Carnegie Mellon University

CARNEGIE INSTITUTE OF TECHNOLOGY

THESIS

SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS

FOR THE DEGREE OF Doctor of Philosophy

TITLE Techno-economic evaluation of coal-to-liquids (CTL) plants and their effects on environment and resources

PRESENTED BY **Hari Chandan Mantripragada**

ACCEPTED BY THE DEPARTMENT OF

Engineering and Public Policy

ADVISOR, MAJOR PROFESSOR DATE

DEPARTMENT HEAD DATE

APPROVED BY THE COLLEGE COUNCIL

DEAN DATE

Techno-economic Evaluation of Coal-to-Liquids (CTL) Plants and Their Effects on Environment and Resources

Submitted in partial fulfillment of the requirements for

the degree of

Doctor of Philosophy

in

Department of Engineering and Public Policy

Hari C. Mantripragada

B.Tech, Mechanical Engineering, Indian Institute of Technology, Chennai
M.Tech, Energy Systems Engineering, Indian Institute of Technology, Mumbai

Carnegie Mellon University
Pittsburgh, PA

May, 2010

Acknowledgements

I express my sincere appreciation to my doctoral thesis committee members Prof. Edward S. Rubin (chair), Prof. Jay Apt, Prof. Granger Morgan and Dr. John M. Marano, for their expert guidance and support in the finishing of this thesis. I acknowledge the financial support provided by US DOE/NETL and the Department of Engineering and Public Policy at Carnegie Mellon University.

I owe my deepest thanks to my advisor Prof. Ed Rubin for his excellent guidance throughout the course of this research. His constant support through the ups and downs of my PhD was an invaluable component in the successful completion of this thesis.

I thank EPP for providing me an opportunity to pursue research in this special place. I will forever cherish the academic as well as personal experiences gained in the past few years here. My special thanks to all the faculty, staff and fellow students of EPP.

I sincerely acknowledge the support provided my research group, particularly Sean McCoy, Mike Berkenpas and Karen Kietzke.

I want to express my greatest gratitude to my family and friends in the US and back home in India for their invaluable moral support over the past few years.

Abstract

Coal-to-liquids (CTL) process involves gasification of coal to produce syngas which is then catalytically converted into liquid fuels in a Fischer-Tropsch (FT) reactor. Two general configurations of CTL plants are possible – liquids-only and co-production. In the liquids-only configuration the unconverted syngas from the FT reactor is recycled to the reactor to increase the productivity of the liquids. In the co-production configuration, the unconverted syngas from the FT reactor, instead of being recycled, is combusted in a gas turbine steam turbine combined cycle power plant to generate electricity. The by-product electricity can be sold to the grid.

In this thesis, techno-economic models are developed to evaluate the performance and costs of CTL plants using different component technologies and process configurations and under different carbon constraints. The results are used to study the implications of large-scale deployment of CTL plants on the environment and resource consumption, particularly in terms of:

- Emissions of CO_2
- Consumption of resources such as coal, water and land
- Economic benefits/costs of transport fuels derived from coal

It was found that, depending on various factors, the costs of liquid product from both liquids-only and co-production plants are in the range of \$40 - \$100/barrel. CTL plants are highly capital intensive, with the capital cost component accounting for about half the total product cost. Carbon capture and sequestration (CCS) is cheaper than paying a CO_2 price of more than \$12/tonne for liquids-only plant and more than \$30/tonne for co-production plants

Co-production plants, with or without CCS consume less coal and emit less CO_2 than separate production of liquids and power. Co-production CTL plants with CCS, supplying 20% of petroleum demand, can meet around 30% of US electricity demand (energy basis) and by displacing conventional coal power plants, have the potential of reducing the US CO_2 emissions by 9% from the 2008 emissions.

In summary it can be said that CTL has significant scope for producing domestic liquid fuels from the abundant coal resources. The commercialization of the technology depends on how the investors and regulatory agencies deal with the economic and environmental risks associated with CTL.

Table of Contents

List of Tables

List of Figures

Chapter 1: Background

The world is going through an energy crisis with the twin problems of depleting fossil fuel reserves and increasing threat of climate change. Oil prices have been consistently increasing in the last decade and more so in the last couple of years. Particularly in the first half 2008, the price of crude oil rose close to $150 per barrel and speculations that the prices will rise to $200 per barrel by the end of this decade were not uncommon in the news. However, for various reasons (mainly an economic downturn), late 2008 saw oil prices dropping again close to $40 per barrel (Fig 1.1). Owing to such uncertainties in the availability of oil and the volatility of prices, there is a growing interest in the production of synthetic liquid fuels. Synthetic liquids from fossil sources like coal, natural gas, oil shale, tar sands or biomass have been used in the past or are being used today. Though such endeavors have proved uneconomical in the past, if the crude oil prices are sufficiently high, these technologies have the potential to become economically feasible.

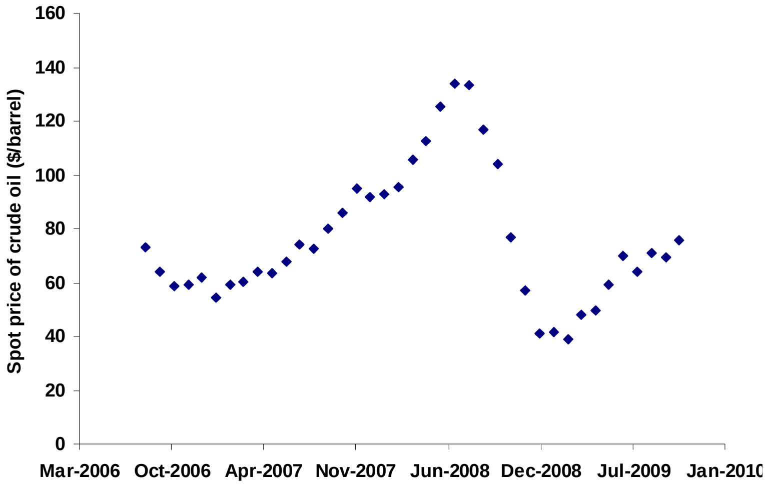


Figure 1.1: Monthly crude oil prices [Source: www.eia.doe.gov]

1.1 Synthetic Liquid Fuels from Coal

Coal-to-liquids (CTL) technology, which produces liquid transportation fuels like diesel and gasoline, is of particular interest to the US because of the abundance of coal reserves in this country. CTL technology was widely used in the World War II era, mostly in Germany and Japan. During the first oil shock of 1970's, there was renewed interest in CTL technology which later faded when the oil prices began to fall [Schulz, 1999; Steynberg and Dry, 2004].

1.1.1 Coal-to-liquids (CTL) process

The CTL process involves gasification of coal to produce synthesis gas which is then catalytically converted into liquid fuels in a Fischer-Tropsch (FT) reactor [Probstein and Hicks, 1985]. Two general configurations of CTL plants are possible as shown in Fig 1.2. In a typical commercial CTL plant shown in Fig 1.2(a), the unconverted syngas from the FT reactor is recycled to the reactor to increase the productivity of the liquids. In this paper, such plants are called 'liquids-only' plants. Another configuration shown in Fig 1.2(b), though not yet commercial, is also possible in which the unconverted syngas from the FT reactor, instead of being recycled, is combusted in a gas turbine steam turbine combined cycle power plant to generate electricity. Plants with such configuration are called 'co-production' plants in this paper. The by-product electricity can be sold to the grid.

