48.6         30.4
PRODUCTION COSTS                 £/t     ECU/t
Diesel                         230.7     346.1
Gasoline                       256.1     384.1
Kerosine                       138.0     207.1

PLANT CAPITAL COST             606.8 M pounds,     910.2 M ECU
```

B.1.3.5 SMDS

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Shell SMDS                  FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,   24096.4 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield        Effic.
Diesel                        1880.0      18.8     33.5         23.7
Naphtha                        470.8       4.7      8.4          5.9
Kerosine                       767.0       7.7     13.7          9.7

TOTAL ENERGY PRODUCTS         3117.7      31.2     55.5         39.3
PRODUCTION COSTS                 £/t     ECU/t
Diesel                         355.8     533.6
Naphtha                        353.4     530.1
Kerosine                       400.4     600.6

PLANT CAPITAL COST             587.2 M pounds,     880.8 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================
RUN: Shell SMDS                  FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,   24096.4 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield        Effic.
Diesel                        1880.0      18.8     33.5         23.7
Naphtha                        470.8       4.7      8.4          5.9
Kerosine                       767.0       7.7     13.7          9.7

TOTAL ENERGY PRODUCTS         3117.7      31.2     55.5         39.3
PRODUCTION COSTS                 £/t     ECU/t
Diesel                         186.6     280.0
Naphtha                        185.4     278.1
Kerosine                       210.1     315.1

PLANT CAPITAL COST             587.2 M pounds,     880.8 M ECU
```

B.2 Texaco

B.2.1 Point of Ayr

B.2.1.1 Methanol

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: Texaco Methanol               FINANCIAL CASE : 54.3 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy     % C.Conv.
                                  t/d     yield    yield        Effic.
Methanol                       8811.7      88.1     58.8          39.5

TOTAL ENERGY PRODUCTS          8811.7      88.1     58.8          39.5

PRODUCTION COSTS
                                  £/t     ECU/t
Methanol                        137.2     205.8

PLANT CAPITAL COST              453.0 M pounds,     679.5 M ECU
```

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: Texaco Methanol               FINANCIAL CASE : 0 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy     % C.Conv.
                                  t/d     yield    yield        Effic.
Methanol                       8811.7      88.1     58.8          39.5

TOTAL ENERGY PRODUCTS          8811.7      88.1     58.8          39.5
PRODUCTION COSTS                  £/t     ECU/t
Methanol                         75.6     113.3

PLANT CAPITAL COST              453.0 M pounds,     679.5 M ECU
```

B.2.1.2 Fuel Alcohol

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================
RUN: Texaco F/A                    FINANCIAL CASE : 54.3 £/te 0 ROI
FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy     % C.Conv.
                                  t/d     yield    yield        Effic.
Fuel alcohol                   4691.4      46.9     40.7          25.6

TOTAL ENERGY PRODUCTS          4715.0      47.2     40.7          25.6

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                    219.5     329.2

PLANT CAPITAL COST              459.6 M pounds,     689.5 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: Texaco F/A                 FINANCIAL CASE : 0 £/te 0 ROI

FEEDSTOCK:
Point of Ayr               10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield       Effic.
Fuel alcohol                 4691.4     46.9     40.7         25.6

TOTAL ENERGY PRODUCTS        4715.0     47.2     40.7         25.6
PRODUCTION COSTS                £/t    ECU/t
Fuel alcohol                  103.7    155.6

PLANT CAPITAL COST            459.6 M pounds,     689.5 M ECU
```

B.2.1.3 MTG

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: Texaco F/A                 FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Point of Ayr               10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield       Effic.
Gasoline                     3186.0     31.9     43.0         28.6
Propane LPG                   176.3      1.8      2.6          1.7
Butane LPG                    423.1      4.2      6.1          4.2

TOTAL ENERGY PRODUCTS        3785.5     37.9     51.7         34.5
PRODUCTION COSTS                £/t    ECU/t
Gasoline                      356.2    534.3
Propane LPG                   303.1    454.7
Butane LPG                    303.1    454.7

PLANT CAPITAL COST            546.6 M pounds,     819.9 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: Texaco F/A                 FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Point of Ayr               10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield       Effic.
Gasoline                     3186.0     31.9     43.0         28.6
Propane LPG                   176.3      1.8      2.6          1.7
Butane LPG                    423.1      4.2      6.1          4.2

TOTAL ENERGY PRODUCTS        3785.5     37.9     51.7         34.5
PRODUCTION COSTS                £/t    ECU/t
Gasoline                      209.3    314.0
Propane LPG                   178.1    267.2
Butane LPG                    178.1    267.2

PLANT CAPITAL COST            546.6 M pounds,     819.9 M ECU
```

B.2.1.4 MOGD

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================
RUN: Texaco                      FINANCIAL CASE : 54.3 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Diesel                        317.2       3.2       4.3          2.8
Gasoline                     2205.6      22.1      29.8         19.8
Kerosine                     1048.6      10.5      13.5          9.4

TOTAL ENERGY PRODUCTS        3571.4      35.7      47.5         32.0
PRODUCTION COSTS                £/t     ECU/t
Diesel                        381.6     572.3
Gasoline                      423.5     635.2
Kerosine                      228.3     342.4

PLANT CAPITAL COST            614.9 M pounds,     922.3 M ECU
```

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================
RUN: Texaco                      FINANCIAL CASE : 0 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Diesel                        317.2       3.2       4.3          2.8
Gasoline                     2205.6      22.1      29.8         19.8
Kerosine                     1048.6      10.5      13.5          9.4

TOTAL ENERGY PRODUCTS        3571.4      35.7      47.5         32.0
PRODUCTION COSTS                £/t     ECU/t
Diesel                        221.5     332.2
Gasoline                      245.8     368.7
Kerosine                      132.5     198.8

PLANT CAPITAL COST            614.9 M pounds,     922.3 M ECU
```

B.2.1.5 SMDS

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================
RUN: Texaco                      FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Diesel                       2460.5      24.6      33.0         25.2
Naphtha                       616.1       6.2       8.3          6.3
Kerosine                     1003.8      10.0      13.5         10.3

TOTAL ENERGY PRODUCTS        4080.4      40.8      54.7         41.8
PRODUCTION COSTS                £/t     ECU/t
Diesel                        310.3     465.4
Naphtha                       308.2     462.3
Kerosine                      349.2     523.8

PLANT CAPITAL COST            594.8 M pounds,     892.2 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Texaco                       FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow   % mass   % energy    % C.Conv.
                                  t/d    yield     yield       Effic.
Diesel                         2460.5     24.6      33.0         25.2
Naphtha                         616.1      6.2       8.3          6.3
Kerosine                       1003.8     10.0      13.5         10.3

TOTAL ENERGY PRODUCTS          4080.4     40.8      54.7         41.8

PRODUCTION COSTS
                                  £/t    ECU/t
Diesel                          181.0    271.6
Naphtha                         179.8    269.8
Kerosine                        203.8    305.6

PLANT CAPITAL COST              594.8 M pounds,     892.2 M ECU
```

B.2.2 Sub-bituminous

B.2.2.1 Methanol

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Texaco Methanol              FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow   % mass   % energy    % C.Conv.
                                  t/d    yield     yield       Effic.
Methanol                       7587.6     75.9      56.4         36.1

TOTAL ENERGY PRODUCTS          7587.6     75.9      56.4         36.1

PRODUCTION COSTS                  £/t    ECU/t
Methanol                        154.1    231.2

PLANT CAPITAL COST              432.2 M pounds,     648.4 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Texaco Methanol              FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow   % mass   % energy    % C.Conv.
                                  t/d    yield     yield       Effic.
Methanol                       7587.6     75.9      56.4         36.1

TOTAL ENERGY PRODUCTS          7587.6     75.9      56.4         36.1
PRODUCTION COSTS                  £/t    ECU/t
Methanol                         82.6    123.9

PLANT CAPITAL COST              432.2 M pounds,     648.4 M ECU
```

B.2.2.2 Fuel Alcohol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Texaco F/A                FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                      Flow    % mass   % energy    % C.Conv.
                                t/d     yield     yield        Effic.
Fuel alcohol                 4040.0      40.4      39.1          23.4

TOTAL ENERGY PRODUCTS        4060.3      40.6      39.1          23.4

PRODUCTION COSTS
                                £/t     ECU/t
Fuel alcohol                  251.3     377.0

PLANT CAPITAL COST            438.8 M pounds,     658.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Texaco F/A                FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                      Flow    % mass   % energy    % C.Conv.
                                t/d     yield     yield        Effic.
Fuel alcohol                 4040.0      40.4      39.1          23.4

TOTAL ENERGY PRODUCTS        4060.3      40.6      39.1          23.4

PRODUCTION COSTS                £/t     ECU/t
Fuel alcohol                  116.9     175.4

PLANT CAPITAL COST            438.8 M pounds,     658.2 M ECU
```

B.2.2.3 MTG

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

                               FINANCIAL CASE : 54.3 £/te
RUN: Texaco MTG
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d
PRODUCTS:                      Flow    % mass   % energy    % C.Conv.
                                t/d     yield     yield        Effic.
                             2743.4      27.4      41.2          26.1
Gasoline                      151.8       1.5       2.5           1.6
Propane LPG                   364.4       3.6       5.9           3.8
Butane LPG

TOTAL ENERGY PRODUCTS        3259.6      32.6      49.6          31.5

                                £/t     ECU/t
PRODUCTION COSTS              396.7     595.0
Gasoline                      337.6     506.4
Propane LPG                   337.6     506.4
Butane LPG

PLANT CAPITAL COST            513.1 M pounds,     769.6 M ECU
```

```
                   ASTON LIQUID FUELS PRODUCTION MODEL
                   ===================================

RUN: Texaco MTG                   FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                      Flow    % mass   % energy    % C.Conv.
                                t/d     yield     yield        Effic.
Gasoline                     2743.4      27.4      41.2         26.1
Propane LPG                   151.8       1.5       2.5          1.6
Butane LPG                    364.4       3.6       5.9          3.8

TOTAL ENERGY PRODUCTS        3259.6      32.6      49.6         31.5
PRODUCTION COSTS                £/t     ECU/t
Gasoline                      226.1     339.1
Propane LPG                   192.4     288.6
Butane LPG                    192.4     288.6

PLANT CAPITAL COST            513.1 M pounds,     769.6 M ECU
```

B.2.2.4 MOGD

```
                   ASTON LIQUID FUELS PRODUCTION MODEL
                   ===================================

RUN: Texaco MOGD                  FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d
PRODUCTS:                      Flow    % mass   % energy    % C.Conv.
                                t/d     yield     yield        Effic.
Diesel                        273.2       2.7       4.1          2.6
Gasoline                     1899.2      19.0      28.5         18.1
Kerosine                      902.9       9.0      12.9          8.6

TOTAL ENERGY PRODUCTS        3075.3      30.8      45.5         29.3
PRODUCTION COSTS                £/t     ECU/t
Diesel                        426.7     640.0
Gasoline                      473.6     710.4
Kerosine                      255.3     382.9

PLANT CAPITAL COST            577.2 M pounds,     865.9 M ECU
```

```
                   ASTON LIQUID FUELS PRODUCTION MODEL
                   ===================================
RUN: Texaco MOGD                  FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d
PRODUCTS:                      Flow    % mass   % energy    % C.Conv.
                                t/d     yield     yield        Effic.
Diesel                        273.2       2.7       4.1          2.6
Gasoline                     1899.2      19.0      28.5         18.1
Kerosine                      902.9       9.0      12.9          8.6

TOTAL ENERGY PRODUCTS        3075.3      30.8      45.5         29.3
PRODUCTION COSTS                £/t     ECU/t
Diesel                        240.8     361.2
Gasoline                      267.3     400.9
Kerosine                      144.1     216.1

PLANT CAPITAL COST            577.2 M pounds,     865.9 M ECU
```

B.2.2.5 SMDS

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: Texaco SMDS                  FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield    yield       Effic.
Diesel                          2105.1      21.1     31.5        22.9
Naphtha                          527.1       5.3      7.9         5.7
Kerosine                         858.8       8.6     12.8         9.3

TOTAL ENERGY PRODUCTS           3491.0      34.9     52.2        38.0
PRODUCTION COSTS                   £/t     ECU/t
Diesel                           348.6     522.9
Naphtha                          346.3     519.4
Kerosine                         392.3     588.5

PLANT CAPITAL COST               557.4 M pounds,      836.1 M ECU
```

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: Texaco SMDS                  FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield    yield       Effic.
Diesel                          2105.1      21.1     31.5        22.9
Naphtha                          527.1       5.3      7.9         5.7
Kerosine                         858.8       8.6     12.8         9.3

TOTAL ENERGY PRODUCTS           3491.0      34.9     52.2        38.0
PRODUCTION COSTS                   £/t     ECU/t
Diesel                           197.6     296.3
Naphtha                          196.2     294.4
Kerosine                         222.3     333.5

PLANT CAPITAL COST               557.4 M pounds,      836.1 M ECU
```

B.2.3 Lignite

B.2.3.1 Methanol

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================
RUN: Teaxco Methanol              FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d
PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield    yield       Effic.
Methanol                        4008.1      40.1     35.5        22.1

TOTAL ENERGY PRODUCTS           4008.1      40.1     35.5        22.1
PRODUCTION COSTS                   £/t     ECU/t
Methanol                         310.7     466.1

PLANT CAPITAL COST               379.1 M pounds,      568.6 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Teaxco Methanol              FINANCIAL CASE : 5

FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy     % C.Conv.
                                  t/d     yield    yield        Effic.
Methanol                       4008.1      40.1     35.5          22.1

TOTAL ENERGY PRODUCTS          4008.1      40.1     35.5          22.1
PRODUCTION COSTS                  £/t     ECU/t
Methanol                        175.2     262.9

PLANT CAPITAL COST              379.1 M pounds,     568.6 M ECU
```

B.2.3.2 Fuel Alcohol

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Texaco F/A                    FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy     % C.Conv.
                                  t/d     yield    yield        Effic.
Fuel alcohol                   2135.1      21.4     24.6          14.3

TOTAL ENERGY PRODUCTS          2145.8      21.5     24.6          14.3
PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                    550.6     825.9

PLANT CAPITAL COST              397.5 M pounds,     596.3 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Texaco F/A                    FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy     % C.Conv.
                                  t/d     yield    yield        Effic.
Fuel alcohol                   2135.1      21.4     24.6          14.3

TOTAL ENERGY PRODUCTS          2145.8      21.5     24.6          14.3

PRODUCTION COSTS
                                  £/t     ECU/t
Fuel alcohol                    296.3     444.4

PLANT CAPITAL COST              397.5 M pounds,     596.3 M ECU
```

B.2.3.3 MTG

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: Texaco MTG                   FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Gasoline                        1449.2      14.5      26.0        16.0
Propane LPG                       80.2       0.8       1.6         1.0
Butane LPG                       192.5       1.9       3.7         2.3

TOTAL ENERGY PRODUCTS           1721.8      17.2      31.2        19.3
PRODUCTION COSTS                   £/t     ECU/t
Gasoline                         772.0    1157.9
Propane LPG                      656.9     985.4
Butane LPG                       656.9     985.4

PLANT CAPITAL COST               427.7 M pounds,     641.5 M ECU
```

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: Texaco MTG                   FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Gasoline                        1449.2      14.5      26.0        16.0
Propane LPG                       80.2       0.8       1.6         1.0
Butane LPG                       192.5       1.9       3.7         2.3

TOTAL ENERGY PRODUCTS           1721.8      17.2      31.2        19.3
PRODUCTION COSTS                   £/t     ECU/t
Gasoline                         449.0     673.5
Propane LPG                      382.1     573.1
Butane LPG                       382.1     573.1

PLANT CAPITAL COST               427.7 M pounds,     641.5 M ECU
```

B.2.3.4 MOGD

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: Texaco MOGD                  FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d
PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Diesel                           144.3       1.4       2.6         1.6
Gasoline                        1003.2      10.0      18.0        11.1
Kerosine                         477.0       4.8       8.1         5.3