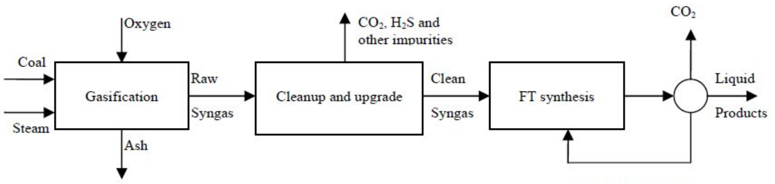


Figure 1 (a): Liquids-only configuration

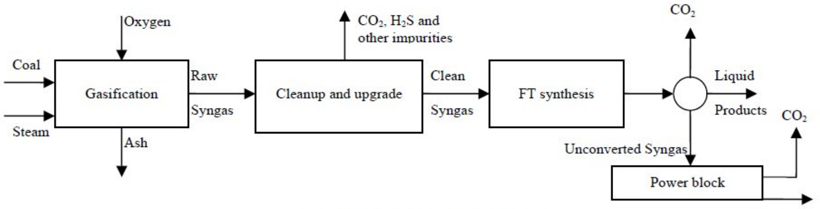


Figure 1 (b):Co-production configuration

Figure 1.2: Liquids-only and co-production configurations of CTL plants

1.1.2 Benefits and risks of CTL technology

Coal liquids, as substitutes for crude-derived fuels, offer certain clear benefits. Deriving liquid fuels from coal helps reduce the dependence on crude oil imports and supplies liquid fuels at a reasonable price. In terms of the environment, FT liquids are clean burning fuels with negligible emissions of conventional air pollutants like sulfur and nitrogen oxides. FT diesel in particular has been proved an excellent automobile fuel owing mainly to its very high cetane value [Dry, 1999; Norton et al, 1998]. Moreover, co-production plants can produce significant electrical outputs which can be sold to the grid to add another stream of revenue [Neathery et al, 1999; Williams et al, 2009].

On the other hand, implementing CTL on a large scale raises a few significant concerns, whose knowledge is important in making informed policy decisions. These concerns are explained below, including the environmental and economic impacts of CTL.

CTL and CO_2 emissions

Coal is predominantly a carbon-rich feedstock whereas liquid fuels are rich in hydrogen. In the process of converting coal to liquids, the excess carbon in coal is emitted in the form of CO_2. Combustion of liquid products in automobiles also generates CO_2. As a result, coal liquids have at least double the life cycle CO_2 emissions compared to conventional crude oil-derived liquid fuels [Farrell and Brandt, 2006; Jaramillo, 2007]. CO_2 is one of the major greenhouse gases that are the cause of global warming and subsequent climate change. This problem becomes magnified if CTL is chosen to be implemented on a large scale, supplying a significant fraction of the country's oil demand. Consequently, it becomes very important to mitigate the CO_2 emissions from coal liquids.

The plant level CO_2 emissions can be mitigated using the carbon capture and sequestration (CCS) technology in which the CO_2 is captured and transported to a geological sequestration site. However, CCS can offer only a partial solution because even though CO_2 emissions at the plant level are eliminated, those produced during downstream combustion of liquid fuels in automobiles are still emitted into the atmosphere.

CTL plants can be utilized in such a way as to reduce the overall global emissions of CO_2 by using the more efficient co-production plants to displace conventional coal power plants. But this depends strongly on whether CCS becomes commercially viable or not. Without CCS, CO_2 emissions will increase significantly.

CTL and resource consumption

Large scale implementation of CTL plants will significantly impact the nation's coal consumption, since coal is also the primary fuel used for power-generation in the US. Coal consumption is lower in the case of co-production as compared to separate generation of liquids and power. Increased coal consumption is associated with increased coal mining and transport, both the processes having their own environmental impacts.

The other resource which is pertinent to CTL processes is water. Water is a key input into any process concerning coal. It is used almost in every stage of the process starting from coal cleaning and scrubbing, in preparing coal slurry, in scrubbing of syngas, ash treatment, in producing steam and so on. Not only is water an input to the process, it is also produced in both the gasification and FT reactions. Understanding water implications of large scale implementation of CTL is thus important.

CTL and land-use issues

A CTL plant can be compared closely to an IGCC power plant because of the use of gasification and combined cycle power plant technologies. However, CTL plants have additional process areas in the form of FT synthesis. Thus CTL plants are likely to use larger amounts of land than equivalent IGCC power plants. With the popular opposition to the siting of coal plants in many states, the land use by CTL plants poses a problem of siting them appropriately. It is important to know the amount of land required for a CTL plant of a particular capacity and the overall land requirement in the case of large-scale nation-wide implementation of CTL plants.

Economic impacts of CTL

Substituting crude oil-derived liquid fuels with coal liquids decreases the amount of imported oil. If the crude oil prices remain steadily high, then CTL might result in significant economic benefits in terms of the savings because of avoided imports. However, CTL processes are highly capital-intensive in that the capital costs of the plants are significantly higher than the operation and maintenance costs, hence being financially risky to investors. There is also a risk of CTL becoming uneconomical were the current crude oil prices to fall.

1.2 Motivation for Research

Proponents of CTL argue that coal liquids lead to less dependency on imported oil and hence is worthy of large-scale implementation. CCS is cited as the solution to the CO_2 problem arising from CTL plants. However, as discussed previously, CCS can offer only a partial solution to the problem of CO_2 emissions and global warming. Moreover, availability of relatively cheaper liquid fuels from coal could lead to increased use of fossil fuels and consequently to increased CO_2 emissions. It is estimated that using a quarter of world's coal reserves to produce liquid fuels increases the atmospheric greenhouse gas concentration by approximately 300 ppm without CCS and about half that if CCS is used [Farrell and Brandt, 2006]. Thus, even with CCS, CTL poses a significant environmental risk. Even though producing synthetic liquid fuels from coal could play an important role in improving the nation's energy security by providing less expensive and reliable supply of transportation fuels, there are considerable economic and environmental risks involved in the process, especially when implemented on a large scale. There have been a few techno-economic analyses of CTL plants in the recent past [NETL 2007a, Williams et al, 2009, SSEB 2006]. Most of these studies are limited in their scope, analyzing a specific technology or a particular configuration. However, CTL is a complex engineering process in which the choice and combination of different technologies has impacts on the plant performance and costs. Moreover, the effects of producing liquid fuels from coal extend beyond the boundaries of the production plant, including pre-production processes such as coal mining and transport and post-production impacts such as emissions of CO_2 and other pollutants into the atmosphere. There is need for a more systematic study of the effects of technology choice on the plant performance and cost and their implications on the overall national environment and resource consumption. Such an understanding is important for making policies such that implementation of CTL offers the benefits of energy security and minimizes risk to the investors and to the environment.

1.3 Objective of this Thesis

The objective of this thesis is to build comprehensive techno-economic models to evaluate the performance and costs of CTL plants using different component technologies and process configurations and to use the results from the models to study the implications of large-scale deployment of CTL plants on the environment and resource consumption, particularly in terms of:

- Emissions of CO_2
- Consumption of resources such as coal, water and land
- Economic benefits/costs of transport fuels derived from coal

1.4 Framing the Problem

Analysis of CTL technology can be considered at two levels – plant level and large scale. A plant level analysis gives us an idea of cost and energy requirements to produce liquid fuels from coal. A bigger picture analysis of how CTL technology fits into different scenarios helps in understanding the impacts of large scale CTL implementation and helps in formulating policies regarding that. In this thesis, performance, cost and impact assessment models are developed for techno-economic evaluation of CTL technology.