TOTAL ENERGY PRODUCTS           1624.5      16.2      28.7        17.9
PRODUCTION COSTS                   £/t     ECU/t
Diesel                           836.0    1254.1
Gasoline                         927.9    1391.9
Kerosine                         500.1     750.2

PLANT CAPITAL COST               462.9 M pounds,     694.3 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Texaco MOGD                    FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d
PRODUCTS:                       Flow     % mass   % energy    % C.Conv.
                                 t/d      yield     yield       Effic.
Diesel                         144.3        1.4       2.6          1.6
Gasoline                      1003.2       10.0      18.0         11.1
Kerosine                       477.0        4.8       8.1          5.3

TOTAL ENERGY PRODUCTS         1624.5       16.2      28.7         17.9
PRODUCTION COSTS                 £/t      ECU/t
Diesel                         484.1      726.2
Gasoline                       537.3      806.0
Kerosine                       289.6      434.4

PLANT CAPITAL COST             462.9 M pounds,     694.3 M ECU
```

B.2.3.5 SMDS

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Texaco SMDS                    FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d
PRODUCTS:                       Flow     % mass   % energy    % C.Conv.
                                 t/d      yield     yield       Effic.
Diesel                        1150.2       11.5      20.5         14.5
Naphtha                        288.0        2.9       5.1          3.6
Kerosine                       469.2        4.7       8.4          5.9

TOTAL ENERGY PRODUCTS         1907.4       19.1      34.0         24.0
PRODUCTION COSTS                 £/t      ECU/t
Diesel                         671.9     1007.8
Naphtha                        667.4     1001.1
Kerosine                       756.2     1134.2

PLANT CAPITAL COST             477.3 M pounds,     716.0 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Texaco SMDS                    FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                       Flow     % mass   % energy    % C.Conv.
                                 t/d      yield     yield       Effic.
Diesel                        1150.2       11.5      20.5         14.5
Naphtha                        288.0        2.9       5.1          3.6
Kerosine                       469.2        4.7       8.4          5.9

TOTAL ENERGY PRODUCTS         1907.4       19.1      34.0         24.0
PRODUCTION COSTS                 £/t      ECU/t
Diesel                         395.5      593.2
Naphtha                        392.8      589.2
Kerosine                       445.1      667.6

PLANT CAPITAL COST             477.3 M pounds,     716.0 M ECU
```

B.3 KRW

B.3.1 Point of Ayr

B.3.1.1 Methanol

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================

RUN: KRW Methanol                   FINANCIAL CASE : 54.3 £/te 0 ROI
FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Methanol                     10583.9     105.8      65.6         47.5

TOTAL ENERGY PRODUCTS        10583.9     105.8      65.6         47.5

PRODUCTION COSTS                 £/t     ECU/t
Methanol                       119.5     179.2

PLANT CAPITAL COST             553.3 M pounds,     829.9 M ECU
```

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================

RUN: KRW Methanol                   FINANCIAL CASE : 0 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Methanol                     10583.9     105.8      65.6         47.5

TOTAL ENERGY PRODUCTS        10583.9     105.8      65.6         47.5

PRODUCTION COSTS                 £/t     ECU/t
Methanol                        68.1     102.2

PLANT CAPITAL COST             553.3 M pounds,     829.9 M ECU
```

B.3.1.2 Fuel Alcohol

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================

RUN: KRW F/A                        FINANCIAL CASE : 54.3 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Fuel alcohol                  6904.5      69.0      55.6         37.7

TOTAL ENERGY PRODUCTS         6939.2      69.4      55.6         37.7
PRODUCTION COSTS                 £/t     ECU/t
Fuel alcohol                   175.3     263.0

PLANT CAPITAL COST             647.7 M pounds,     971.6 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: KRW F/A                    FINANCIAL CASE : 0 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Fuel alcohol                  6904.5      69.0      55.6         37.7

TOTAL ENERGY PRODUCTS         6939.2      69.4      55.6         37.7
PRODUCTION COSTS                 £/t     ECU/t
Fuel alcohol                    96.7     145.0

PLANT CAPITAL COST             647.7 M pounds,     971.6 M ECU
```

B.3.1.3 MTG

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: KRW MTG                    FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Gasoline                      3826.8      38.3      47.9         34.3
Propane LPG                    211.8       2.1       2.9          2.1
Butane LPG                     508.2       5.1       6.8          5.0

TOTAL ENERGY PRODUCTS         4546.8      45.5      57.7         41.4
PRODUCTION COSTS                 £/t     ECU/t
Gasoline                       312.7     469.1
Propane LPG                    266.1     399.2
Butane LPG                     266.1     399.2

PLANT CAPITAL COST             656.0 M pounds,     984.0 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: KRW MTG                    FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Gasoline                      3826.8      38.3      47.9         34.3
Propane LPG                    211.8       2.1       2.9          2.1
Butane LPG                     508.2       5.1       6.8          5.0

TOTAL ENERGY PRODUCTS         4546.8      45.5      57.7         41.4
PRODUCTION COSTS                 £/t     ECU/t
Gasoline                       190.4     285.6
Propane LPG                    162.1     243.1
Butane LPG                     162.1     243.1

PLANT CAPITAL COST             656.0 M pounds,     984.0 M ECU
```

B.3.1.4 MOGD

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: KRW MOGD                      FINANCIAL CASE : 54.3 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow     % mass  % energy    % C.Conv.
                                  t/d      yield     yield       Effic.
Diesel                          381.0        3.8       4.7          3.4
Gasoline                       2649.2       26.5      33.2         23.7
Kerosine                       1259.5       12.6      15.0         11.3

TOTAL ENERGY PRODUCTS          4289.7       42.9      53.0         38.4
PRODUCTION COSTS                  £/t      ECU/t
Diesel                          334.3      501.4
Gasoline                        371.0      556.5
Kerosine                        200.0      299.9

PLANT CAPITAL COST              738.4 M pounds,    1107.7 M ECU
```

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: KRW MOGD                      FINANCIAL CASE : 0 £/te 0 ROI
FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d
PRODUCTS:                        Flow     % mass  % energy    % C.Conv.
                                  t/d      yield     yield       Effic.
Diesel                          381.0        3.8       4.7          3.4
Gasoline                       2649.2       26.5      33.2         23.7
Kerosine                       1259.5       12.6      15.0         11.3

TOTAL ENERGY PRODUCTS          4289.7       42.9      53.0         38.4
PRODUCTION COSTS                  £/t      ECU/t
Diesel                          201.0      301.5
Gasoline                        223.1      334.6
Kerosine                        120.2      180.4

PLANT CAPITAL COST              738.4 M pounds,    1107.7 M ECU
```

B.3.1.5 SMDS

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================
RUN: KRW SMDS                      FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d
PRODUCTS:                        Flow     % mass  % energy    % C.Conv.
                                  t/d      yield     yield       Effic.
Diesel                         2906.1       29.1      36.2         29.8
Naphtha                         727.7        7.3       9.1          7.5
Kerosine                       1185.6       11.9      14.8         12.1

TOTAL ENERGY PRODUCTS          4819.4       48.2      60.0         49.4
PRODUCTION COSTS                  £/t      ECU/t
Diesel                          267.9      401.8
Naphtha                         266.1      399.2
Kerosine                        301.5      452.2

PLANT CAPITAL COST              685.2 M pounds,    1027.8 M ECU
```

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================

RUN: KRW SMDS                        FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                          Flow    % mass   % energy    % C.Conv.
                                    t/d     yield     yield       Effic.
Diesel                           2906.1      29.1      36.2        29.8
Naphtha                           727.7       7.3       9.1         7.5
Kerosine                         1185.6      11.9      14.8        12.1

TOTAL ENERGY PRODUCTS            4819.4      48.2      60.0        49.4
PRODUCTION COSTS                    £/t     ECU/t
Diesel                            158.5     237.7
Naphtha                           157.4     236.1
Kerosine                          178.4     267.5

PLANT CAPITAL COST                685.2 M pounds,    1027.8 M ECU
```

B.3.2 Sub-bituminous

B.3.2.1 Methanol

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================

RUN: KRW Methanol                    FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit         10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                          Flow    % mass   % energy    % C.Conv.
                                    t/d     yield     yield       Effic.
Methanol                         9074.4      90.7      66.7        43.2

TOTAL ENERGY PRODUCTS            9074.4      90.7      66.7        43.2
PRODUCTION COSTS                    £/t     ECU/t
Methanol                          132.2     198.3

PLANT CAPITAL COST                529.4 M pounds,     794.0 M ECU
```

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================

RUN: KRW Methanol                    FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit         10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                          Flow    % mass   % energy    % C.Conv.
                                    t/d     yield     yield       Effic.
Methanol                         9074.4      90.7      66.7        43.2

TOTAL ENERGY PRODUCTS            9074.4      90.7      66.7        43.2

PRODUCTION COSTS                    £/t     ECU/t
Methanol                           72.3     108.5

PLANT CAPITAL COST                529.4 M pounds,     794.0 M ECU
```

B.3.2.2 Fuel Alcohol

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: KRW F/A                         FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit      10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass   % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Fuel alcohol                   6257.9      62.6      59.8         36.2

TOTAL ENERGY PRODUCTS          6289.4      62.9      59.8         36.2

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                    189.1     283.7

PLANT CAPITAL COST              609.9 M pounds,     914.9 M ECU
```

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: KRW F/A                         FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit      10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass   % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Fuel alcohol                   6257.9      62.6      59.8         36.2

TOTAL ENERGY PRODUCTS          6289.4      62.9      59.8         36.2

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                    102.4     153.6

PLANT CAPITAL COST              609.9 M pounds,     914.9 M ECU
```

B.3.2.3 MTG

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: KRW MTG                         FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit      10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass   % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Gasoline                       3281.0      32.8      48.7         31.2
Propane LPG                     181.6       1.8       2.9          1.9
Butane LPG                      435.7       4.4       7.0          4.6

TOTAL ENERGY PRODUCTS          3898.3      39.0      58.7         37.7

PRODUCTION COSTS                  £/t     ECU/t
Gasoline                        343.1     514.6
Propane LPG                     291.9     437.9
Butane LPG                      291.9     437.9

PLANT CAPITAL COST              617.4 M pounds,     926.1 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: KRW MTG                    FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Gasoline                      3281.0      32.8      48.7         31.2
Propane LPG                    181.6       1.8       2.9          1.9
Butane LPG                     435.7       4.4       7.0          4.6

TOTAL ENERGY PRODUCTS         3898.3      39.0      58.7         37.7
PRODUCTION COSTS                 £/t     ECU/t
Gasoline                       200.4     300.6
Propane LPG                    170.5     255.8
Butane LPG                     170.5     255.8

PLANT CAPITAL COST             617.4 M pounds,     926.1 M ECU
```

B.3.2.4 MOGD

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================
RUN: KRW MOGD                   FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Diesel                         326.7       3.3       4.8          3.1
Gasoline                      2271.3      22.7      33.7         21.6
Kerosine                      1079.9      10.8      15.3         10.3

TOTAL ENERGY PRODUCTS         3677.8      36.8      53.9         35.0
PRODUCTION COSTS                 £/t     ECU/t
Diesel                         368.3     552.5
Gasoline                       408.8     613.2
Kerosine                       220.4     330.5

PLANT CAPITAL COST             694.7 M pounds,    1042.1 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================
RUN: KRW MOGD                   FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d
PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Diesel                         326.7       3.3       4.8          3.1
Gasoline                      2271.3      22.7      33.7         21.6
Kerosine                      1079.9      10.8      15.3         10.3

TOTAL ENERGY PRODUCTS         3677.8      36.8      53.9         35.0
PRODUCTION COSTS                 £/t     ECU/t
Diesel                         212.9     319.4
Gasoline                       236.3     354.5
Kerosine                       127.4     191.1

PLANT CAPITAL COST             694.7 M pounds,    1042.1 M ECU
```

B.3.2.5 SMDS

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: KRW SMDS                   FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Diesel                         2483.1      24.8      36.7         27.0
Naphtha                         621.8       6.2       9.2          6.8
Kerosine                       1013.0      10.1      15.0         11.0

TOTAL ENERGY PRODUCTS          4118.0      41.2      60.9         44.8
PRODUCTION COSTS                  £/t     ECU/t
Diesel                          298.2     447.2
Naphtha                         296.2     444.3
Kerosine                        335.6     503.3

PLANT CAPITAL COST              645.3 M pounds,      967.9 M ECU
```

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: KRW SMDS                   FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Diesel                         2483.1      24.8      36.7         27.0
Naphtha                         621.8       6.2       9.2          6.8
Kerosine                       1013.0      10.1      15.0         11.0

TOTAL ENERGY PRODUCTS          4118.0      41.2      60.9         44.8
PRODUCTION COSTS                  £/t     ECU/t
Diesel                          170.1     255.2
Naphtha                         169.0     253.5
Kerosine                        191.5     287.2

PLANT CAPITAL COST              645.3 M pounds,      967.9 M ECU
```

B.3.3 Lignite

B.3.3.1 Methanol

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: KRW Methanol               FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal         10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                       7871.5      78.7      72.8         43.5

TOTAL ENERGY PRODUCTS          7871.5      78.7      72.8         43.5
PRODUCTION COSTS                  £/t     ECU/t
Methanol                        140.2     210.3

PLANT CAPITAL COST              513.1 M pounds,      769.6 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: KRW Methanol                 FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow     % mass   % energy     % C.Conv.
                                   t/d      yield     yield        Effic.
Methanol                        7871.5      78.7      72.8          43.5

TOTAL ENERGY PRODUCTS           7871.5      78.7      72.8          43.5

PRODUCTION COSTS                   £/t     ECU/t
Methanol                          71.2     106.8

PLANT CAPITAL COST              513.1 M pounds,     769.6 M ECU
```

B.3.3.2 Fuel Alcohol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: KRW F/A                      FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow     % mass   % energy     % C.Conv.
                                   t/d      yield     yield        Effic.
Fuel alcohol                    5365.1      53.7      64.5          36.0

TOTAL ENERGY PRODUCTS           5392.0      53.9      64.5          36.0

PRODUCTION COSTS                   £/t     ECU/t
Fuel alcohol                     195.1     292.6

PLANT CAPITAL COST              618.3 M pounds,     927.4 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: KRW F/A                      FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow     % mass   % energy     % C.Conv.
                                   t/d      yield     yield        Effic.
Fuel alcohol                    5365.1      53.7      64.5          36.0

TOTAL ENERGY PRODUCTS           5392.0      53.9      64.5          36.0

PRODUCTION COSTS
                                   £/t     ECU/t
Fuel alcohol                      93.9     140.8

PLANT CAPITAL COST              618.3 M pounds,     927.4 M ECU
```

B.3.3.3 MTG

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================
RUN: KRW MTG                        FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal            10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                          Flow    % mass  % energy    % C.Conv.
                                    t/d     yield     yield       Effic.
Gasoline                         2846.1      28.5      53.2         31.4
Propane LPG                       157.5       1.6       3.2          1.9
Butane LPG                        378.0       3.8       7.6          4.6

TOTAL ENERGY PRODUCTS            3381.6      33.8      64.0         37.9
PRODUCTION COSTS                    £/t     ECU/t
Gasoline                          363.5     545.2
Propane LPG                       309.3     464.0
Butane LPG                        309.3     464.0

PLANT CAPITAL COST                596.9 M pounds,     895.3 M ECU
```

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================
RUN: KRW MTG                        FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal            10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                          Flow    % mass  % energy    % C.Conv.
                                    t/d     yield     yield       Effic.
Gasoline                         2846.1      28.5      53.2         31.4
Propane LPG                       157.5       1.6       3.2          1.9
Butane LPG                        378.0       3.8       7.6          4.6

TOTAL ENERGY PRODUCTS            3381.6      33.8      64.0         37.9
PRODUCTION COSTS                    £/t     ECU/t
Gasoline                          199.0     298.5
Propane LPG                       169.4     254.0
Butane LPG                        169.4     254.0

PLANT CAPITAL COST                596.9 M pounds,     895.3 M ECU
```

B.3.3.4 MOGD

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================
RUN: KRW MOGD                       FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal            10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                          Flow    % mass  % energy    % C.Conv.
                                    t/d     yield     yield       Effic.
Diesel                            283.4       2.8       5.3          3.1
Gasoline                         1970.2      19.7      36.8         21.7
Kerosine                          936.7       9.4      16.7         10.3

TOTAL ENERGY PRODUCTS            3190.3      31.9      58.8         35.2
PRODUCTION COSTS                    £/t     ECU/t
Diesel                            390.2     585.3
Gasoline                          433.1     649.7
Kerosine                          233.4     350.2

PLANT CAPITAL COST                662.0 M pounds,     993.1 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: KRW MOGD                  FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Diesel                         283.4       2.8       5.3          3.1
Gasoline                      1970.2      19.7      36.8         21.7
Kerosine                       936.7       9.4      16.7         10.3

TOTAL ENERGY PRODUCTS         3190.3      31.9      58.8         35.2
PRODUCTION COSTS                 £/t     ECU/t
Diesel                         211.0     316.6
Gasoline                       234.2     351.4
Kerosine                       126.3     189.4

PLANT CAPITAL COST             662.0 M pounds,     993.1 M ECU
```

B.3.3.5 SMDS

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: KRW SMDS                  FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Diesel                        2157.4      21.6      40.1         27.2
Naphtha                        540.2       5.4      10.0          6.8
Kerosine                       880.1       8.8      16.4         11.1

TOTAL ENERGY PRODUCTS         3577.8      35.8      66.5         45.1
PRODUCTION COSTS                 £/t     ECU/t
Diesel                         314.2     471.3
Naphtha                        312.1     468.2
Kerosine                       353.6     530.5

PLANT CAPITAL COST             634.5 M pounds,     951.7 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: KRW SMDS                  FINANCIAL CASE : 0 £/te 10 ROI
FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield     yield       Effic.
Diesel                        2906.1      29.1      36.2         29.8
Naphtha                        727.7       7.3       9.1          7.5
Kerosine                      1185.6      11.9      14.8         12.1

TOTAL ENERGY PRODUCTS         4819.4      48.2      60.0         49.4
PRODUCTION COSTS                 £/t     ECU/t
Diesel                         199.1     298.6
Naphtha                        197.8     296.6
Kerosine                       224.1     336.1

PLANT CAPITAL COST             685.2 M pounds,    1027.8 M ECU
```

B.4 HTW

B.4.1 Lignite

B.4.1.1 Methanol

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN:                          FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal      10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Methanol                     7979.4      79.8      73.0        44.1

TOTAL ENERGY PRODUCTS        7979.4      79.8      73.0        44.1

PRODUCTION COSTS                £/t     ECU/t
Methanol                      132.4     198.6

PLANT CAPITAL COST            502.1 M pounds,      753.2 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN:                          FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal      10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Methanol                     7979.4      79.8      73.0        44.1

TOTAL ENERGY PRODUCTS        7979.4      79.8      73.0        44.1

PRODUCTION COSTS                £/t     ECU/t
Methanol                      132.4     198.6

PLANT CAPITAL COST            502.1 M pounds,      753.2 M ECU
```

B.4.1.2 Fuel Alcohol

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: HTW F/A                  FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal      10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Fuel alcohol                 6970.2      69.7      82.9        46.8

TOTAL ENERGY PRODUCTS        7005.3      70.1      82.9        46.8
PRODUCTION COSTS                £/t     ECU/t
Fuel alcohol                  174.0     261.0

PLANT CAPITAL COST            656.0 M pounds,      983.9 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: HTW F/A                          FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal         10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d    yield    yield        Effic.
Fuel alcohol                 6970.2     69.7     82.9         46.8

TOTAL ENERGY PRODUCTS        7005.3     70.1     82.9         46.8
PRODUCTION COSTS                £/t    ECU/t
Fuel alcohol                   96.1    144.2

PLANT CAPITAL COST            656.0 M pounds,     983.9 M ECU
```

B.4.1.3 MTG

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: HTW MTG                          FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal         10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d    yield    yield        Effic.
Gasoline                     2885.1     28.9     53.3         31.8
Propane LPG                   159.7      1.6      3.2          1.9
Butane LPG                    383.2      3.8      7.6          4.7

TOTAL ENERGY PRODUCTS        3427.9     34.3     64.1         38.4
PRODUCTION COSTS                £/t    ECU/t
Gasoline                      344.8    517.2
Propane LPG                   293.4    440.1
Butane LPG                    293.4    440.1

PLANT CAPITAL COST            587.0 M pounds,     880.6 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: HTW MTG                          FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal         10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d    yield    yield        Effic.
Gasoline                     2885.1     28.9     53.3         31.8
Propane LPG                   159.7      1.6      3.2          1.9
Butane LPG                    383.2      3.8      7.6          4.7

TOTAL ENERGY PRODUCTS        3427.9     34.3     64.1         38.4
PRODUCTION COSTS                £/t    ECU/t
Gasoline                      182.6    273.8
Propane LPG                   155.4    233.0
Butane LPG                    155.4    233.0

PLANT CAPITAL COST            587.0 M pounds,     880.6 M ECU
```

B.4.1.4 MOGD

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: HTW MOGD                  FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal         10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield        Effic.
Diesel                        287.3       2.9      5.3           3.2
Gasoline                     1997.3      20.0     36.9          22.0
Kerosine                      949.6       9.5     16.7          10.5

TOTAL ENERGY PRODUCTS        3234.1      32.3     58.9          35.7
PRODUCTION COSTS                £/t     ECU/t
Diesel                        369.8     554.7
Gasoline                      410.4     615.6
Kerosine                      221.2     331.8

PLANT CAPITAL COST            652.6 M pounds,     978.9 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================
RUN: HTW MOGD                  FINANCIAL CASE : 0 £/t
FEEDSTOCK:
Rhenisch Brown Coal         10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield        Effic.
Diesel                        287.3       2.9      5.3           3.2
Gasoline                     1997.3      20.0     36.9          22.0
Kerosine                      949.6       9.5     16.7          10.5

TOTAL ENERGY PRODUCTS        3234.1      32.3     58.9          35.7
PRODUCTION COSTS                £/t     ECU/t
Diesel                        193.0     289.5
Gasoline                      214.2     321.4
Kerosine                      115.5     173.2

PLANT CAPITAL COST            652.6 M pounds,     978.9 M ECU
```

B.4.1.5 SMDS

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================
RUN: HTW SMDS                  FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal         10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield        Effic.
Diesel                       2188.5      21.9     40.2          27.6
Naphtha                       548.0       5.5     10.1           6.9
Kerosine                      892.8       8.9     16.4          11.3

TOTAL ENERGY PRODUCTS        3629.4      36.3     66.7          45.7
PRODUCTION COSTS                £/t     ECU/t
Diesel                        296.2     444.2
Naphtha                       294.2     441.3
Kerosine                      333.3     499.9

PLANT CAPITAL COST            626.5 M pounds,     939.7 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: HTW SMDS                   FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                       Flow   % mass  % energy   % C.Conv.
                                 t/d    yield     yield     Effic.
Diesel                        2188.5     21.9      40.2      27.6
Naphtha                        548.0      5.5      10.1       6.9
Kerosine                       892.8      8.9      16.4      11.3

TOTAL ENERGY PRODUCTS         3629.4     36.3      66.7      45.7
PRODUCTION COSTS                 £/t    ECU/t
Diesel                         150.9    226.3
Naphtha                        149.9    224.8
Kerosine                       169.8    254.7

PLANT CAPITAL COST             626.5 M pounds,     939.7 M ECU
```

B.5 Lurgi

B.5.1 Point of Ayr

B.5.1.1 Methanol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi Methanol             FINANCIAL CASE : 54.3 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow   % mass  % energy   % C.Conv.
                                 t/d    yield     yield     Effic.
Methanol                      5326.3     53.3      35.6      23.9

TOTAL ENERGY PRODUCTS         5326.3     53.3      35.6      23.9
PRODUCTION COSTS                 £/t    ECU/t
Methanol                       161.4    242.0

PLANT CAPITAL COST             323.9 M pounds,     485.8 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi Methanol             FINANCIAL CASE : 0 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                       Flow   % mass  % energy   % C.Conv.
                                 t/d    yield     yield     Effic.
Methanol                      5326.3     53.3      35.6      23.9

TOTAL ENERGY PRODUCTS         5326.3     53.3      35.6      23.9
PRODUCTION COSTS                 £/t    ECU/t
Methanol                        59.4     89.1

PLANT CAPITAL COST             323.9 M pounds,     485.8 M ECU
```

B.5.1.2 Fuel Alcohol

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: Lurgi F/A                     FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield       Effic.
Fuel alcohol                   2260.6      22.6     19.6         12.3

TOTAL ENERGY PRODUCTS          2271.9      22.7     19.6         12.3

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                    302.8     454.2

PLANT CAPITAL COST              326.2 M pounds,     489.3 M ECU
```

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: Lurgi F/A                     FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield       Effic.
Fuel alcohol                   2260.6      22.6     19.6         12.3

TOTAL ENERGY PRODUCTS          2271.9      22.7     19.6         12.3

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                     62.6      93.9

PLANT CAPITAL COST              326.2 M pounds,     489.3 M ECU
```

B.5.1.3 MTG

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: Lurgi MTG                     FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield       Effic.
Gasoline                       1925.8      19.3     26.0         17.3
Propane LPG                     106.6       1.1      1.6          1.0
Butane LPG                      255.8       2.6      3.7          2.5

TOTAL ENERGY PRODUCTS          2288.2      22.9     31.3         20.8
PRODUCTION COSTS                  £/t     ECU/t
Gasoline                        415.7     623.6
Propane LPG                     353.8     530.7
Butane LPG                      353.8     530.7

PLANT CAPITAL COST              388.0 M pounds,     581.9 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi MTG                    FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Point of Ayr                   10000.0 daf t/d,    13422.8 raw t/d
PRODUCTS:                         Flow     % mass  % energy     % C.Conv.
                                   t/d      yield    yield        Effic.
Gasoline                        1925.8       19.3     26.0          17.3
Propane LPG                      106.6        1.1      1.6           1.0
Butane LPG                       255.8        2.6      3.7           2.5

TOTAL ENERGY PRODUCTS           2288.2       22.9     31.3          20.8
PRODUCTION COSTS                   £/t      ECU/t
Gasoline                         172.7      259.1
Propane LPG                      147.0      220.5
Butane LPG                       147.0      220.5

PLANT CAPITAL COST               388.0 M pounds,     581.9 M ECU
```

B.5.1.4 MOGD

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi MOGD                   FINANCIAL CASE : 54.3 £/te 0 ROI
FEEDSTOCK:
Point of Ayr                   10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow     % mass  % energy     % C.Conv.
                                   t/d      yield    yield        Effic.
Diesel                           191.7        1.9      2.6           1.7
Gasoline                        1333.2       13.3     18.0          11.9
Kerosine                         633.8        6.3      8.1           5.7

TOTAL ENERGY PRODUCTS           2158.7       21.6     28.7          19.3
PRODUCTION COSTS                   £/t      ECU/t
Diesel                           445.5      668.2
Gasoline                         494.4      741.6
Kerosine                         266.5      399.7

PLANT CAPITAL COST               425.7 M pounds,     638.5 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi MOGD                   FINANCIAL CASE : 0 £/te 0 ROI
FEEDSTOCK:
Point of Ayr                   10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow     % mass  % energy     % C.Conv.
                                   t/d      yield    yield        Effic.
Diesel                           191.7        1.9      2.6           1.7
Gasoline                        1333.2       13.3     18.0          11.9
Kerosine                         633.8        6.3      8.1           5.7

TOTAL ENERGY PRODUCTS           2158.7       21.6     28.7          19.3
PRODUCTION COSTS                   £/t      ECU/t
Diesel                           180.7      271.0
Gasoline                         200.5      300.8
Kerosine                         108.1      162.1

PLANT CAPITAL COST               425.7 M pounds,     638.5 M ECU
```

B.5.1.5 SMDS

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi SMDS                   FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,   13422.8 raw t/d
PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Diesel                        1629.0      16.3     21.9        16.7
Naphtha                        407.9       4.1      5.5         4.2
Kerosine                       664.6       6.6      8.9         6.8

TOTAL ENERGY PRODUCTS         2701.5      27.0     36.2        27.7

PRODUCTION COSTS                 £/t     ECU/t
Diesel                         463.3     695.0
Naphtha                        460.2     690.3
Kerosine                       521.4     782.1

PLANT CAPITAL COST             525.6 M pounds,     788.4 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi SMDS                   FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,   13422.8 raw t/d
PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Diesel                        1629.0      16.3     21.9        16.7
Naphtha                        407.9       4.1      5.5         4.2
Kerosine                       664.6       6.6      8.9         6.8

TOTAL ENERGY PRODUCTS         2701.5      27.0     36.2        27.7
PRODUCTION COSTS                 £/t     ECU/t
Diesel                         268.1     402.2
Naphtha                        266.4     399.5
Kerosine                       301.8     452.7

PLANT CAPITAL COST             525.6 M pounds,     788.4 M ECU
```

B.5.2 Sub-bituminous

B.5.2.1 Methanol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi Methanol               FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,   13736.3 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Methanol                      4294.8      42.9     31.9        20.5

TOTAL ENERGY PRODUCTS         4294.8      42.9     31.9        20.5
PRODUCTION COSTS                 £/t     ECU/t
Methanol                       188.6     282.9

PLANT CAPITAL COST             305.3 M pounds,     457.9 M ECU
```

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================

RUN: Lurgi Methanol               FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit         10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass   % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                       4294.8      42.9      31.9         20.5

TOTAL ENERGY PRODUCTS          4294.8      42.9      31.9         20.5

PRODUCTION COSTS                  £/t     ECU/t
Methanol                         62.1      93.2

PLANT CAPITAL COST              305.3 M pounds,     457.9 M ECU
```

B.5.2.2 Fuel Alcohol

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================

RUN: Lurgi F/A                    FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit         10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass   % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Fuel alcohol                   1822.8      18.2      17.6         10.5

TOTAL ENERGY PRODUCTS          1831.9      18.3      17.6         10.5

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                    365.4     548.0

PLANT CAPITAL COST              307.7 M pounds,     461.6 M ECU
```

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================

RUN: Lurgi F/A                    FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit         10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass   % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Fuel alcohol                   1822.8      18.2      17.6         10.5

TOTAL ENERGY PRODUCTS          1831.9      18.3      17.6         10.5

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                     67.5     101.2

PLANT CAPITAL COST              307.7 M pounds,     461.6 M ECU
```

B.5.2.3 MTG

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================

RUN: Lurgi                      FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Gasoline                     1552.9      15.5      23.3         14.8
Propane LPG                    85.9       0.9       1.4          0.9
Butane LPG                    206.2       2.1       3.3          2.2

TOTAL ENERGY PRODUCTS        1845.0      18.5      28.1         17.8

PRODUCTION COSTS                £/t     ECU/t
Gasoline                      480.7     721.1
Propane LPG                   409.1     613.7
Butane LPG                    409.1     613.7

PLANT CAPITAL COST            357.3 M pounds,     535.9 M ECU
```

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================
RUN: Lurgi                      FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Gasoline                     1552.9      15.5      23.3         14.8
Propane LPG                    85.9       0.9       1.4          0.9
Butane LPG                    206.2       2.1       3.3          2.2

TOTAL ENERGY PRODUCTS        1845.0      18.5      28.1         17.8
PRODUCTION COSTS                £/t     ECU/t
Gasoline                      179.3     269.0
Propane LPG                   152.6     228.9
Butane LPG                    152.6     228.9