1.4.1 Large-scale implementation of CTL – a policy framework

To assess the impacts of large-scale implementation of CTL processes on the environment and resource consumption, it is necessary to define a scenario in which such an implementation might occur. As discussed previously, the co-production configuration with CCS has the capability to induce a net reduction in CO_2 emissions if they can also displace conventional coal-fired power plants. But it is also possible that co-production plants are built solely because of their economic attractiveness while conventional coal power plants also continue to run. Assuming that CTL is implemented on a large scale to supply a significant fraction of US oil demand – diesel or gasoline or both – the following are a few scenarios that are possible:

1) Only liquids-only CTL plants are built and conventional coal-fired power plants continue
2) Only co-production plants are built and conventional coal-fired power plants continue
3) Only co-production plants are built and conventional coal-fired power plants are displaced
4) – 6) All the above cases are combined with the use of CCS to minimize CO_2 emissions

The above scenarios will have different impacts and costs. Thus, it is important to evaluate them all to identify the least cost options across a spectrum of policies regarding energy and the environment.

1.4.2 CTL process – a problem of technology choice

CTL process is a complicated chemical engineering process with many sub-processes at each stage. The main process areas can be divided into three categories – syngas production and gas cleanup, FT synthesis and power generation. The performance and cost of the whole CTL plant depend on the choice of technology made in each of these process sections. The choice of technology again depends on a variety of factors, including the type of coal and the products of interest [Steynberg and Dry, 2004]. Different coal types require different types of gasifiers for effective gasification. Again, the type of gasifier influences the composition of syngas it produces and hence the downstream treatment steps of syngas. The choice of gasifier also has an important effect on the energy and resource usage of the whole plant. The choice of FT reactor technology depends on the desired liquid products. If the predominant product is diesel, then the better reactor to use is a low temperature FT (LTFT). On the other hand, if the desired product is gasoline, high temperature FT (HTFT) will be the technology of choice. Even within each type of FT reactor, there can be different kinds of catalysts. Catalysts are usually iron (Fe) or cobalt (Co) based. The choice of catalyst again depends on the composition of syngas. If the syngas is rich in CO, then there is no need for its upgrading if an iron catalyst is used. If the catalyst is Co-based, then the syngas needs to be upgraded with a water gas shift reaction to adjust the ratio of CO and H_2 for FT reaction. The choice of gas cleanup technology also depends on the type of gasifier and the composition of syngas.

All these different technologies play a major role in determining the performance and cost characteristics of the overall CTL plant. Such technology choice will also have environmental, economic and strategic implications at a higher level. More details about a few of these technologies are given in the following subsections.

1.4.3 Research Questions

The preceding description about the complexities involved in CTL processes and the policy context in which this technology must be evaluated. This motivates the following research questions, answers to which are of prime importance in identifying policy options that lead to a strengthening of the nation's energy security with minimum damage on the environment.

The key questions addressed in this thesis are:

Q1. *If liquids are to be produced from coal, what is the effect of technology choice on performance, plant configuration and coal type on cost and emissions of the plant?*

This question has been graphically illustrated in Fig 1.3. For a desired product (gasoline or diesel), there are different types of FT reactors. The choice of gasifier depends mainly on the type of coal (bituminous, sub-bituminous, lignite) and the same coal type can be gasified using different technologies. The upgrade process (adjusting CO/H2 ratio before FT synthesis) depends on the type of FT reactor and the catalyst used. The type and number of CO_2 removal units depends on the process configuration (liquids-only or co-production), the type of FT reactor and the catalyst used.

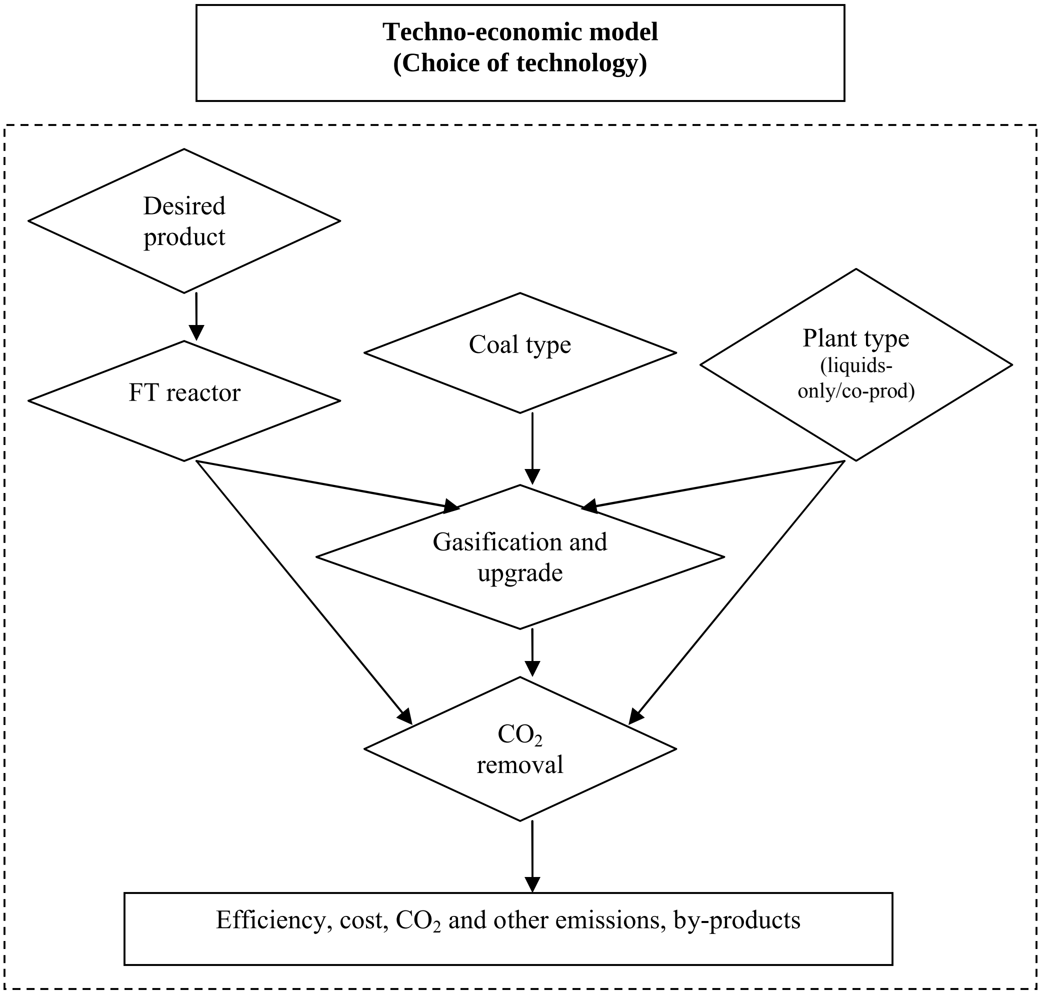


Figure 1.3: Schematic representation of technology choice involved in CTL processes

Q2. *For a particular plant design and configuration, what are the impacts on emissions and resource consumptions in the different scenarios explained in section 3?*

Because each configuration has different performance and costs, they will have different impacts on the larger environment and resource consumption. For example, it might be better to build CTL plants using one type of coal rather than another because of the availability of reserves of that coal type. Such policy-relevant estimates can be made using the results obtained from the plant-level techno-economic simulations. This has been pictorially described in Fig 1.4.

Q3. *What are the effects on coal consumption, water use and CO_2 emissions when coal liquids are used on a large scale?*

Large-scale implementation of CTL is associated with increases in coal consumption, water use, land use and CO_2 emissions. If coal liquids were to replace a fraction of liquid-fuel demand currently supplied by crude-oil based liquids, what would be the increase in resource consumption and CO_2 emissions? Such estimates are required in assessing the role of coal liquids under different policies.

Q4. *Can CTL plants be used to achieve a net reduction in CO_2 emissions?*

Co-production of liquids and electricity has the potential to be more efficient compared to separate production. If co-production CTL with CCS can be used to supply both liquids and electricity on a large-scale, while displacing conventional coal-fired power plants, it is possible to achieve a net reduction in CO_2 emissions. This possibility will be explored so that the role of coal liquids can be evaluated to achieve certain environmental goals.

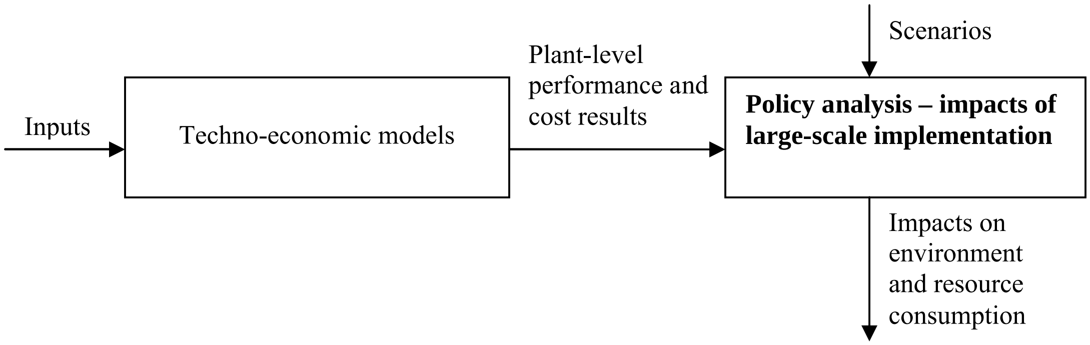


Figure 1.4: Schematic representation of the impact assessment model

1.5 Structure of the Thesis

Chapter 2 explains the different processes of a CTL plant in detail. Recent literature on techno-economic modeling is reviewed. This chapter forms the basis on which the process performance models are built. Chapter 3 deals with the development of process performance models of CTL, using Aspen Plus simulation software. The types of results obtained from this model are also explained. The subject of Chapter 4 is the development of cost-estimation models for the processes evaluated and modeled. Methods used to estimate the cost of FT technology from data available in literature are explained. Chapter 5 next deals with the large-scale impact assessment methodology, including the estimation of life cycle CO_2 emissions of CTL, the increase in coal usage because of large-scale CTL deployment, and the increased water usage and land use assessments. Chapters 6 – 9 deal with the application of performance and cost models to different case studies. Finally, broad conclusions and policy recommendations are detailed in Chapter 10.

Chapter 2: Coal-to-Liquids – Literature Review

Coals to liquids technologies produce liquids such as fuels or chemicals using coal as the feedstock. This involves the conversion of solid coal which is high in carbon to liquids which are high in hydrogen. An ideal coal liquefaction process is one which makes fewest changes to a material's native structure using the least amount of hydrogen. There are three ways in which coal can be liquefied [Probstein and Hicks, 1985; Matar, 1982]:

1. *Pyrolysis*: natural oil is distilled out of coal by rapid heating and the oil vapors are then condensed and cleaned.
2. *Direct Liquefaction*: Solid coal is converted directly to liquid under conditions of high pressure and a reducing H_2 atmosphere
3. *Indirect Liquefaction*: Coal is first gasified into synthesis gas, which is then converted to liquid fuels. Most frequently used syngas to liquid conversion process is the Fischer-Tropsch Process.

This chapter introduces indirect coal liquefaction technology using the FT process. A historical overview of the development of commercial CTL technologies is given. Depending on the commercially operating plants, the CTL process is explained. An overview of recent literature on the techno-economic modeling of CTL plants is also provided.

2.1 History and Current Status

Historically coal liquids have been prevalent in the industrial world, particularly in Germany and Japan before the Second World War and in South Africa later. The roots of Fischer-Tropsch process lie in Kaiser Wilhelm Institute for Coal Research in Germany where scientists Franz Fischer and Hanz Tropsch worked to produce hydrocarbon molecules from coal-derived gas, the ultimate goal being the production of fuels and chemicals. The main products during this time period were middle distillates and wax. About 800,000 barrels/year of FT fuels and chemicals were produced in Germany during World War II [Steynberg and Dry, 2004; Schulz, 1999]. Apart from the nine FT plants in Germany, Japan and France also had their share of coal-derived FT liquids. Most of these FT reactors can be classified under the modern low temperature (LTFT) reactor category. The first high temperature reactors (HTFT) were built in the US during the 1950's at Brownsville, Texas. But these reactors were fed by syngas derived using natural gas. But because of the availability of cheaper crude oil, FT liquids did not find their base in the US market.

After the war, mainly because of the discovery of new crude oil reserves in the Middle East and the availability of cheap liquid fuels, coal liquids lost their place, the only country in which liquid fuels were produced from coal being South Africa, whose Coal, Oil and Gas Corporation (SASOL) produced motor fuels both for commercial and developmental purposes. These plants still form a significant fraction of South African liquid fuels and chemicals production and SASOL has been a pioneer in the development of FT technology ever since the 1950's. Apart from the SASOL plants, a couple of CTL plants are in operation in Malaysia and Qatar.

After a two decade lull in FT research in the US, it again gained a lot of attention particularly from the government, during the high crude-oil periods of the 1970's and 80's. But the interest died down again because of cheaper availability of crude oil again. It is only after 2000 that CTL started gaining importance again in the US. During the high oil-price period of 2006 – 2008, a significant number of projects were being considered by both industry and government [CTL newsletter]. However, this time there was also opposition to CTL mainly because of the high CO_2 emissions from coal liquids compared to crude oil-derived liquids.

This historical perspective of CTL in general and FT liquids in particular makes it clear that coal liquids face a stiff competition from crude oil-derived liquids and that unless crude oil prices are high, investing in CTL can be financially a risky venture. The success of CTL in South Africa could not have been possible without government support [Dry, 1999].

2.2 Coal-to-Liquids Technology

A CTL plant is a complex chemical engineering process involving the use of a wide range of technologies. A typical CTL plant consists of the following basic steps:

- Synthesis gas production
- FT synthesis
- Product upgrading
- Power block

Synthesis gas production step involves a coal gasification process and subsequent gas cleaning and upgrade steps to prepare a syngas which results in maximum yield in the FT reactor. The cleaning of syngas involves an acid gas removal step in which most of the sulfur containing products are removed, along side CO_2. In some cases, the syngas is subjected to a water gas shift (WGS) reaction to adjust the H_2/CO ratio suitable for FT synthesis.

The syngas thus prepared goes through FT synthesis process section where it is converted to liquids. As explained in chapter 1, the unconverted syngas is either recycled to the FT reactor or is combusted in a power block to produce electricity.

The liquid products from the FT reactor are sent to a product upgrading section where they are refined to the required fuels and chemicals. Depending on the desired final products, the steps involved in this are oligomerization for shifting light HC to heavier HCs, hydrocracking for shifting heavy products to light HCs and hydrogenation to convert olefins to paraffins. In this thesis, this section of the CTL plant has not been modeled.

The unconverted syngas is either recycled into the FT reactor (liquids-only configuration) or combusted in a gas turbine (co-production configuration) to generate electricity. In the combined cycle power plant, heat from the gas turbine exhaust gases is used to generate high pressure supercritical steam (9.8 MPa, 538 ^{o}C) in a heat recovery steam generator (HRSG). This steam is expanded in a 3-stage (9.8 MPa, 2.1 MPa and 0.28 MPa) steam turbine with intermediate reheating to generate additional electricity. The cooling of hot syngas from the gasifier is another source of high-pressure steam and cooling of the FT reactor is a source of intermediate-pressure steam. Both of these are also sent to HRSG and used to generate electricity. For the liquids-only configuration, electricity is produced from waste heat in an amount that is just sufficient to meet the internal requirements of the plant, with no export to the grid.