PLANT CAPITAL COST            357.3 M pounds,     535.9 M ECU
```

B.5.2.4 MOGD

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================
RUN: Lurgi MOGD                 FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Diesel                        154.6       1.5       2.3          1.5
Gasoline                     1075.0      10.7      16.2         10.2
Kerosine                      511.1       5.1       7.3          4.9

TOTAL ENERGY PRODUCTS        1740.7      17.4      25.8         16.6
PRODUCTION COSTS                £/t     ECU/t
Diesel                        518.1     777.2
Gasoline                      575.1     862.6
Kerosine                      310.0     464.9

PLANT CAPITAL COST            393.2 M pounds,     589.7 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================
RUN: Lurgi MOGD                  FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow   % mass  % energy    % C.Conv.
                                  t/d    yield    yield       Effic.
Diesel                          154.6      1.5      2.3         1.5
Gasoline                       1075.0     10.7     16.2        10.2
Kerosine                        511.1      5.1      7.3         4.9

TOTAL ENERGY PRODUCTS          1740.7     17.4     25.8        16.6
PRODUCTION COSTS                  £/t    ECU/t
Diesel                          189.7    284.6
Gasoline                        210.6    315.8
Kerosine                        113.5    170.2

PLANT CAPITAL COST              393.2 M pounds,     589.7 M ECU
```

B.5.2.5 SMDS

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Lurgi SMDS                  FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow   % mass  % energy    % C.Conv.
                                  t/d    yield    yield       Effic.
Diesel                         1339.2     13.4     20.0        14.6
Naphtha                         335.3      3.4      5.0         3.6
Kerosine                        546.3      5.5      8.2         5.9

TOTAL ENERGY PRODUCTS          2220.9     22.2     33.2        24.1
PRODUCTION COSTS                  £/t    ECU/t
Diesel                          518.4    777.6
Naphtha                         514.9    772.4
Kerosine                        583.4    875.1

PLANT CAPITAL COST              485.2 M pounds,     727.9 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Lurgi SMDS                  FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow   % mass  % energy    % C.Conv.
                                  t/d    yield    yield       Effic.
Diesel                         1339.2     13.4     20.0        14.6
Naphtha                         335.3      3.4      5.0         3.6
Kerosine                        546.3      5.5      8.2         5.9

TOTAL ENERGY PRODUCTS          2220.9     22.2     33.2        24.1
PRODUCTION COSTS                  £/t    ECU/t
Diesel                          281.0    421.4
Naphtha                         279.1    418.6
Kerosine                        316.2    474.3

PLANT CAPITAL COST              485.2 M pounds,     727.9 M ECU
```

B.5.3 Lignite

B.5.3.1 Methanol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN:                           FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal       10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                    Flow    % mass  % energy    % C.Conv.
                              t/d     yield     yield       Effic.
Methanol                   2875.6      28.8      25.5         15.9

TOTAL ENERGY PRODUCTS      2875.6      28.8      25.5         15.9

PRODUCTION COSTS              £/t     ECU/t
Methanol                    249.1     373.7

PLANT CAPITAL COST          275.7 M pounds,     413.5 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN:                           FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal       10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                    Flow    % mass  % energy    % C.Conv.
                              t/d     yield     yield       Effic.
Methanol                   2875.6      28.8      25.5         15.9

TOTAL ENERGY PRODUCTS      2875.6      28.8      25.5         15.9

PRODUCTION COSTS              £/t     ECU/t
Methanol                     60.3      90.4

PLANT CAPITAL COST          275.7 M pounds,     413.5 M ECU
```

B.5.3.2 Fuel Alcohol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi F/A                 FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal       10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                    Flow    % mass  % energy    % C.Conv.
                              t/d     yield     yield       Effic.
Fuel alcohol               1220.4      12.2      14.1          8.2

TOTAL ENERGY PRODUCTS      1226.6      12.3      14.1          8.2

PRODUCTION COSTS              £/t     ECU/t
Fuel alcohol                515.0     772.6

PLANT CAPITAL COST          293.2 M pounds,     439.8 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi F/A                   FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Fuel alcohol                   1220.4      12.2      14.1          8.2

TOTAL ENERGY PRODUCTS          1226.6      12.3      14.1          8.2

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                     70.1     105.2

PLANT CAPITAL COST              293.2 M pounds,     439.8 M ECU
```

B.5.3.3 MTG

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi MTG                   FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Gasoline                       1039.7      10.4      18.6         11.5
Propane LPG                      57.5       0.6       1.1          0.7
Butane LPG                      138.1       1.4       2.7          1.7

TOTAL ENERGY PRODUCTS          1235.3      12.4      22.4         13.8

PRODUCTION COSTS                  £/t     ECU/t
Gasoline                        630.8     946.2
Propane LPG                     536.8     805.2
Butane LPG                      536.8     805.2

PLANT CAPITAL COST              322.8 M pounds,     484.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi MTG                   FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Gasoline                       1039.7      10.4      18.6         11.5
Propane LPG                      57.5       0.6       1.1          0.7
Butane LPG                      138.1       1.4       2.7          1.7

TOTAL ENERGY PRODUCTS          1235.3      12.4      22.4         13.8

PRODUCTION COSTS                  £/t     ECU/t
Gasoline                        180.6     270.9
Propane LPG                     153.7     230.5
Butane LPG                      153.7     230.5

PLANT CAPITAL COST              322.8 M pounds,     484.2 M ECU
```

B.5.3.4 MOGD

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Lurgi MOGD                 FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal         10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield        Effic.
Diesel                        103.5       1.0      1.8          1.1
Gasoline                      719.8       7.2     12.9          7.9
Kerosine                      342.2       3.4      5.8          3.8

TOTAL ENERGY PRODUCTS        1165.5      11.7     20.6         12.9
PRODUCTION COSTS                £/t     ECU/t
Diesel                        678.6    1017.9
Gasoline                      753.2    1129.8
Kerosine                      406.0     608.9

PLANT CAPITAL COST            340.9 M pounds,     511.3 M ECU
```

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================
RUN: Lurgi MOGD                 FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal         10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield        Effic.
Diesel                        103.5       1.0      1.8          1.1
Gasoline                      719.8       7.2     12.9          7.9
Kerosine                      342.2       3.4      5.8          3.8

TOTAL ENERGY PRODUCTS        1165.5      11.7     20.6         12.9
PRODUCTION COSTS                £/t     ECU/t
Diesel                        188.1     282.2
Gasoline                      208.8     313.2
Kerosine                      112.5     168.8

PLANT CAPITAL COST            340.9 M pounds,     511.3 M ECU
```

B.5.3.5 SMDS

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Lurgi SMDS                 FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal         10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield        Effic.
Diesel                        992.7       9.9     17.7         12.5
Naphtha                       248.6       2.5      4.4          3.1
Kerosine                      405.0       4.0      7.2          5.1

TOTAL ENERGY PRODUCTS        1646.3      16.5     29.3         20.7
PRODUCTION COSTS                £/t     ECU/t
Diesel                        631.7     947.6
Naphtha                       627.5     941.3
Kerosine                      711.0    1066.5

PLANT CAPITAL COST            445.5 M pounds,     668.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Lurgi SMDS                   FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Diesel                          992.7       9.9      17.7         12.5
Naphtha                         248.6       2.5       4.4          3.1
Kerosine                        405.0       4.0       7.2          5.1

TOTAL ENERGY PRODUCTS          1646.3      16.5      29.3         20.7

PRODUCTION COSTS                  £/t     ECU/t
Diesel                          311.5     467.2
Naphtha                         309.4     464.1
Kerosine                        350.5     525.8

PLANT CAPITAL COST              445.5 M pounds,     668.2 M ECU
```

B.6 BGL

B.6.1 Point of Ayr

B.6.1.1 Methanol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL Methanol                 FINANCIAL CASE : 54.3 £/te 0 ROI

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                      10395.0     103.9      66.0         46.7

TOTAL ENERGY PRODUCTS         10395.0     103.9      66.0         46.7
PRODUCTION COSTS                  £/t     ECU/t
Methanol                        102.8     154.1

PLANT CAPITAL COST              483.8 M pounds,     725.7 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL Methanol                 FINANCIAL CASE : 0 £/te 0 ROI
FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                      10395.0     103.9      66.0         46.7

TOTAL ENERGY PRODUCTS         10395.0     103.9      66.0         46.7
PRODUCTION COSTS                  £/t     ECU/t
Methanol                         50.5      75.8

PLANT CAPITAL COST              483.8 M pounds,     725.7 M ECU
```

B.6.1.2 Fuel Alcohol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL F/A                  FINANCIAL CASE : 54.3 £/te 0 ROI

FEEDSTOCK:
Point of Ayr               10000.0 daf t/d,     13422.8 raw t/d

PRODUCTS:                     Flow    % mass   % energy     % C.Conv.
                               t/d     yield     yield        Effic.
Fuel alcohol                9111.3      91.1      75.2          49.7

TOTAL ENERGY PRODUCTS       9157.1      91.6      75.2          49.7

PRODUCTION COSTS               £/t     ECU/t
Fuel alcohol                 137.6     206.3

PLANT CAPITAL COST           653.3 M pounds,     979.9 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL F/A                  FINANCIAL CASE : 0 £/te 0 ROI

FEEDSTOCK:
Point of Ayr               10000.0 daf t/d,     13422.8 raw t/d

PRODUCTS:                     Flow    % mass   % energy     % C.Conv.
                               t/d     yield     yield        Effic.
Fuel alcohol                9111.3      91.1      75.2          49.7

TOTAL ENERGY PRODUCTS       9157.1      91.6      75.2          49.7

PRODUCTION COSTS               £/t     ECU/t
Fuel alcohol                  78.0     116.9

PLANT CAPITAL COST           653.3 M pounds,     979.9 M ECU
```

B.6.1.3 MTG

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL MTG                  FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Point of Ayr               10000.0 daf t/d,     13422.8 raw t/d

PRODUCTS:                     Flow    % mass   % energy     % C.Conv.
                               t/d     yield     yield        Effic.
Gasoline                    3758.5      37.6      48.2          33.7
Propane LPG                  208.0       2.1       2.9           2.0
Butane LPG                   499.2       5.0       6.9           4.9

TOTAL ENERGY PRODUCTS       4465.7      44.7      58.0          40.7

PRODUCTION COSTS               £/t     ECU/t
Gasoline                     272.9     409.4
Propane LPG                  232.3     348.4
Butane LPG                   232.3     348.4

PLANT CAPITAL COST           584.7 M pounds,     877.0 M ECU
```

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================
RUN: BGL MTG                   FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Point of Ayr              10000.0 daf t/d,   13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Gasoline                     3758.5      37.6      48.2         33.7
Propane LPG                   208.0       2.1       2.9          2.0
Butane LPG                    499.2       5.0       6.9          4.9

TOTAL ENERGY PRODUCTS        4465.7      44.7      58.0         40.7
PRODUCTION COSTS                £/t     ECU/t
Gasoline                      148.4     222.6
Propane LPG                   126.3     189.4
Butane LPG                    126.3     189.4

PLANT CAPITAL COST            584.7 M pounds,    877.0 M ECU
```

B.6.1.4 MOGD

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: BGL MOGD                  FINANCIAL CASE : 54.3 £/te 0 ROI
FEEDSTOCK:
Point of Ayr              10000.0 daf t/d,   13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Diesel                        374.2       3.7       4.8          3.4
Gasoline                     2601.9      26.0      33.4         23.3
Kerosine                     1237.0      12.4      15.1         11.1

TOTAL ENERGY PRODUCTS        4213.1      42.1      53.2         37.8

PRODUCTION COSTS                £/t     ECU/t
Diesel                        291.0     436.5
Gasoline                      323.0     484.5
Kerosine                      174.1     261.1

PLANT CAPITAL COST            666.5 M pounds,    999.8 M ECU
```

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: BGL MOGD                  FINANCIAL CASE : 0 £/te 0 ROI
FEEDSTOCK:
Point of Ayr              10000.0 daf t/d,   13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Diesel                        374.2       3.7       4.8          3.4
Gasoline                     2601.9      26.0      33.4         23.3
Kerosine                     1237.0      12.4      15.1         11.1

TOTAL ENERGY PRODUCTS        4213.1      42.1      53.2         37.8
PRODUCTION COSTS                £/t     ECU/t
Diesel                        155.3     233.0
Gasoline                      172.4     258.6
Kerosine                       92.9     139.4

PLANT CAPITAL COST            666.5 M pounds,    999.8 M ECU
```

B.6.1.5 SMDS

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL SMDS                  FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,   13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy   % C.Conv.
                                t/d     yield     yield      Effic.
Diesel                       2933.0      29.3      37.4        30.0
Naphtha                       734.5       7.3       9.4         7.5
Kerosine                     1196.5      12.0      15.3        12.3

TOTAL ENERGY PRODUCTS        4864.0      48.6      62.0        49.8
PRODUCTION COSTS                £/t     ECU/t
Diesel                        226.7     340.0
Naphtha                       225.2     337.7
Kerosine                      255.1     382.6

PLANT CAPITAL COST            626.3 M pounds,     939.5 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL SMDS                  FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,   13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy   % C.Conv.
                                t/d     yield     yield      Effic.
Diesel                       2933.0      29.3      37.4        30.0
Naphtha                       734.5       7.3       9.4         7.5
Kerosine                     1196.5      12.0      15.3        12.3

TOTAL ENERGY PRODUCTS        4864.0      48.6      62.0        49.8
PRODUCTION COSTS                £/t     ECU/t
Diesel                        118.3     177.4
Naphtha                       117.5     176.2
Kerosine                      133.1     199.7

PLANT CAPITAL COST            626.3 M pounds,     939.5 M ECU
```

B.6.2 Sub-bituminous

B.6.2.1 Methanol

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL Methanol              FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit       10000.0 daf t/d,   13736.3 raw t/d

PRODUCTS:                      Flow    % mass  % energy   % C.Conv.
                                t/d     yield     yield      Effic.
Methanol                     8659.7      86.6      65.8        41.3

TOTAL ENERGY PRODUCTS        8659.7      86.6      65.8        41.3
PRODUCTION COSTS                £/t     ECU/t
Methanol                      115.8     173.7

PLANT CAPITAL COST            435.2 M pounds,     652.8 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: BGL Methanol                  FINANCIAL CASE : 0 £/te

FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                       8659.7      86.6      65.8         41.3

TOTAL ENERGY PRODUCTS          8659.7      86.6      65.8         41.3

PRODUCTION COSTS                  £/t     ECU/t
Methanol                         53.1      79.7

PLANT CAPITAL COST              435.2 M pounds,     652.8 M ECU
```

B.6.2.2 Fuel Alcohol

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: BGL F/A                       FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Fuel alcohol                   7146.7      71.5      70.6         41.4

TOTAL ENERGY PRODUCTS          7182.6      71.8      70.6         41.4

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                    155.1     232.7

PLANT CAPITAL COST              577.1 M pounds,     865.6 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: BGL F/A                       FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Fuel alcohol                   7146.7      71.5      70.6         41.4

TOTAL ENERGY PRODUCTS          7182.6      71.8      70.6         41.4

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                     79.2     118.7

PLANT CAPITAL COST              577.1 M pounds,     865.6 M ECU
```

B.6.2.3 MTG

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: BGL MTG                      FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit      10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield       Effic.
Gasoline                     3131.5      31.3     48.1        29.8
Propane LPG                   173.3       1.7      2.9         1.8
Butane LPG                    415.9       4.2      6.9         4.4

TOTAL ENERGY PRODUCTS        3720.7      37.2     57.8        36.0
PRODUCTION COSTS                £/t     ECU/t
Gasoline                      305.2     457.8
Propane LPG                   259.7     389.6
Butane LPG                    259.7     389.6

PLANT CAPITAL COST            527.3 M pounds,     790.9 M ECU
```

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================
RUN: BGL MTG                      FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit      10000.0 daf t/d,    13736.3 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield    yield       Effic.
Gasoline                     3131.5      31.3     48.1        29.8
Propane LPG                   173.3       1.7      2.9         1.8
Butane LPG                    415.9       4.2      6.9         4.4

TOTAL ENERGY PRODUCTS        3720.7      37.2     57.8        36.0
PRODUCTION COSTS                £/t     ECU/t
Gasoline                      155.7     233.6
Propane LPG                   132.5     198.8
Butane LPG                    132.5     198.8

PLANT CAPITAL COST            527.3 M pounds,     790.9 M ECU
```

B.6.2.4 MOGD

```
                ASTON LIQUID FUELS PRODUCTION MODEL
                ===================================

RUN: BGL MOGD                     FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit      10000.0 daf t/d,    13736.3 raw t/d

                                                           % C.Conv.
PRODUCTS:                      Flow    % mass  % energy      Effic.
                                t/d     yield    yield
                                                   4.8         3.0
Diesel                        311.8       3.1     33.3        20.6
Gasoline                     2167.8      21.7     15.1         9.8
Kerosine                     1030.6      10.3
                                                  53.1        33.4
TOTAL ENERGY PRODUCTS        3510.2      35.1
PRODUCTION COSTS                £/t     ECU/t
Diesel                        326.1     489.1
Gasoline                      361.9     542.9
Kerosine                      195.1     292.6
                                                  892.5 M ECU
PLANT CAPITAL COST            595.0 M pounds,
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL MOGD                     FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,     13736.3 raw t/d

PRODUCTS:                        Flow     % mass   % energy    % C.Conv.
                                  t/d      yield     yield       Effic.
Diesel                          311.8       3.1       4.8         3.0
Gasoline                       2167.8      21.7      33.3        20.6
Kerosine                       1030.6      10.3      15.1         9.8

TOTAL ENERGY PRODUCTS          3510.2      35.1      53.1        33.4
PRODUCTION COSTS                  £/t     ECU/t
Diesel                          163.2     244.9
Gasoline                        181.2     271.8
Kerosine                         97.7     146.5

PLANT CAPITAL COST              595.0 M pounds,     892.5 M ECU
```

B.6.2.5 SMDS

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL SMDS                     FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,     13736.3 raw t/d

PRODUCTS:                        Flow     % mass   % energy    % C.Conv.
                                  t/d      yield     yield       Effic.
Diesel                         2428.7      24.3      37.1        26.4
Naphtha                         608.2       6.1       9.3         6.6
Kerosine                        990.8       9.9      15.1        10.8

TOTAL ENERGY PRODUCTS          4027.6      40.3      61.5        43.8
PRODUCTION COSTS                  £/t     ECU/t
Diesel                          259.7     389.5
Naphtha                         257.9     386.9
Kerosine                        292.2     438.4

PLANT CAPITAL COST              574.7 M pounds,     862.1 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL SMDS                     FINANCIAL CASE : 0 £/te
FEEDSTOCK:
South African Sub-bit        10000.0 daf t/d,     13736.3 raw t/d

PRODUCTS:                        Flow     % mass   % energy    % C.Conv.
                                  t/d      yield     yield       Effic.
Diesel                         2428.7      24.3      37.1        26.4
Naphtha                         608.2       6.1       9.3         6.6
Kerosine                        990.8       9.9      15.1        10.8

TOTAL ENERGY PRODUCTS          4027.6      40.3      61.5        43.8
PRODUCTION COSTS                  £/t     ECU/t
Diesel                          128.8     193.1
Naphtha                         127.9     191.9
Kerosine                        144.9     217.4

PLANT CAPITAL COST              574.7 M pounds,     862.1 M ECU
```

B.6.3 Lignite

B.6.3.1 Methanol

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================

RUN: BGL Methanol                       FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield       Effic.
Methanol                       7236.3      72.4     70.1         40.0

TOTAL ENERGY PRODUCTS          7236.3      72.4     70.1         40.0

PRODUCTION COSTS                  £/t     ECU/t
Methanol                        134.6     201.9

PLANT CAPITAL COST              428.9 M pounds,    643.4 M ECU
```

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================

RUN: BGL Methanol                       FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield       Effic.
Methanol                       7236.3      72.4     70.1         40.0

TOTAL ENERGY PRODUCTS          7236.3      72.4     70.1         40.0

PRODUCTION COSTS                  £/t     ECU/t
Methanol                         59.6      89.4

PLANT CAPITAL COST              428.9 M pounds,    643.4 M ECU
```

B.6.3.2 Fuel Alcohol

```
                         ASTON LIQUID FUELS PRODUCTION MODEL
                         ===================================

RUN: BGL F/A                            FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield       Effic.
Fuel alcohol                   6161.3      61.6     77.6         41.3

TOTAL ENERGY PRODUCTS          6192.2      61.9     77.6         41.3

PRODUCTION COSTS                  £/t     ECU/t
Fuel alcohol                    175.1     262.7

PLANT CAPITAL COST              564.8 M pounds,    847.2 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: BGL F/A                      FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Fuel alcohol                    6161.3      61.6      77.6         41.3

TOTAL ENERGY PRODUCTS           6192.2      61.9      77.6         41.3
PRODUCTION COSTS                   £/t     ECU/t
Fuel alcohol                      87.0     130.5

PLANT CAPITAL COST               564.8 M pounds,     847.2 M ECU
```

B.6.3.3 MTG

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: BGL MTG                      FINANCIAL CASE : 54.3 £/te

FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Gasoline                        2616.5      26.2      51.2         28.9
Propane LPG                      144.8       1.4       3.1          1.7
Butane LPG                       347.5       3.5       7.3          4.2

TOTAL ENERGY PRODUCTS           3108.7      31.1      61.6         34.8
PRODUCTION COSTS                   £/t     ECU/t
Gasoline                         350.2     525.2
Propane LPG                      298.0     447.0
Butane LPG                       298.0     447.0

PLANT CAPITAL COST               506.0 M pounds,     759.1 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: BGL MTG                      FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal           10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Gasoline                        2616.5      26.2      51.2         28.9
Propane LPG                      144.8       1.4       3.1          1.7
Butane LPG                       347.5       3.5       7.3          4.2

TOTAL ENERGY PRODUCTS           3108.7      31.1      61.6         34.8
PRODUCTION COSTS                   £/t     ECU/t
Gasoline                         171.3     256.9
Propane LPG                      145.7     218.6
Butane LPG                       145.7     218.6

PLANT CAPITAL COST               506.0 M pounds,     759.1 M ECU
```

B.6.3.4 MOGD

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================

RUN: BGL MOGD                    FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield       Effic.
Diesel                          260.5       2.6      5.1         2.9
Gasoline                       1811.3      18.1     35.4        20.0
Kerosine                        861.1       8.6     16.1         9.5

TOTAL ENERGY PRODUCTS          2932.9      29.3     56.6        32.3
PRODUCTION COSTS                  £/t     ECU/t
Diesel                          376.3     564.5
Gasoline                        417.7     626.5
Kerosine                        225.1     337.7

PLANT CAPITAL COST              568.9 M pounds,     853.4 M ECU
```

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================
RUN: BGL MOGD                    FINANCIAL CASE : 0 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield       Effic.
Diesel                          260.5       2.6      5.1         2.9
Gasoline                       1811.3      18.1     35.4        20.0
Kerosine                        861.1       8.6     16.1         9.5

TOTAL ENERGY PRODUCTS          2932.9      29.3     56.6        32.3
PRODUCTION COSTS                  £/t     ECU/t
Diesel                          181.4     272.1
Gasoline                        201.4     302.0
Kerosine                        108.5     162.8

PLANT CAPITAL COST              568.9 M pounds,     853.4 M ECU
```

B.6.3.5 SMDS

```
                     ASTON LIQUID FUELS PRODUCTION MODEL
                     ===================================

RUN: BGL SMDS                    FINANCIAL CASE : 54.3 £/te
FEEDSTOCK:
Rhenisch Brown Coal          10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                                % mass  % energy    % C.Conv.
                                 Flow     yield    yield       Effic.
                                  t/d              39.8        25.8
Diesel                         2044.1      20.4     10.0         6.5
Naphtha                         511.9       5.1     16.2        10.5
Kerosine                        833.9       8.3
                                                    66.0        42.7
TOTAL ENERGY PRODUCTS          3389.9      33.9
PRODUCTION COSTS                  £/t     ECU/t
Diesel                          295.1     442.7
Naphtha                         293.2     439.7
Kerosine                        332.1     498.2
                                                    829.6 M ECU
PLANT CAPITAL COST              553.1 M pounds,
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: BGL SMDS                     FINANCIAL CASE : 0 £/te

FEEDSTOCK:
Rhenisch Brown Coal             10000.0 daf t/d,    24096.4 raw t/d

PRODUCTS:                          Flow    % mass  % energy    % C.Conv.
                                    t/d     yield     yield       Effic.
Diesel                           2044.1      20.4      39.8        25.8
Naphtha                           511.9       5.1      10.0         6.5
Kerosine                          833.9       8.3      16.2        10.5

TOTAL ENERGY PRODUCTS            3389.9      33.9      66.0        42.7

PRODUCTION COSTS                    £/t     ECU/t
Diesel                            139.6     209.4
Naphtha                           138.7     208.0
Kerosine                          157.1     235.7

PLANT CAPITAL COST                553.1 M pounds,     829.6 M ECU
```

B.7 Sensitivity Results On Base Case

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Lifetime +10%

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow     % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                       9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS          9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                  £/t     ECU/t
Methanol                        124.3     186.4

PLANT CAPITAL COST              511.4 M pounds,     767.2 M ECU
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Lifetime -10%

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow     % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                       9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS          9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                  £/t     ECU/t
Methanol                        126.8     190.2

PLANT CAPITAL COST              511.4 M pounds,     767.2 M ECU
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : 365 days/year

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow     % mass  % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                       9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS          9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                  £/t     ECU/t
Methanol                        123.3     185.0

PLANT CAPITAL COST              511.4 M pounds,     767.2 M ECU
=
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : 309 days/year

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Methanol                        9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS           9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                   £/t     ECU/t
Methanol                         128.5     192.7

PLANT CAPITAL COST               511.4 M pounds,     767.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Interest +10%

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Methanol                        9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS           9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                   £/t     ECU/t
Methanol                         126.2     189.3

PLANT CAPITAL COST               511.4 M pounds,     767.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Interest -10%

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Methanol                        9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS           9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                   £/t     ECU/t
Methanol                         124.7     187.1

PLANT CAPITAL COST               511.4 M pounds,     767.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Inflation +10%

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield        Effic.
Methanol                       9449.1      94.5     63.1         42.4

TOTAL ENERGY PRODUCTS          9449.1      94.5     63.1         42.4

PRODUCTION COSTS
                                  £/t     ECU/t
Methanol                        125.3     188.0

PLANT CAPITAL COST              511.4 M pounds,     767.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Inflation -10%

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield        Effic.
Methanol                       9449.1      94.5     63.1         42.4

TOTAL ENERGY PRODUCTS          9449.1      94.5     63.1         42.4

PRODUCTION COSTS
                                  £/t     ECU/t
Methanol                        125.5     188.3

PLANT CAPITAL COST              511.4 M pounds,     767.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Feed Cost +10%

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                        Flow    % mass  % energy    % C.Conv.
                                  t/d     yield    yield        Effic.
Methanol                       9449.1      94.5     63.1         42.4

TOTAL ENERGY PRODUCTS          9449.1      94.5     63.1         42.4

PRODUCTION COSTS
                                  £/t     ECU/t
Methanol                        131.1     196.7

PLANT CAPITAL COST              511.4 M pounds,     767.2 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Feed Cost -10%

FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Methanol                     9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS        9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                £/t     ECU/t
Methanol                      120.2     180.3

PLANT CAPITAL COST            511.4 M pounds,     767.2 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Labour cost +10%

FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Methanol                     9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS        9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                £/t     ECU/t
Methanol                      125.4     188.2

PLANT CAPITAL COST            511.4 M pounds,     767.2 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Labour cost -10%

FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow    % mass  % energy    % C.Conv.
                                t/d     yield     yield       Effic.
Methanol                     9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS        9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                £/t     ECU/t
Methanol                      125.4     188.1

PLANT CAPITAL COST            511.4 M pounds,     767.2 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Maintenance +10%

FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow     % mass  % energy    % C.Conv.
                                t/d      yield    yield        Effic.
Methanol                     9449.1       94.5     63.1          42.4

TOTAL ENERGY PRODUCTS        9449.1       94.5     63.1          42.4

PRODUCTION COSTS
                                £/t      ECU/t
Methanol                      125.8      188.7

PLANT CAPITAL COST            511.4 M pounds,     767.2 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Maintenance -10%

FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow     % mass  % energy    % C.Conv.
                                t/d      yield    yield        Effic.
Methanol                     9449.1       94.5     63.1          42.4

TOTAL ENERGY PRODUCTS        9449.1       94.5     63.1          42.4

PRODUCTION COSTS
                                £/t      ECU/t
Methanol                      125.1      187.6

PLANT CAPITAL COST            511.4 M pounds,     767.2 M ECU
```

```
                  ASTON LIQUID FUELS PRODUCTION MODEL
                  ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Overheads +10%

FEEDSTOCK:
Point of Ayr                10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                      Flow     % mass  % energy    % C.Conv.
                                t/d      yield    yield        Effic.
Methanol                     9449.1       94.5     63.1          42.4

TOTAL ENERGY PRODUCTS        9449.1       94.5     63.1          42.4

PRODUCTION COSTS
                                £/t      ECU/t
Methanol                      126.2      189.3

PLANT CAPITAL COST            511.4 M pounds,     767.2 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: Data:coal.dat:10 % sense    FINANCIAL CASE : Overheads -10%

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:
                                 Flow    % mass   % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                       9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS          9449.1      94.5      63.1         42.4

PRODUCTION COSTS

                                  £/t     ECU/t
Methanol                        124.6     186.9

PLANT CAPITAL COST              511.4 M pounds,     767.2 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: Data:coal.dat:10 % sense    FINANCIAL CASE : HP Steam +10%

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:
                                 Flow    % mass   % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                       9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS          9449.1      94.5      63.1         42.4

PRODUCTION COSTS

                                  £/t     ECU/t
Methanol                        125.3     187.9

PLANT CAPITAL COST              511.4 M pounds,     767.2 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: Data:coal.dat:10 % sense    FINANCIAL CASE : HP Steam -10%

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:
                                 Flow    % mass   % energy    % C.Conv.
                                  t/d     yield     yield       Effic.
Methanol                       9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS          9449.1      94.5      63.1         42.4

PRODUCTION COSTS

                                  £/t     ECU/t
Methanol                        125.6     188.4

PLANT CAPITAL COST              511.4 M pounds,     767.2 M ECU
```

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : LP Steam +10%

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                          Flow    % mass  % energy     % C.Conv.
                                    t/d     yield     yield        Effic.
Methanol                         9449.1      94.5      63.1          42.4

TOTAL ENERGY PRODUCTS            9449.1      94.5      63.1          42.4

PRODUCTION COSTS
                                    £/t     ECU/t
Methanol                          125.6     188.3

PLANT CAPITAL COST                511.4 M pounds,     767.2 M ECU
```

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : LP Steam -10%

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                          Flow    % mass  % energy     % C.Conv.
                                    t/d     yield     yield        Effic.
Methanol                         9449.1      94.5      63.1          42.4

TOTAL ENERGY PRODUCTS            9449.1      94.5      63.1          42.4

PRODUCTION COSTS
                                    £/t     ECU/t
Methanol                          125.3     187.9

PLANT CAPITAL COST                511.4 M pounds,     767.2 M ECU
```

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Process water +10%

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                          Flow    % mass  % energy     % C.Conv.
                                    t/d     yield     yield        Effic.
Methanol                         9449.1      94.5      63.1          42.4

TOTAL ENERGY PRODUCTS            9449.1      94.5      63.1          42.4

PRODUCTION COSTS
                                    £/t     ECU/t
Methanol                          125.4     188.1

PLANT CAPITAL COST                511.4 M pounds,     767.2 M ECU
```

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Process water -10%

FEEDSTOCK:
Point of Ayr                   10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield    yield        Effic.
Methanol                        9449.1      94.5     63.1         42.4

TOTAL ENERGY PRODUCTS           9449.1      94.5     63.1         42.4

PRODUCTION COSTS
                                   £/t     ECU/t
Methanol                         125.4     188.1

PLANT CAPITAL COST               511.4 M pounds,     767.2 M ECU
```

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Cooling water +10%

FEEDSTOCK:
Point of Ayr                   10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield    yield        Effic.
Methanol                        9449.1      94.5     63.1         42.4

TOTAL ENERGY PRODUCTS           9449.1      94.5     63.1         42.4

PRODUCTION COSTS
                                   £/t     ECU/t
Methanol                         125.5     188.3

PLANT CAPITAL COST               511.4 M pounds,     767.2 M ECU
```