2.3 Fischer-Tropsch Technology

Fischer Tropsch reactors convert syngas to hydrocarbon chains of varying lengths. The distribution of chain lengths depends mainly on the catalyst used and the operating temperature.

The Fischer-Tropsch process is essentially a catalytic reaction between CO and H_2, the main components of syngas, as shown in Eqn 1:

$$n\,CO + 2n\,H_2 \rightarrow (\text{--}CH_2\text{--})_n + n\,H_2O \qquad (1)$$

where n is the number of carbon atoms in the hydrocarbon molecule.

The stoichiometric ratio of H_2 to CO in the reactants is 2:1. Thus, it is effective if the syngas entering the FT reactor has a H2/CO ratio close to 2.

Apart from the generic reaction producing olefins, as shown in Eqn 1, a few other reactions also take place, resulting in the formation of products like methane, paraffins and alcohols.

$$CO + 3\,H_2 \Leftrightarrow CH_4 + H_2O \qquad (2)$$

$$nCO + 2nH_2 \Leftrightarrow C_nH_{2n+2}O + (n-1)H_2O \qquad (3)$$

$$(n+1)\,H_2 + 2n\,CO == C_nH_{(2n+2)} + n\,CO_2 \qquad (4)$$

Another important reaction that takes place in the FT reactor and has considerable effect on the whole process is the water gas shift reaction (WGS), shown in Eqn 5.

$$CO + H_2O \rightarrow CO_2 + H_2 \qquad (5)$$

The extent to which all these reactions take place depends on the reactor design, operating conditions like pressure and temperature, composition of inlet syngas and the catalyst used. The effects of these factors are explained in the following subsections.

2.3.1 Fischer-Tropsch Reactors

Based on the temperature at which they operate, FT reactors can be classified as low temperature (LTFT, 220 – 250^{o}C) and high temperature (HTFT, 320 – 350^{o}C). FT reaction kinetics dictates that the products contain shorter chain lengths as the temperature increases. Consequently, HTFT products tend to contain higher amount of shorter chain hydrocarbons compared to those of LTFT. As a result, HTFT reactors are optimized to produce hydrocarbons in the gasoline range and LTFT reactors are designed to optimize the production of longer-chained hydrocarbons in the diesel and wax range [Dry, 1996; Steynberg and Dry, 2004].

In each category, there are different reactor designs. HTFT reactors come in circulating fluidized bed and turbulent or fixed fluidized bed designs whereas LTFT reactors can be obtained in tubular fixed bed reactors and three-phase slurry based reactors. Of these, the fixed fluidized bed HTFT and tubular fixed bed LTFT reactors are the ones mostly used in commercial operations. Nevertheless, the three-phase slurry based LTFT is expected to be the design of choice in new plants because of its adaptability to coal-based syngas and economic attractiveness over fixed bed LTFT. However, so far, using slurry-based LTFT reactors in liquids-only CTL configuration have not been commercially proposed.

2.3.1.1 Low Temperature FT Reactors

LTFT synthesis is used mainly to produce longer chain hydrocarbons such as waxes. These waxes can be refined downstream to produce diesel fuel of very high cetane number [Dry, 1999]. Two types of reactors currently used in commercial applications are the tubular fixed-bed reactors and slurry-bed reactors [Espinoza et al, 1999].

Tubular Fixed Bed Reactors

In this kind of reactors, shown in Fig 2.1, syngas flows through tubes packed with catalyst. Outside the tubes (shell-side), water is continually circulated to cool the tubes in which the highly exothermic FT reactions take place. The key design criterion is to enable effective heat transfer between the catalyst particles on whom the reactions take place and the cooling medium outside the tubes. Temperature control is an important parameter in the conversion of syngas to products. To improve the heat transfer and conversion, some portion of the tail gas is usually recycled to the reactor.

To improve conversion per pass, it is better to have smaller catalyst particles. To improve the heat transfer, it is better to have narrower tubes. Tubes of 5cm diameter are used commercially for Fe-based catalysts while narrower tubes are required for Co-based catalysts because of their higher activity and consequently higher heat generation. A combination of these factors means that the differential pressure over the length of a tube will be high as a result of which gas compression costs might go up. Also, loading of catalyst into such narrow tubes poses operational difficulties. Replacing catalyst in these reactors is a lengthy process. Because of the behavior of catalysts, the temperature gradients in both the axial and radial directions in the tubes are not optimal. Since thousands of tubes are required in a reactor vessel, the reactors themselves are very heavy.

The advantage of a multi-tube fixed bed reactor is its ease of operation. The liquid wax formed in the FT products trickles down the bed because of its heavy weight this eliminating a need for catalyst-wax separation equipment. Also, prediction of performance of this kind of reactor is relatively easy. Hence, it is easy to design large scale facilities based on pilot plant performance. In case of sulfur-poisoning because of malfunction of upstream gas purification steps, only a portion of the catalyst bed is deactivated thereby not overly affecting the performance of the whole reactor.

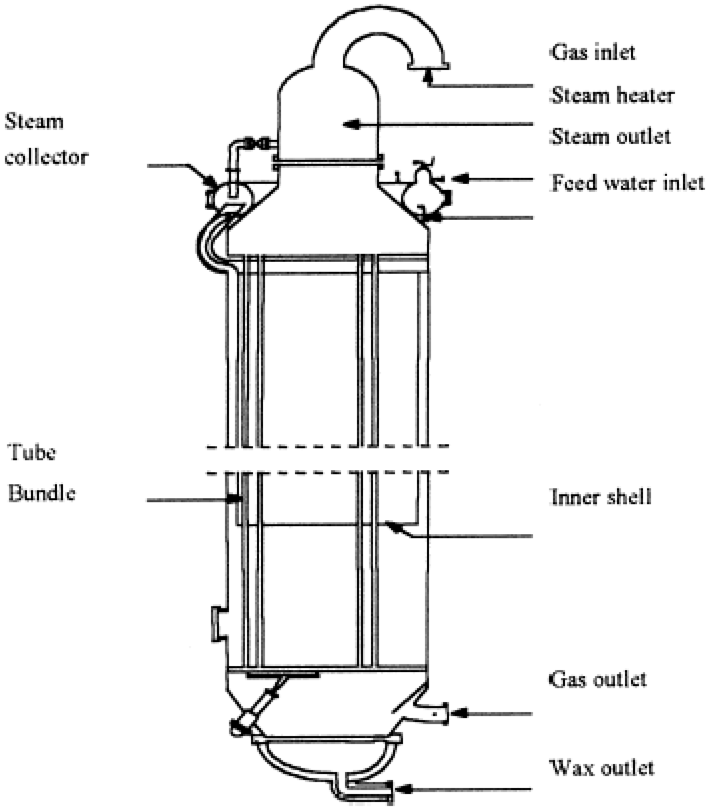


Figure 2.1: Tubular fixed bed reactor [Espinoza et al, 1999]

Fixed bed reactors are not suitable for high temperature operation because of the predominance of carbon deposition on catalyst particles at high temperatures.

<u>Slurry phase reactors</u>

The slurry phase reactor design varies a lot from that of the fixed bed reactor. In a slurry bed reactor (Fig 2.2), the cooling water flows through the tubes and reactions take place on the shell side. The slurry is made up of FT product wax mixed with catalyst particles. Syngas enters the slurry at the bottom and reactions take place as it moves upwards. The gaseous products diffuse to the top and the heavier products form part of the slurry. Unlike in the tubular reactors, the catalyst here must be separated from the wax in separate equipment. The slurry is continuously circulated leading to uniformly distributed catalyst particles and temperatures. The advantage of this circulation is that conversions can be achieved with lower catalyst loading. The disadvantage is that deactivation of catalyst also takes place uniformly. However, because of continuous circulation, catalyst can be replaced during operation without any reactor downtime. Full load catalyst change is also easier than in the fixed-bed case. The catalyst particles are also smaller than in the fixed-bed case. The reactor size is also much smaller than the fixed-bed reactor. Overall, it is estimated that the cost of a reactor train is only 25% of multi-tubular fixed bed reactor train of similar capacity. The pressure drop across the reactor is also lower thus lowering the operating costs of gas compression.