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Cooling water -10%

FEEDSTOCK:
Point of Ayr                   10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield    yield        Effic.
Methanol                        9449.1      94.5     63.1         42.4

TOTAL ENERGY PRODUCTS           9449.1      94.5     63.1         42.4

PRODUCTION COSTS
                                   £/t     ECU/t
Methanol                         125.3     188.0

PLANT CAPITAL COST               511.4 M pounds,     767.2 M ECU
```

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Fuel gas +10%

FEEDSTOCK:
Point of Ayr                    10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                           Flow    % mass  % energy    % C.Conv.
                                     t/d     yield     yield       Effic.
Methanol                          9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS             9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                     £/t     ECU/t
Methanol                           124.9     187.4

PLANT CAPITAL COST                 511.4 M pounds,     767.2 M ECU
```

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Fuel gas -10%

FEEDSTOCK:
Point of Ayr                    10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                           Flow    % mass  % energy    % C.Conv.
                                     t/d     yield     yield       Effic.
Methanol                          9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS             9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                     £/t     ECU/t
Methanol                           125.9     188.8

PLANT CAPITAL COST                 511.4 M pounds,     767.2 M ECU
```

```
                      ASTON LIQUID FUELS PRODUCTION MODEL
                      ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Oxygen +10%

FEEDSTOCK:
Point of Ayr                    10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                           Flow    % mass  % energy    % C.Conv.
                                     t/d     yield     yield       Effic.
Methanol                          9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS             9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                     £/t     ECU/t
Methanol                           129.7     194.5

PLANT CAPITAL COST                 511.4 M pounds,     767.2 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Oxygen -10%

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,   13422.8 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Methanol                      9449.1     94.5     63.1        42.4

TOTAL ENERGY PRODUCTS         9449.1     94.5     63.1        42.4

PRODUCTION COSTS
                                 £/t    ECU/t
Methanol                       121.2    181.8

PLANT CAPITAL COST             511.4 M pounds,    767.2 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Power +10%

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,   13422.8 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Methanol                      9449.1     94.5     63.1        42.4

TOTAL ENERGY PRODUCTS         9449.1     94.5     63.1        42.4

PRODUCTION COSTS
                                 £/t    ECU/t
Methanol                       125.4    188.1

PLANT CAPITAL COST             511.4 M pounds,    767.2 M ECU
```

```
                 ASTON LIQUID FUELS PRODUCTION MODEL
                 ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Power -10%

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,   13422.8 raw t/d

PRODUCTS:                       Flow    % mass  % energy    % C.Conv.
                                 t/d     yield    yield       Effic.
Methanol                      9449.1     94.5     63.1        42.4

TOTAL ENERGY PRODUCTS         9449.1     94.5     63.1        42.4

PRODUCTION COSTS
                                 £/t    ECU/t
Methanol                       125.4    188.1

PLANT CAPITAL COST             511.4 M pounds,    767.2 M ECU
```

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Capital Cost +10%

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Methanol                        9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS           9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                   £/t     ECU/t
Methanol                         128.4     192.6

PLANT CAPITAL COST               562.4 M pounds,     843.7 M ECU
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:10 % sense   FINANCIAL CASE : Capital Cost -10%

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Methanol                        9449.1      94.5      63.1         42.4

TOTAL ENERGY PRODUCTS           9449.1      94.5      63.1         42.4

PRODUCTION COSTS
                                   £/t     ECU/t
Methanol                         122.7     184.0

PLANT CAPITAL COST               465.0 M pounds,     697.4 M ECU
```

B.8 Ideal Gasifier, Methanol Case

```
                    ASTON LIQUID FUELS PRODUCTION MODEL
                    ===================================

RUN: Data:coal.dat:Ideal Gas    FINANCIAL CASE : 'Ideal' Gasifier

FEEDSTOCK:
Point of Ayr                  10000.0 daf t/d,    13422.8 raw t/d

PRODUCTS:                         Flow    % mass  % energy    % C.Conv.
                                   t/d     yield     yield       Effic.
Methanol                       20951.2     209.5     139.9         93.9

TOTAL ENERGY PRODUCTS          20951.2     209.5     139.9         93.9

PRODUCTION COSTS
                                   £/t     ECU/t
Methanol                          75.2     112.8

PLANT CAPITAL COST               752.5 M pounds,    1128.7 M ECU
```

B.9 Shell With Methane, No Reformer Case

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: Data:coal.dat:testalance   FINANCIAL CASE : Runname

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,   13422.8 raw t/d

PRODUCTS:                       Flow   % mass  % energy   % C.Conv.
                                 t/d    yield    yield      Effic.
Methanol                      8221.0     82.2     54.9        36.9

TOTAL ENERGY PRODUCTS         8221.0     82.2     54.9        36.9

PRODUCTION COSTS
                                 £/t    ECU/t
Methanol                       125.8    188.6

PLANT CAPITAL COST             472.1 M pounds,    708.2 M ECU
```

B.9 Shell With Methane, Reformer Case

```
                        ASTON LIQUID FUELS PRODUCTION MODEL
                        ===================================

RUN: Data:coal.dat:5 % meth r   FINANCIAL CASE : Runname

FEEDSTOCK:
Point of Ayr                 10000.0 daf t/d,   13422.8 raw t/d

PRODUCTS:                       Flow   % mass  % energy   % C.Conv.
                                 t/d    yield    yield      Effic.
Methanol                     10040.9    100.4     67.0        45.1

TOTAL ENERGY PRODUCTS        10040.9    100.4     67.0        45.1

PRODUCTION COSTS
                                 £/t    ECU/t
Methanol                       122.4    183.6

PLANT CAPITAL COST             556.0 M pounds,    834.0 M ECU
```

Appendix C

Derivation of Equations Developed by John Brown Engineers and Constructors Ltd to model Syngas Conditioning Steps.

C.1 Summary of Variables Used

C.1.1 Main Streams

	Raw Syngas	Actual Shift Feed	Actual Shift Product	Shift By-pass	Total Shift Product	H_2S Plant Product	H_2S Plant Reject	CO_2 Plant Feed	CO_2 Plant Product
H_2	F1	EF1	EP1	EB1	L1	N1	RH1	W1	Q1
CO	F2	EF2	EP2	EB2	L2	N2	RH2	W2	Q2
CO_2	F3	EF3	EP3	EB3	L3	N3	RH3	W3	Q3
C_1	F4	EF4	EP4	EB4	L4	N4	RH4	W4	Q4
C_2	F5	EF5	EP5	EB5	L5	N5	RH5	W5	Q5
N_2	F6	EF6	EP6	EB6	L6	N6	RH6	W6	Q6
H_2O	F7	EF7	EP7	EB7	L7	N7	RH7	W7	Q7
C_3	-	-	-	-	-	-	-	W11	Q11
C_4	-	-	-	-	-	-	-	W12	Q12
C_5	-	-	-	-	-	-	-	W13	Q13
H_2S	F14	EF14	EP14	EB14	L14	N14	RH14	-	-
COS	F15	EF15	EP15	EB15	L15	N15	RH15	-	-
SO_2	F16	EF16	EP16	EB16	L16	N16	RH16	-	-
CS_2	F17	EF17	EP17	EB17	L17	N17	RH17	-	-
Mercaptan	F18	EF18	EP18	EB18	L18	N18	RH18	-	-
Thiophene	F19	EF19	EP19	EB19	L19	N19	RH19	-	-
Total	FT	EFT	EPT	EBT	LT	NT	RHT	WT	QT

Notes: all components variables in program are one dimensional arrays eg F1 is F[1].

	CO_2 Plant Reject	Alcohol Feed to Synthesis	Total Alcohol Offgas	Purge Gas	Reformer Feed	Reformer Product	PSA Feed	PSA Product	PSA Reject	Recycle to CO_2 Plant
H_2	RC1	QA1	B1	G1	R1	P1	PS1	PP1	PG1	HS1
CO	RC2	QA2	B2	G2	R2	P2	PS2	-	PG2	HS2
CO_2	RC3	QA3	B3	G3	R3	P3	PS3	-	PG3	HS3
C_1	RC4	QA4	B4	G4	R4	P4	PS4	PP4	PG4	HS4
C_2	RC5	QA5	B5	G5	R5	-	PS5	-	PG5	HS5
N_2	RC6	QA6	B6	G6	R6	P6	PS6	PP6	PG6	HS6
H_2O	RC8	QA8	B8	G8	R8	P8	PS8	-	PG8	HS8
C_3	RC11	QA11	B11	G11	R11	-	PS11	-	PG11	HS11
C_4	RC12	QA12	B12	G12	R12	-	PS12	-	PG12	HS12
C_5	RC13	QA13	B13	G13	R13	-	PS13	-	PG13	HS13
Total	RCT	QAT	BT	GT	RT	PT	PST	PPT	PGT	HST

C.1.2 General

T1$	Case Title
T$[N]	Component titles
T2$	Recycle system - recycle, reformer, PSA

C.1.3 Shift

S	Mol / h CO to be shifted to CO_2
SQ	Shift Required, 1 = Yes, 0 = No
HS	Mols Steam Added
HP	Minimum mols H_2O in actual shift feed
K1	Mol fraction CO converted in shift K2 minimum mols H_2O / mol dry gas in shift feed
Z1	Mol fraction of total shift routed to shift dry basis
F[N]	Feed kg mol / h from gasifier / feed compression
PH	Feed pressure , bar (abs)
DPS	Pressure drop, bar
TS	Temperature downstream of shift cooler
VP2	SVP water at TS
HT	Mols H_2O condensed in shift product cooler
HTS	Saturated mols water in gas from shift product cooler
HT1	Mols water in gas to shift product cooler
CK1 to CK6	Constant in equations for calculating mols CO to be shifted
S[N]	Mols CO shifted on successive iterations to eliminate the shift

C.1.4 H_2S Removal

LH[N]	Mol fraction of light ends over plant
DPH	Pressure drop, bar (abs)
HQ	Selexol plant required (1) or not required (0)
HH	Mols H_2O condensed in feed cooler
HHS	Saturated mols water in gas from feed cooler
HH1	Mols water in gas from feed cooler.

C.1.5 CO_2 Removal Plant

A	Mol fractions CO_2 in outlet from CO_2 plant, dry basis
R	Mol / h CO_2 to be removed in CO_2 plant
LC[N]	Mol-fraction recoveries of light ends over plant
DPC	Pressure drop, bar (abs)

C.1.6 Alcohol Unit

Alcohols	Wt. Fraction Alcohols in Alcohol Product	Mol Fraction Alcohols in Alcohol Product	MW	Alcoholskg mol / h
CH_3OH	WFA[1]	MFA[1]	MWA[1]	MA[1]
C_2H_5OH	WFA[2]	MFA[2]	MWA[2]	MA[2]
C_3H_7OH	WFA[3]	MFA[3]	MWA[3]	MA[3]
C_4H_9OH	WFA[4]	MFA[4]	MWA[4]	MA[4]
$C_5H_{11}OH$	WFA[5]	MFA[5]	MWA[5]	MA[5]
$C_6H_{13}OH$	WFA[6]	MFA[6]	MWA[6]	MA[6]
H_2O				MA[8]
Total				MAT

	Wt. Fraction HC's in HC's Produced	Mol Fraction HC's in HC's Produced	MW HC's	kg mol / h HC's
C_1H_4	WFG[1]	MFG[1]	MWG[1]	MG[1]
C_2H_6	WFG[2]	MFG[2]	MWG[2]	MG[2]
C_3H_8	WFG[3]	MFG[3]	MWG[3]	MG[3]
C_4H_{10}	WFG[4]	MFG[4]	MWG[4]	MG[4]
C_5H_{12}	WFG[5]	MFG[5]	MWG[5]	MG[5]
Total				MGT

WMA	Sum of alcohol wt fractions / MW
WMG	Sum of hydrocarbon wt fractions / MW
KMA	Mols CO - required to produce one mol of final alcohol product
KMG	Mols CO - required to produce one mol of final hydrocarbon product
MCA	kg mol / h CO - converted to alcohols
MCH	kg mol / h CO - converted to hydrocarbons
MCT	kg mol / h CO - converted to alcohols & hydrocarbons
SA	kg mol / h CO - shifted to CO_2 in alcohol plant
SM	Mol fraction CO - shifted to CO_2 in alcohol plant
SAC	Mol fraction CO - selectivity to alcohols
CNV	Mol fraction CO - converted to alcohols & hydrocarbons
RH	Required feed H_2 : CO molar ratio
UHA	Mols H_2 consumed in production of alcohols
UHG	Mols H_2 consumed in production of hydrocarbons
UWA	Mols H_2O produced in production of alcohols
UWG	Mols H_2O produced in production of hydrocarbons
AA	Mol fraction CO_2 in alcohol plant recycle / offgas, dry basis
R	kg mol / h CO_2 removed from recycle / offgas
MK[50]	Calculated total mols alcohols (dry) in each iteration
CLA	% closure on total mols alcohols (dry) after final iteration
PM1	Pressure, bar (abs), downstream feed compressor
PM2	Pressure, bar (abs), in product HP separator
VP1	Pressure, bar (abs), SVP H_2O @ 38 °C
HM1	Mols steam to alcohol plant from syngas feed compressor (actual)
HM2	Mols water knocked out in syngas feed compressor coolers
HM3	Mols steam to alcohol plant from syngas feed compressor (saturated)

C.1.7 PSA Unit

H3	Mol fraction H_2 in PSA product
H4	Mol fraction H_2 recover over PSA Unit

C.1.8 Reformer

C9	Mol fraction of methane in raw syngas feed converted in reformer
Z	Mol fraction of hydrocarbons converted to CO
D	Required mol fraction of methane in exit from reformer, dry basis
HR	Mols steam added
SH	Mol ratio steam / hydrocarbon
CLC	% error on closure methane in reformer product
HF	Mols condensed in product cooler
HFS	Saturated mols water in gas from product cooler
HF1	Mols water in gas to product cooler
KS	Constant D / (1-D)

C.1.9 Recycle System

RR	Molar recycle ratio, recycle / purge dry basis
RQ	Type of recycle system required: = 0 for recycle system required; = 1 for reformer; = 2 for PSA.
SK	Recycle convergence required to calculate required recycle ratio to eliminate shift: = 0 convergence not required; = 1 convergence required
RR[50]	Values of recycle ratio in each iteration
CLR	% closure on recycle closure

C.2 Summary of Equations

This section contains a summary of the major equations used in the program and in the equations described in section 3.6

C.2.1 First Estimate of Mols of Recycle Stream to Feed

	Variable	Reformer Case	PSA case	Recycle Case
H_2	HS1	(3F4 + 5F5) x 0.8	0.2 x F1	0.2 x F1
CO	HS2	(F4 + F5) x 0.6	-	0.03 x F2
CO_2	HS3	(F4 + F5) x 0.4	-	0.6 x HS2
C_1	HS4	F4 x 0.2	-	1.2 x F4
C_2	HS5	0	-	F5
N_2	HS6	F6 x 2	HS1 x (1-H3) / H3	F6

Amounts of C_3, C_4, C_5 are ignored for the first estimate

C.2.2 Mols CO Shifted, CO_2 Removed

Shift constants:

CK1 = (F1LH1 + HS1) + (F2LH2 + HS2)LC2 + (F3LH£ + HS3)LC3
    + (F4LH4 + HS4)LC4 + (F5LH5 + HS5) + (F6LH6 + HS6)LC6
CK2 = LH1LC1 - LH2LC2 + LH3
CK3 = LH3 - ACK2 / (1-A)
CK4 = F3LH3+HS3 - ACK1 / (1-A)
CK5 = RHLC2(F2LH2+HS2) - LC1(F1LH1+HS1)
CK6 = LH1LC1 + RHLH2LC2

Mols to be shifted	S = K5 / K6
Mols CO_2 to be removed in CO_2 removal plant	R = S CK3 + CK4

C.2.3 Shift Product

H_2	L1 = F1 + S	CO	L2 = F2 - S
CO_2	L3 = F3 + S	C_1	L4 = F4
C_2	L5 = F5	N_2	L6 = F6
H_2S	L14 = F14	COS	L15 = F15
SO_2	L16 = F16	CS_2	L17 = F17
Mercaptan	L18 = L18	Thiophene	L19 = F19

C.2.4 H_2S Plant

	Product	Reject to Sulphur Recovery
H_2	N1 = L1 LH1	RH1 = L1 - N1
CO	N2 = L2 LH2	RH2 = L2 - N2
CO_2	N3 = L3 LH3	RH3 = L3 - N3
C_1	N4 = L4 LH4	RH4 = L4 - N4
C_2	N5 = L5 LH5	RH5 = L5 - N5
N_2	N6 = L6 LH6	RH6 = L6 - N6

C.2.5 CO_2 Plant

	Feed	Product	Reject
H_2	W1 = N1 + HS1	Q1 = W1LC1	RC1 = W1 - Q1
CO	W2 = N2 + HS2	Q2 = W2LC2	RC2 = W2 - Q2
CO_2	W3 = N3 + HS3	Q3 = W3 - R	RC3 = R
C_1	W4 = N4 + HS4	Q4 = W4LC4	RC4 = W4 - Q4
C_2	W5 = N5 + HS5	Q5 = W5LC5	RC5 = W5 - Q5
N_2	W6 = N6 + HS6	Q6 = W6LC6	RC6 = W6 - Q6
C_3	W11 = HS11	Q11 = W11	
C_4	W12 = HS12	Q12 = W12	
C_5	W13 = HS13	Q13 = W13	

C.2.6 Alcohol Plant

C.2.6.1 Synthesis Section Feed

Mols CO shifted: SA = SM x Q2

H_2 QA1 = Q1+SA   CO QA2 = Q2 - SA
CO_2 QA3 = Q3 + SA C_1 QA4 = Q4
C_2 QA5 = Q5 N_2 QA6 = Q6
C_3QA11 = Q11 C_4 QA12 = Q12
C_5QA13 = Q13

C.2.6.2 Mols Alcohols & Hydrocarbons Produced

Mols CO to	- alcohols + HC's	MCT = QA2 x CNV
	- alcohols	MCA = MCT x SAC
	- hydrocarbons	MCH = MCT - MCA
Total mols	- alcohols produced	MAT = MCA / KMA
	- H / C's Produced	MGT = MCH / KMG

Mols alcohols produced

C_1OH	MA1 = MAT x MFA1	C_2OH	MA2 = MAT x MFA2
C_3OH	MA3 = MAT x MFA3	C_4OH	MA4 = MAT x MFA4
C_5OH	MA5 = MAT x MFA5	C_6OH	MA6 = MAT x MFA6

Mols hydrocarbons produced

C_1	MG4 = MGT x MFG1	C_2	MG5 = MGT x MFG2
C_3	MG11 = MGT x MFG3	C_4	MG12 = MGT x MFG4
C_5	MG13 = MGT x MFG5		

C.2.6.3 Mols Hydrocarbons in Total Offgas

C_1	$B4 = MG4 + QA4$	C_2	$B5 = MG5 + QA5$
C_3	$B11 = MG11 + QA11$	C_4	$B12 = MG12 + QA12$
C_5	$B13 = MG13 + QA13$		

C.2.6.4 Mols H_2 Consumed, H_2O Produced

Mols H_2 consumed in alcohol production.

$$UHA = 2MA1 + 4MA2 + 6MA3 + 8MA4 + 10MA5 + 12MA6$$

Mols H_2O produced in alcohol production.

$$UWA = MA2 + 2MA3 + 3MA4 + 4MA5 + 5MA6$$

Mols H_2 consumed in hydrocarbon production.

$$UHG = 3MG4 + 5MG5 + 7MG11 + 9MG12 + 11MG13$$

Mols H_2 produced in hydrocarbon production.

$$UWG = MG4 + 2MG5 + 3MG11 + 4MG12 + 5MG13$$

C.2.6.5 Complete Offgas, Excluding CO_2

H_2	$B1 = QA1 - UHA - UHG$
CO	$B2 = QA2 - MCT$
N_2	$B6 = QA6$

Total Offgas, excluding CO_2

$$BT = \sum_{13}^{1} B\ (N)$$

C.2.6.6 6 CO_2 Removal in Alcohol Unit.

CO removed

$$RA = QA_3 - \frac{AA * BT}{(1 - AA)}$$

CO in offgas $B3 = QA3 - RA$

Total Offgas $BT = BT + B3$

C.2.6.7 7 Purge Gas

H_2 G1 = B1 / (1 + RR)
CO_2 G3 = B3 / (1 + RR)
C_2 G5 = B5 / (1 + RR)
C_3 G11 = B11 / (1 + RR)
C_5 G13 = B13 / (1 + RR)

CO G2 = B2 / (1 + RR)
C_1 G4 = B4 / (1 + RR)
N_2 G6 = B6 / (1 + RR)
C_4 G12 = B12 / (1 + RR)

C.2.7 Reformer in Recycle Stream

C.2.7.1 Reformer Feed

H_2 R1 = B1 - G1
CO_2 R3 = B3 - G3
C_2 R5 = B5 - G5
C_3 R11 = B11 - G11
C_5 R13 = B13 - G13

CO R2 = B2 - G2
C_1 R4 = B4 - G4
N_2 R6 = B6 - G6
C_4 R12 = B12 - G12

C.2.7.2 Reformer Product.

Note: the following equations are applicable for a feed including C_6 (R14). In the program.

R14 is set as 0.

Constant K5 = D / (1 - D)

Fraction of methane in reformer feed converted

C9 = {R4 - K5[R1 + R2 + R3 + R6 + R5(9 - 2Z) + R11(13 - 3Z) + R12(17 - 4Z) + R13(215Z) + R14(25 - 6Z)]} / R4[1+K5(5-Z)]

H_2 P1 = R1 + R4(9(4 - Z) + R5(7 - 2Z) + R11(10 - 3Z) + R12(13 - 4Z) + R13(16 - 5Z) + R14(19 - 6Z)
CO P2 = R2 +Z[R4C9+2R5+3R11+4R12+5R13+6R14]
CO_2 P3 = P3 +(1-Z)[R4C9+2R5+3R11+4R12+5R13+6R14]
C_1 P4 = R4(1-C9)
C_2 P5 = 0
N_2 P6 = R6

C.2.7.3 Recycle to Feed

H_2 HS1 = P1
CO_2 HS3 = P3
C_2 HS5 = P5

CO HS2 = P2
C_1 HS4 = P4
N_2 HS6 = P6

C.2.7.4 Recycle Case ie No Reformer PSA

H_2 HS1 = B1 - G1
CO_2 HS3 = B3 - G3
C_2 HS5 = B5 - G5
C_3 HS11 = B11 - G11
C_5 HS13 = B13 - G13

CO HS2 = B2 - G2
C_1 HS4 = B3 - G4
N_2 HS6 = B6 - G6
C_4 HS12 = B12 - G12

C.2.8 PSA in Recycle Stream

C.2.8.1 PSA Feed

H_2	PS1 = B1 - G1	CO	PS2 = B2 - G2
CO_2	PS3 = B3 - G3	C_1	PS4 = B4 - G4
C_2	PS5 = B5 - G5	N_2	PS6 = B6 - G6
C_3	PS11 = B11 - G11	C_4	PS12 = B12 - G12
C_5	PS13 = B13 - G13		

C.2.8.2 PSA, Excluding H_2

CO	PG2 = PS2	CO_2	PG3 = PS3
C_1	PG4 = PS4	C_2	PG5 = PS5
N_2	PG6 = PS6	C_3	PG11 = PS11
C_4	PG12 = PS12	C_5	PG13 = PS13

C.2.8.3 H_2 in PSA Product / Reject Streams

H_2 in product	PP1 = PS1 x H4
H_2 in reject	PG1 = PS1 - PP1

C.2.8.4 Contaminant in PSA Product / Reject Streams

N_2 in product	PP6 = PP1 x (1 - H3) / H3

If there is no N_2 in feed, C_1 is used as contaminant in feed then

- C_1 in product	PP4 = PP6
- N_2 in product	PP6 = 0
- C_1 in reject	PG4 = PS4 - PP4
- N_2 in reject	PG6 = PS6 - PP6

C.2.8.5 Recycle to Feed

H_2	HS1 = PP1
C_1	HS4 = PP4
N_2	HS6 = PP6

All other components are zero.

C.2.9 Calculations for Next Iteration

C.2.9.1 Recycle Gas Composition For Next Mols Alcohol Calculation.

If closure has not been reached on the mols of alcohols from successive iterations, the composition of the recycle gas to reformer / PSA etc is simply taken as the composition calculated from the last iteration.

C.2.9.2 Convergence on Recycle Ratio to Eliminate Shift

For the first trial, the recycle ratio used is the value selected internally by the program. The second trial uses the recycle ratio from the first trial, adjusted as follows:

- x 1.2 if calculated mols shifted > 0;
- / 1.2 if calculated mols shifted < 0.

For subsequent trials, the next value of the recycle ratio is calculated by linear interpolation from the previous trials eg for the third trial:

RR = RR2 + S2 x (R2 - R1) / (S1 - S2)

C.2.10 Steam Totals Dry

For N = 1 to 19

FT = F[N] - F [8]
QAT = QA[N]
PT = P[N]
PST = PS[N]
LT = L[N]

WT = W[N]
BT = B[N]
PGT = PG[N]
PPT = PP[N]
NT = N[N]

QT = Q[N]
GT = G[N]
HST = HS[N]
RT = R[N]

C.2.11 Complete Water Offgas, Purge Gas

Offgas B8 = Bt x VP1 / (PM2 - VP1)
Purge gas G8 = GT x VP1 / (PM2 - VP1)

C.2.11.1 Water Balance Reformer Case

H_2O required is feed to reformer:

R8 = SH x [R4 + R5 + R11 + R12 + R13 + R14]