At high temperatures, the wax in the slurry starts to get hydrocracked as a result of which fresh wax feed requirement increases. For this reason, slurry bed reactors are not suitable for high temperature operation.

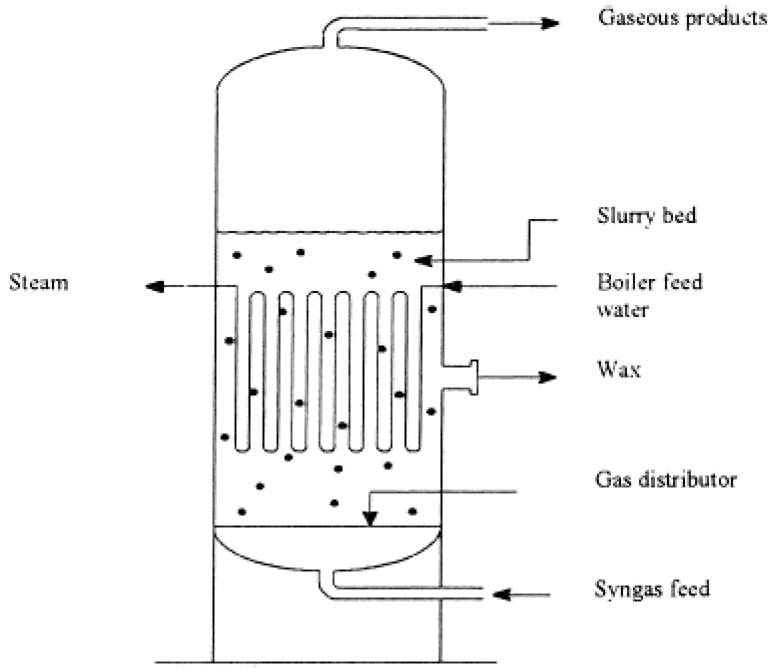


Figure 2.2: Slurry bed LTFT reactor [Espinoza et al, 1999]

2.3.1.2 High Temperature Fischer Tropsch Reactors

HTFT reactors are used specifically when lighter hydrocarbons like gasoline are the preferred products. Fluidized bed reactors are generally used for this purpose. The high rates of heat generation associated with high temperature FT conversion can be efficiently removed using this design. The bed consists of catalyst particles with syngas as the fluidizing medium. Currently, there are two kinds of fluidized bed reactors – circulating fluidized bed (Synthol reactors), shown in Fig 2.3 and turbulent fluidized bed (Sasol Advanced Synthol reactor / SAS reactor), shown in Fig 2.4. To remove heat in both these designs, steam at 40 bar is produced from the cooling water [Steynberg et al, 1999].

Circulating fluidized bed reactors

Catalyst particles are carried into the reactor section by syngas which has been preheated to about 200 °C. Heat exchangers within the reactor remove about 40% of the heat while producing steam. The catalyst is re-circulated after being separated from the product gases. Carbon deposition on the catalyst particles causes operational problems in this kind of reactors. A more advanced reactor design is the turbulent fluidized bed design.

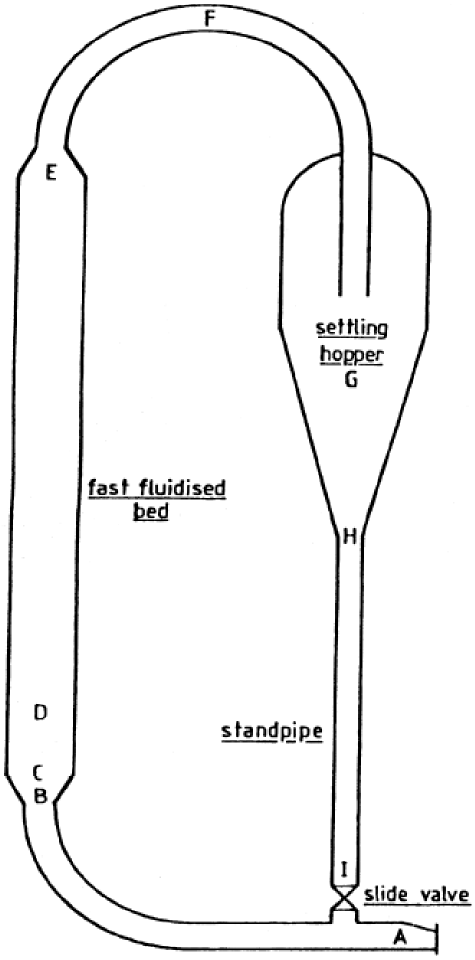


Figure 2.3: Circulating fluidized bed reactor HTFT [Steynberg et al, 1999]

Turbulent fluidized bed reactor

These reactors are conventional fluidized bed reactors which can operate at pressures in the range of 20 – 40 bar. For similar operating conditions as the CFB reactors, these reactors have higher capacities because of higher conversions levels. Owing to their smaller size, these reactors cost 40% lower than a corresponding CFB reactor. This is also much easier to operate. As a result, this reactor design is mostly used in the currently commercial applications.

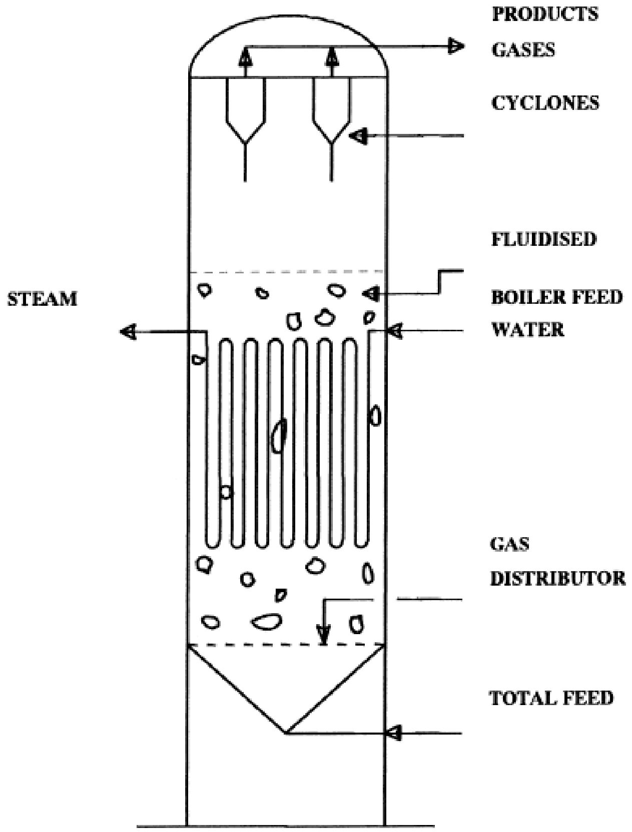


Figure 2.4: SAS reactor [Steynberg et al, 1999]

2.3.4 Fischer-Tropsch Catalysts

Another important variable in the FT reactor technology is the type of catalyst. Catalysts that are currently commercial are either iron (Fe) or cobalt (Co) based. For FT synthesis, as seen in Eqn 3, the ratio of moles of CO to H_2 should be 1:2. To adjust the composition of syngas to this ratio, the fraction of CO has to be reduced and that of H_2 has to be increased. This can be achieved by a water gas shift (WGS) reaction in which steam is used to oxidize CO and produce H_2 (Eqn 5).