H_2O added to Feed:

HR = R8 - RT x VP1 / (PM2 - VP1)

H_2O in reformer product u/s cooler:

HF1 = R8 - (2 - Z) x [R4C9 + 2RS + 3R11 + 4R12 + 5R13 + 6R14]

Water KO'd in cooler:

HFS = PT x VP1 / (PH-DPS-DPH-VP1)
P[8] = HFS
HF = HF1 - HFS

C.2.11.2 Water Balance Recycle Case

H_2O in recycle to feed: HS8 = B8 - G8

C.2.11.3 Water Balance PSA Case.

H_2O in PSA feed: PS8 = B8 - G8
H_2O in PSA reject: PG8 = PS8

C.2.11.4 Shift By-pass and Shift Water Balance

Mol fraction total feed to shift	Z1 = S / K1 x F2
Minimum mols H_2O in shift feed	HP = K2Z1FT
Total mols actual shift feed, day	EFT = Z1FT
H_2O added to shift	HS = HP - Z1E8
H_2O in actual shift feed	EF8 = HP

H_2O In actual shift product

HT1 = HP - S (upstream shift cooler)

	Actual Shift Feed	Actual Shift Product	Shift by-pass
H_2	EF1 = F1Z1	EP1 = EF1 + S	EB1 = F1 - EF1
CO	EF2 = F2Z1	EP2 = EF2 - S	EB2 = F2 - EF2
CO_2	EF3 = F3Z1	EP3 = EF3 + S	EB3 = F3 - EF3
C_1	EF4 = F4Z1	EP4 = EF4	EB4 = F4 - EF4
C_2	EF5 = F5Z1	EP5 = EF5	EB5 = F5 - EF5
N_2	EF6 = F6Z1	EP6 = EF6	EB6 = F6 - EF6
H_2S	EF14 = F14Z1	EP14 = EF14	EB14 = F14 - EF14
COS	EF15 = F15Z1	EP15 = EF15	EB15 = F15 - EF15
SO_2	EF16 = F16Z1	EP16 = EF16	EB16 = F16 - EF16
CS_2	EF17 = F17Z1	EP17 = EF17	EB17 = F17 - EF17
Mercaptan	EF18 = F18Z1	EP18 = EF18	EB18 = F18 - EF18
Thiophene	EF19 = F19Z1	EP19 = EF19	EB19 = F19 - EF19

$$EPT = \sum_{1}^{16} EP\,(N) \qquad HTS = \frac{EPT\ VP2}{(PH - DPS - VP2)}$$

HT = HT1 - HTS

EP [8] = HTS

H_2S Feed:

H_2O	L8 = EP8 + EB8	H_2S	L14 = EP14 + EB14
COS	L15 = EP15 + EB15	SO_2	L16 = EP16 + EB16
CS_2	L18 = EP17 + EB17	Mercaptan	L18 = EP18 + EB18
Thiophene	L19 = EP19 + EB19		

C.2.12 Complete H_2S, CO_2 Plants

$$HHS = \frac{LT * VP1}{(PH - DPS - VP1)}$$

HH = L[8] - HHS

HH1 = HHS

N8 = HH1 x L8

Reject

H_2O:	RH14 = L14	COS:	RH15 = L15
SO_2:	RH16 = L16	CS_2:	RH17 = L17
Mercaptan:	RH18 = L18	Thiophene:	RH19 = L19

Over CO_2 Plant:

W8 = N8 + HS8

Q8 = W8 x LC8

RC8 = W8 - Q8

C.2.13 Water Balance Alcohol Plant

Saturated H_2O in feed	HM3 = QT x VP1 / (PM1 - VP1)
H_2O KO'd in feed compressor	HM2 = Q8 - HM3
H_2O to alcohol plant	HM1 = HM3 (or = Q8 if Q8 < HM3)
Mols H_2O to synthesis section	QA8 = HM1 - SA
Mols H_2O in alcohol product	MA8 = QA8 + UWA +UWG - B8

C.2.14 Steam Totals Wet

water simply added to stream totals dry

C.3 Derivation of Equations

C.3.1 Reformer

C.3.1.1 Basis

- All C_2 to C_6 in feed is converted;
- All reactions are exothermic.

C.3.1.2 Variables

Z Mol fraction hydrocarbons converted to CO_2
D Mol fraction methane in reformer product, dry basis
C_9 Mol fraction methane converted in reformer

	Reformer feed	Reformer Product
H_2	R1	P1
CO	R2	P2
CO_2	R3	P3
C_1	R4	P4
C_2	R5	-
N_2	R6	P6 = R6
H_2O	R8	P8
C_3	R11	-
C_4	R12	-
C_5	R13	-
C_6	R14	-

C.3.1.3 Chemical Reactions

$$CH_4 + H_2O \rightarrow CO + 3H_2$$
$$C_2H_6 + 2H_2O \rightarrow 2CO + 5H_2$$
$$C_3H_8 + 3H_2O \rightarrow 3CO + 7H_2$$
$$C_4H_{10} + 4H_2O \rightarrow 4CO + 9H_2$$
$$C_5H_{12} + 5H_2O \rightarrow 5CO + 11H_2$$
$$C_6H_{14} + 6H_2O \rightarrow 6CO + 13H_2$$

$$CO + H_2O \rightarrow CO_2 + H_2$$

C.3.1.4 Basic Equations

i) For the hydrocarbons converted to 100 % CO, ie no shift to CO_2

H_2 Produced = 3R4C9 + 5R5 + 7R11 + 11R13 + 13R14
CO Produced = R4C9 + 2R5 + 3R11 + 4R12 + 5R13 + 6R14
H_2O Consumed = R4C9 + 2R5 + 3R11 + 4R12 + 5R13 + 6R14

ii) Now part of this CO produced is converted to CO_2

Fraction of feed converted to CO = Z

∴ Fraction of feed converted to CO_2 = (1-Z)

So amounts produced / consumed by this shift reaction are:

H_2 produced (1-Z) [R4C9 + 2R5 + 3R11 + 4R12 + 5R12 + 6R14]
CO consumed (1-Z) [R4C9 + 2R5 + 3R11 + 4R12 + 5R12 + 6R14]
CO_2 produced (1-Z) [R4C9 + 2R5 + 3R11 + 4R12 + 5R12 + 6R14]
H_2O consumed (1-Z) [R4C9 + 2R5 + 3R11 + 4R12 + 5R12 + 6R14]

iii) The reformer product is the sum of (i) + (ii) + the mols in the reformer feed. This gives the following:

H_2: P1 = R1 + 3R4C9 + 5R5 + 7R11 + 9R12 + 11R13 + 13R14
+ (1-Z) [R4C9 + 2R5 + 3R11 + 4R12 + 5R13 + 6R14]
P1 = R1+R4C9(4-Z)+R5(7-2Z)+R11(10-3Z)+R12(13-4Z)
+R13(16-5Z)+R14(19-6Z)

CO: P2 = Z[R4C9+2R5+3R11+4R12+5R13+6R14]
CO_2: P3 = R3 + (1-Z)[R4C9+2R5+3R11+4R12+5R13+6R14]
H_2O: P8 = R8 - (2-Z)[R4C9+2R5+3R11+4R12+5R13+6R14]
C_1: P4 = R4(1-C9)

iv) Calculation of C9 - mol fraction C1 converted in reformer

To meet C1 spec in reformer outlet

$$D = \frac{P4}{P1+P2+P3+P4+P6}$$

∴ P4 = D(P1+P2+P3+P6+DP4

∴ P4(1-D) = D(P1+P2+P3+P6)

Let K5 = D / (1-D)

P4 = K5 (P1+P2+P3+P6)

Substituting for P1,P2,P3,P4 from (iii) above & P6 = R6 gives

∴ R4(1 - C9) = K5[R1 + R4C9(4 - Z)+R5(7 - 2Z) + R11(10 - 3Z) + R2 +
R4C9Z + 2R5Z + 3R11Z + R3 + R4C9(1-Z) + 2R5(1 - Z) +
3R11(1 - Z) + R12(13 - 4R) + R13(16 - 5Z) + R14(19 - 6Z) +
4R12Z + 5R13Z + 6R14Z + 4R12(1-Z) + 5R13(1 - Z) +
6R14(1 - Z)+R6]

∴ R4(1 - C9) = K5[R1 + R2 + R3 + R6 + R4C9(5 - Z] + R5(9 - 2Z] + R11(13
- 3Z] + R12(17 - 4Z] + R13(21 - 5Z] + R14(25 - 6Z]]

∴ R4(1 - C9] - K5R4C9(5 - Z] = K5[R1 + R2 + R3 + R6 + R5(9 - 2Z] +
R11(13 - 3Z] + R12(17 - 4Z] + R13(21 -
5Z] + R14(25 - 6Z]]

$$\therefore \quad R4 - R4C9[1 + K5\{5 - Z]] = K5[R1 + R2 + R3 + R6 + R5(9 - 2Z] + R11(13 - 3Z] + R12(17 - 4Z] + R13(21 - 5Z] + R14(25 - 6Z]]$$

$$\therefore \quad C9 = \{R4 - K5[R1 + R2 + R3 + R6 + R5(9 - 2Z] + R11(13 - 3Z] + R12(17 - 4Z] + R13(21 - 5Z] + R14(25 - 6Z]]\} / R4[1 + K5(5 - Z]]$$

C.3.1.5 Calculation of Mols CO Shifted, CO_2 Removed

	Shift Feed	Shift Product	H_2S Product	Recycle	CO_2 Feed	Methanol Feed
H_2	F1	F1+S	(F1+S)LH1	HS1	(F1+S)LH1+HS1	Q1=[{F1+S)LH1+HS1]LC1
CO	F2	F2-S	(F2-S)LH2	HS2	(F2-S)LH2+HS2	Q2=[(F2-S)LH2+HS2]LC2
CO_2	F3	F3+S	(F3+S)LH3	HS3	(F3+S)LH3+HS3	Q3=[(F3+S)LH3+HS3-R
C_1	F4	F4	F4LH4	HS4	F4LH4+HS4	Q4=[F4LH4+HS4]LC4
C_2	F5	F5	F5LH5	HS5	F5LH5+HS5	Q5=[F5LH5+HS5]LC5
N_2	F6	F6	F6LH6	HS6	F6LH6+HS6	Q6=[F6LH6+HS6]LC6

R = Mols CO_2 produced in CO_2
S = Mols CO shifted
A = Mol fraction CO_2 in outlet from CO_2 plant, dry basis
LH = required molar components passing through H_2S plant to product
LC = required molar components passing through H_2S plant to product

Basic Equations:

To reset specification on CO_2 from CO_2 plant

$$A = Q3 / (Q1+Q2+Q3+Q4+Q5+Q6) \qquad (1)$$

To meet spec on molar ratio H2 : CO to alcohol unit

$$RH = Q1 / Q2$$

Solving equations:

From (1) $\quad Q3 = A\ (Q1+Q2+Q3+Q4+Q5+Q6)$
substituting for Q1 to Q6

$$(F3 + S)LH3 + P3 - R = A \times \{[(F1 + S)LH1 + HS1]LC1 + [(F2 - S)LH2 + HS2]LC2 + (F3 + S)LH3 + HS3 - R + [F4LH4 + HS4]LC4 + [F5LH5 + HS5]LC5 + [F6LH6 + HS6]LC6\}$$

$$= A \times \{[F1H1 + SLH1 + HS1]LC1 + [F2LH2 - SLH2 + HS2]LC2 + [F3LH3 + SLH3 + HS3 - R] + [F4LH4 + HS4]LC4 + [F5LH5 + HS5]LC5 + [F6LH6 + HS6]LC6\}$$

$$= AS \times [LH1LC1 - LH2LC2 + LH3] + A \times \{[F1LH1 + HS1]LC1 + [F2LH2+ HS2]LC2 + F3LH3 + HS3 + [F4LH4 + HS4]LC4 + [F5LH5 + HS5]LC5 + [F6LH6 + HS6]LC6 - AR$$

$$\text{Let } K1 = \{[F1LH1 + HS1]LC1 + [F2LH2 + HS2]LC2 + F3LH3 + HS3 + [F4LH4 + HS4]LC4 + F5LH5 + HS5]LC5 + [F6LH6 + HS6]LC6\}$$

$K2 = LH1LC1 - LH2LC2 + LH3$

$\therefore$ $F3LH3+SLH3+HS3-R = ASK2+AK1-AR$

$\therefore$ $R-AR = F3LH3+SLH3+HS3-ASK2-AK1$

$\therefore$ $R = S(LH3-AK2)+F3LH3+HS3-AK1 / (1-A)$

Let $K3 = LH3 - AK2 / (1-A)$ and $K4 = F3LH3 + HS3 - AK1 / (1-A)$

then $R = SK3+K4$ (3)

From (2), substituting for Q1, Q2.

$Q1 = RHQ2$

$\therefore$ $[(F1 + S)LH1 + P1]LC1 = RH[(F2 - S)LH2 + P2]LC2$

$\therefore$ $[F1LH1 + SLH1 + P1]LC1 = RHLC2[F2LH2 - SLH2 + P2]$

$\therefore$ $SLH1LC1 + [F1LH1 + P1]LC1 = - RHLC2SLH2 + RHLC2[F2LH2 + P2]$

let $K5 = RHLC2[F2LH2 + P2] - LC1[F1LH1 + P1]$

$\therefore$ $S[LH1LC1 + RHLH2LC2] = K5$

let $K6 = LH1LC1 + RHLH2LC2$

$\therefore$ $S = K5 / K6$

C.3.2 Calculation Over Shift (By-pass & H_2O at exit)

C.3.2.1 Basis:

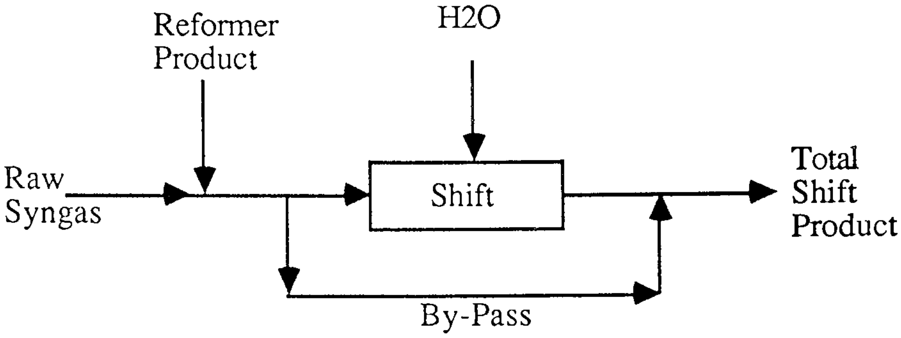
- Already calculated mols CO to be shifted;
- Need to calculate amount of syngas that needs to pass through shift and amount by-passed;
- Amount to shift calculated to meet specification of mol fraction CO converted to CO_2 in shift;
- Also add H_2O if necessary to meet a maximum mols H_2O / mol dry in actual shift feed.

C.3.2.2 Variables:

	Total Shift Feed	Actual Shift Feed	Actual Shift Product	Amount By-passed	Total Shift Product
H_2	E1	E1Z1	E1Z1+S	E1[1-Z1]	E1+S
CO	E2	E2Z1	E2Z1-S	E2[1-Z1]	E2-S
CO_2	E3	E3Z1	E3Z1+S	E3[1-Z1]	E3+S
C_1	E4	E4Z1	E4Z1	E4[1-Z1]	E4
C_2	E5	E5Z1	E5Z1	E5[1-Z1]	E5
N_2	E6	E6Z1	E6Z1	E6[1-Z1]	E6
H_2O	E8	E8Z1	E8Z1-S	E8[1-Z1]	E8-S

S = Mols CO to be shifted
K1 = Mol fraction CO in actual shift feed converted to CO_2
Z1 = Mol fraction total shift feed routed to actual shift dry basis
K2 = Mols water H_2O to be added, i necessary, u/s of shift
HP = Min mols H_2O in actual shift feed

C.3.2.3 Flowsheet



C.3.2.4 Equations

i) Calculation of amount fed to shift

Mols CO in actual shift product $= E2Z1-S$
& also $= E2Z1[1-K1]$

$\therefore$ $Z1 = S / [E2K1]$

ii) Calculation of actual shift feed, product & by - pass (excluding H_2O)

Knowing Z1, the actual mols to / from shift & by-pass can be calculated from equations in (2) on previous page

iii) Water balance

Minimum mols H_2O in actual shift Feed

$$HP = K2 \times Z1[E1+E2+E3+E4+E5+E6]$$

H_2O to be added to actual shift feed

$$HS = HP - E8Z1$$

C.3.3 CO_2 Removal in Alcohol Unit

Mols CO_2 in offgas prior to CO_2 removal = QA3

Total mols offgas excluding CO_2, H_2O = BT mols CO_2 removal = RA Required mol fraction CO_2 in offgas, dry = AA

So mols CO_2 in offgas, dry QA3 - RA
To meet CO_2 spec in offgas

$$AA = QA3 - RA / (BT+QA3-RA)$$

$$\therefore \quad AA \times BT+AA \times QA3-AA \times RA = QA3 - RA$$

$$\therefore \quad RA-AA \times RA = QA3-AA \times QA3-AA \times BT$$

$$\therefore \quad RA[1-AA] = QA3[1-AA]-AA \times BT$$

$$\therefore \quad RA = QA3 - AA \times BT / (1-AA)$$

Appendix D
Capital Cost Raw Data

Feed Preparation Costs

Gasification Process	Preparation Type	Coal Type	Throughput te/d	Capital Cost 10^6 US$	Date	Cap. Cost US$ Mid 88	Ref
Dry Ash Lurgi	Fixed bed	Illin. No.6	9072	48.4	Mid 1982	55.4	1
Dry Ash Lurgi	Fixed bed	New Mexico Sub-bituminous	13435	61.9	Mid 1982	70.9	2
BGC/Lurgi	Fixed bed	Illin. No.6	10632	49.0	Mid 1982	56.1	3
BGC/Lurgi	Fixed bed	Illin. No.6	268	22.9	Jan 1984	33.5	4
BGC/Lurgi	Fixed Bed	Pitt No. 8	1394	12.6	Mid 85	13.3	5
Texaco	Slurry Entrained	Illin. No.6	9979	65.7	Mid 1982	75.2	6
Texaco	Slurry Entrained	Illin. No.6	4457	39.3	Mid 1982	45.0	7
Texaco	Slurry Entrained	Illin. No.6	23059	118.0	Mid 1982	135.1	8
Texaco	Slurry Entrained	Illin. No.6	6153	47.1	Mid 1982	54.3	9
Texaco	Slurry Entrained	Illin. No.6	9663	65.0	Mid 1982	74.4	10
Shell	Dry Entrained	Illin. No.6	10632	78.3	Mid 1982	89.7	11
Shell	Dry Entrained	Texas Lig.	16429	108.2	Mid 1982	123.9	12
KRW	Fluidised bed	Illin. No.6	4794	24.4	Jan 1983	27.3	13
KRW	Fluidised bed	Texas Lig.	7617	29.9	Jan 1983	33.4	14
KRW	Fluidised bed	Texas Lig.	25734	78	Mid 1982	82.3	15
KRW	Fluidised bed	Pitt No 8	8695	48	Mid 85	49.3	16
KRW	Fluidised bed	Pitt No 8	8930	45	Mid 85	46.5	17
KRW	Fluidised bed	Pitt No 8	7058	41	Mid 85	42.5	18
KRW	Fluidised bed	Pitt No 8	7104	42	Mid 85	43.5	19
Lurgi	Fixed Bed	Lignite	16424	37	Mid 85	39.0	20
Lurgi	Fixed Bed	Lignite	25305	52	Mid 82	59.6	21
Lurgi	Fixed Bed	Lignite	36754	68	Mid 82	77.9	22
Winkler	Fluidised bed	N. Dak. Lig.	43341	94.7	Feb 1980	126.9	23

Gasifier Capital Costs

Gasification Process	Coal Type	Throughput (maf) te/d	Cap. Cost 10^6 US$	Date	Cap. Cost 10^6 US$ Mid 88	No. Gasifiers	No Spare	Ref
Dry Ash Lurgi	Illin. No.6	7 820	225.7	Mid-1982	258.5	18	2	1
Dry Ash Lurgi	New Mexico Sub-bituminous	8 329	209.1	Mid-1982	239.5	22	2	2
BGC/Lurgi	Illin. No.6	8 418	257.1	Mid-1982	294.5	16	4	3
BGC/Lurgi	Illin. No.6	3 380	86.7	Jan-1984	94.5	?	?	4
BGC/Lurgi	Pitt No. 8	1 150	37.6	Mid 1985	39.7	?	?	24
Texaco	Illin. No.6	7 903	270.8	Mid-1982	310.1	10	2	5
Texaco	Illin. No.6	3 530	119.9	Mid-1982	137.3	5	1	6
Texaco	Illin. No.6	17 921	546.9	Mid-1982	626.4	?	?	7
Texaco	Illin. No.6	7 472	166.9	Mid-1982	191.2	6	1	8
Texaco	Illin. No.6	8 330	267.8	Mid-1982	306.7	8	2	9
Shell	Illin. No.6	8 419	243.1	Mid-1982	278.4	5	1	10
Shell	Texas Lignite	8 920	237.2	Mid-1982	271.7	5	1	11
KRW	Illin. No.6	3 797	144.8	Jan 1983	161.7	?	?	12
KRW	Texas Lignite	4 136	155.1	Jan 1983	173.2	?	?	13
KRW	Lignite	4 696	145	Mid-1982	166.1	?	?	25
KRW	Pitt No.8	7 060	194	Mid-1985	217.4	?	?	26
KRW	Pitt No.8	5 768	153	Mid-1985	161.5	5	1	27
Dow	Wy. Sub-bit	3 267	78.67	Jan 1988	79.86	2	0	28
Dow	Lignite	5 863	94.4	Jan 1988	95.8	2	0	18
PRENFLO	-	~1 300	80.10^6 DM	~1989	26.7	1	0	29

NB The figures were updated using Process Engineering International cost indices. The figures were converted to £ Sterling for inclusion in the step models.

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Appendix E

Publications

EN3V-0032-UK

PRODUCTION COSTS OF LIQUID FUELS BY INDIRECT COAL LIQUEFACTION

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LIQUID FUELS BY INDIRECT LIQUEFACTION OF COAL: PROCESS IDENTIFICATION AND ASSESSMENT

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