Fe catalysts support WGS reaction even within the FT reactor whereas Co catalysts are not active WGS catalysts. As a result, if Co-based catalysts are used, the CO/H_2 ratio has to be adjusted external to the FT reactor whereas when Fe-based catalyst is used, WGS occurs within FT reactor. Consequently, when an iron catalyst is used, there is some amount of CO_2 generated in the FT reactor which has to be removed downstream of the reactor. On the other hand, there is no CO_2 generation within the FT reactor with a cobalt catalyst but CO_2 is produced upstream of the reactor because WGS reaction is used to adjust the CO/H_2 ratio.

2.3.5 Chemistry of FT reactions

In contrast with the gasification reactions which can be modeled using thermodynamic equilibrium assumptions, reaction kinetics dictates the FT reactions. There is a wide range of literature pertaining to modeling of FT reactions using kinetic rate expressions. These equations can be used in the design and scale-up of FT reactors [Dry, 1996; Mills, 1994; Espinoza et al, 1999; Steynberg and Dry, 2004 and Wender, 1996]. One of the earliest kinetic rate expressions were proposed by Anderson [Espinoza et al, 1999]:

For Fe catalysts, $-r_{FT} = \dfrac{k_{FT}\, P_{CO}\, P_{H_2}}{P_{CO} + b\, P_{H_2O}}$ and

For CO-catalysts, $-r_{FT} = \dfrac{k_{FT}\, P_{CO}\, P_{H_2}^2}{1 + b\, P_{CO}\, P_{H_2}^2}$

There have been numerous studies later but Espinoza et al (1999) note that the common link between most of the studies is that in case of Co-catalysts, the rate expressions contain only terms for H_2 and CO whereas for Fe-catalysts, the rate expressions also include terms for H_2O or CO_2 in some cases.

There are also several studies related to the mechanism of FT reactions. These mechanisms describe how chain hydrocarbon chain initiation, propagation and termination occur on different catalyst surfaces and operating conditions. Proposed reaction mechanisms should account for the following unique features of FT products [Dry, 1996]:

- Predominantly linear compounds, irrespective of the type
- High olefin content compared to paraffins
- Predominantly terminal olefins
- Considerable amount of chain branching, mainly monomethyl branches
- Decreasing degree of branching with increasing chain lengths

Linearity of the FT products is explained by the addition of $–CH_2$- units in chain propagation. It is now widely accepted that CO adsorbed on the catalyst causes the formation of $–CH_2$- blocks, thus helping the chain propagation while H_2 acts as a chain-terminating agent.

2.3.5.1 Ideal H_2/CO ratio in the syngas

As explained before, the ideal ratio of H_2/CO in the syngas for an FT reaction is close to 2. In processes which produce syngas with a lower H_2/CO ratio (e.g. Coal gasification), a water gas shift reaction (WGS) can be used to adjust the ratio by reacting CO in the syngas with steam to form more H_2, CO_2 being the other product.

In some cases, depending on the catalyst and operating temperature, WGS occurs within the FT reactor. This eliminates the need for shifting the syngas prior to the FT reactor. Fe catalysts support WGS reaction even within the FT reactor. Water formed in the FT reaction reacts with CO in the syngas, producing more H_2 to react with CO to form FT products. Thus, syngas with H_2/CO ratio less than 2 can also be used in a FT reactor using Fe catalyst, without the need for an additional WGS reactor upstream of the FT reactor. LTFT slurry bed reactors are specially suited for this purpose and thus are likely to be the reactors of choice for CTL applications.

On the other hand, Co catalysts are not active WGS catalysts. H2/CO ratio has to be adjusted external to the FT reactor, unlike when Fe-based catalysts are used.

Consequently, when an iron catalyst is used, there is some amount of CO_2 generated in the FT reactor which has to be removed downstream of the reactor. On the other hand, there is no CO_2 generation within the FT reactor with a cobalt catalyst but CO_2 is produced upstream of the reactor because WGS reaction is used to adjust the CO/H_2 ratio.

Based on practical knowledge, for a fixed bed LTFT reactor using Fe catalyst, the required H_2/CO ratio is approximately 1.65 [Steynberg and Dry, 2004]. The ratio for HTFT applications should be slightly greater than 2. However, there is no clear indication in the literature as to the ideal syngas H_2/CO ratio for slurry-based LTFT reactors. Most of the studies agree that syngas from coal gasification can be used directly in the FT reactor without any need for prior adjustment of the ratio. Many modeling studies use a syngas H_2/CO ratio ranging from 0.6 – 1 [Gray and Tomlinson, 1990; NETL, 2007a; Williams et al, 2006; Steynberg and Nel, 2004]. Some modeling studies include a WGS reactor to adjust the ratio to 2.0 prior to the FT reactor [Boerrigter and Zwart, 2004].

2.3.5.2 Extent of WGS reaction

The extent of water gas shift reaction within the FT reactor has a significant effect on the ideal usage ratio of H_2/CO in the inlet syngas. The relative rates of FT and WGS reactions have an effect on the amount of H_2 formed within the FT reactor, the product yield and CO_2 formation. Thus, for modeling purposes, it is important to understand the extent of WGS reaction compared to the FT reaction.

Though many studies consider WGS reaction also in the overall reaction mechanism, the knowledge of relative rates of FT and WGS reactions is not straightforward [Patzlaff et al, 1999; Raje and Davis, 1997; Schluz and Claeys, 1999; Shi and Davis, 2004; Sie and Krishna, 1999; van der Laan and Beenackers, 2000]. Raje and Davis (1997) conducted LTFT experiments with syngas H_2/CO ratios of 0.67 and 1.7. The relative rates of FT and WGS reactions were measured and it can be deduced from the results that the ratio of rates of WGS to FT is in the range of 0.54 – 0.92. This can also be understood as the fraction of CO converted in WGS reaction is about 0.54 – 0.92 times that converted in the FT reaction. More detailed explanation of this is given in the next chapter where the process model is discussed.

Since WGS reaction closely follows equilibrium thermodynamics, it can be imagined that the rate of forward reaction will be inversely proportional to increasing H_2/CO ratio in the inlet syngas. If the ratio is low, then the formation of H_2, i.e. the forward WGS reaction will be high. If the ratio is high, the formation of H_2 will be low. This has been observed even in practical systems. Thus, for modeling purposes, the relative rates of WGS and FT reactions should be linked with the H_2/CO ratio of the inlet syngas. This relation will be further explored in the next chapter where the process model is explained.

2.3.6 FT product distribution

FT products contain a large number of hydrocarbon chains ranging from carbon numbers 1 to more than 30. The distribution of chain lengths depends on a parameter called chain growth probability (α) and can be depicted by the Anderson-Schulz-Flory (ASF) equation [Dry, 1999; Mills, 1994] as shown in Eqn 6 and Fig 2.5. The chain growth probability depends on the operating parameters of the FT reactor like temperature and the catalyst used. In the equation, α denotes the chain growth probability.

$$W_n = n(1-\alpha)^2 \alpha^{n-1} \qquad (6)$$

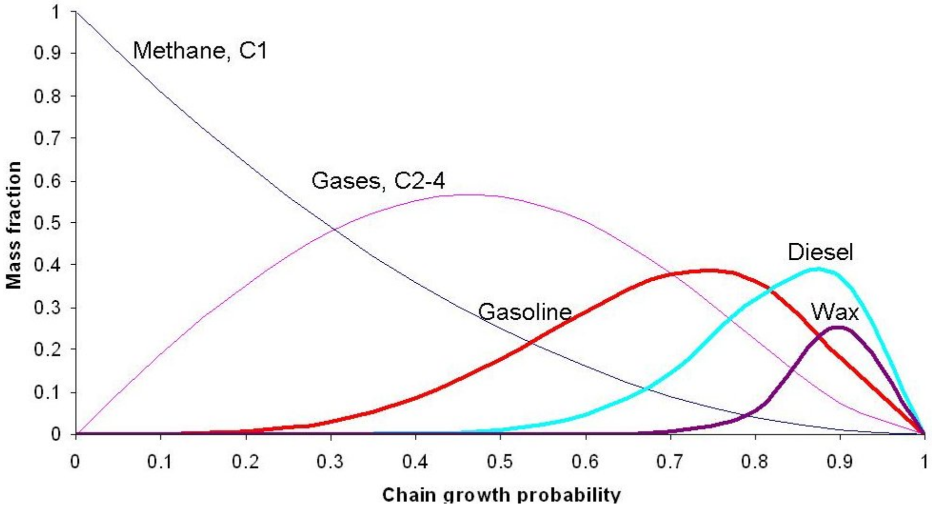


Figure 2.5: Anderson Shulz Flory distribution of FT products

Nickel (Ni) is known to be an active hydrogenation catalyst which enables the formation of high amounts of methane under FT operating conditions. Hence Ni is not used as a catalyst in FT processes. Other metals which are suited for the FT process are ruthenium (Ru), Co and Fe. Since Ru is an expensive material, Co and Fe are the two most widely used FT catalyst materials. Co has higher hydrogenation potential than Fe. Thus FT reactors using Co-based catalysts produce more methane than when Fe-based catalysts are used.

The probability of chain growth decreases with increasing temperature because hydrogenation reactions are more active at higher temperatures. Thus, HTFT products contain more shorter-chained hydrocarbons than LTFT products. Hence, LTFT reactors are more suitable if the desired products are diesel and waxes while HTFT is more suitable for gasoline production.

In most commercial processes, α is in the range of 0.7 to 0.95, depending on the operating conditions. Here, it is assumed to be 0.9, a typical value for the low temperature FT reactors [Steynberg and Dry, 2004].

2.4 Coal Gasification

Gasification of coal is essentially a reaction of carbon in coal with a source of hydrogen (usually steam) and/or oxygen to yield a gas containing predominantly carbon monoxide (CO), hydrogen (H_2), carbon dioxide (CO_2) and methane (CH_4). Coal can be gasified to produce medium calorific value (10 – 16 MJ/m^3) synthesis gas (or syngas), consisting primarily of a mixture of CO and H_2. Synthetic natural gas whose main component is CH_4 can also be produced from coal. Since syngas is the reactant in FT reactions, only those gasifier technologies used to produce syngas are considered here.

Gasifiers that produce syngas generally involve reaction of coal with steam and oxygen in the presence of heat [Probstein and Hicks, 1985]. The main reactions occurring in these gasifiers are:

$$C + H_2O \rightarrow CO + H_2 \qquad \Delta H^o_{1000K} = 135 \text{ kJ/mol} \qquad (7)$$

$$C + \tfrac{1}{2} O_2 \rightarrow CO \qquad \Delta H^o_{1000K} = -112 \text{ kJ/mol} \qquad (8)$$

$$C + O_2 \rightarrow CO_2 \qquad \Delta H^o_{1000K} = -395 \text{ kJ/mol} \qquad (9)$$

Oxygen and steam requirements for coal gasification

To understand the amount of oxygen and steam required to efficiently gasify the carbon in coal, it is helpful to look at the thermal balance of the gasification reactions. Steam gasification of carbon (Eqn 7) is an endothermic reaction needing 135 kJ/mol of heat. This heat can be supplied by the combustion reaction of carbon (Eqn 9). To achieve thermal neutrality, a fraction (0.34) of the combustion reaction needs to take place. The effective reaction then will be:

$$1.34C + 0.34O_2 + H_2O\ (g) \rightarrow 0.34CO_2 + CO + H_2 \qquad \Delta H^{o}_{1000K} = 0 \qquad (10)$$

The stoichiometry of this reaction shows that there should be 0.34 moles of O_2 and 1 mole of H_2O for every 1.34 mole of carbon for thermal neutrality. Hence the stoichiometric ratios of oxygen and steam are as follows:

$$O_2 / C = 0.25\ mol / mol, 0.67 kg / kg$$

$$H_2O / C = 0.75 mol / mol, 1.125 kg / kg$$

Since these ratios don't change much with temperature, they can be taken as representative stoichiometric ratios for steam gasification of coal. Though ideally CO and H_2 are the only desired components in the syngas, in real gasifiers, other reactions also take place, resulting in other components such as CH_4, H_2S, COS and NH_3. Modeling a real gasifier, thus, needs to take into account the formation of other species.

The following are the main reactions that take place in a gasifier (Holt and Alpert, 2001):

$$C + H_2O \rightarrow CO + H_2 \qquad (11)$$

$$C + 0.5\ O_2 \rightarrow CO \qquad (12)$$

$$CO + H_2O \rightarrow CO_2 + H_2 \qquad (13)$$

$$CO_2 + C \rightarrow 2CO \qquad (14)$$

$CH_4 + 1.5\ O_2 \rightarrow CO + 2H_2O$ (15)

$S + H_2 \rightarrow H_2S$ (16)

$N_2 + 3H_2 \rightarrow 2NH_3$ (17)

$CO + H_2S \rightarrow COS + H_2$ (18)

2.4.1 Types of Gasifiers

A gasifier is fundamentally a chemical reactor. Based on the reactor type, gasifiers are classified as fixed/moving bed, fluidized bed or entrained flow gasifiers. Selection of gasifier depends on a number of factors including the coal characteristics, quality requirements of syngas, operating parameters, site-specific requirements and so on. Of the above-mentioned gasifier types, entrained flow design (Fig 2.6) is the most widely used. These gasifiers operate at high temperatures and are characterized by very low residence time of coal (of the order of seconds). High temperatures limit the formation of methane. The advantage of entrained flow gasifiers is the flexibility of using different types of coal. Coal has to be pulverized to help in its rapid gasification. Within the entrained gasifier design, there is variability in the method in which coal is fed into the gasifier. Coal can be fed either dry or in the form of water slurry. In this paper, three commercially used gasifier designs are modeled – (1) GE/Texaco slurry feed, (2) Conoco-Phillips E-Gas slurry feed and (3) Shell dry feed gasifiers. The input variables such as gasification pressure, temperature and the feed rates of oxygen and steam relative to coal are based on the values reported in NETL baseline study of thermal power plants [NETL 2007b]. A comparison of these gasifiers is given in table 2.1.

GE/Texaco Gasifier

GE gasifier (earlier Texaco/Chevron Texaco) is a cylindrical pressure vessel in which coal is fed in the form of water slurry and the oxidant is pure oxygen (95% purity, in this case). The operating temperature is 1,316 ^{o}C and pressure is 5.6 MPa. Ash is removed in the form of molten slag. The gasifier uses a radiant cooling technology to cool the raw syngas.

GE gasifier (earlier Texaco/Chevron Texaco) is a cylindrical pressure vessel in which coal is fed in the form of water slurry and the oxidant is either pure oxygen or air. The operating temperatures are in the range of 1250^{o}C to 1450^{o}C and at pressures slightly greater than 40 bar. Ash is removed in the form of molten slag. Because of the operating conditions, the product syngas contains more of CO than H_2. Depending on the cooling system used, cold gas efficiency varies from 75% to 95%. The disadvantage of GE gasifier is that handling low rank coal becomes uneconomical.

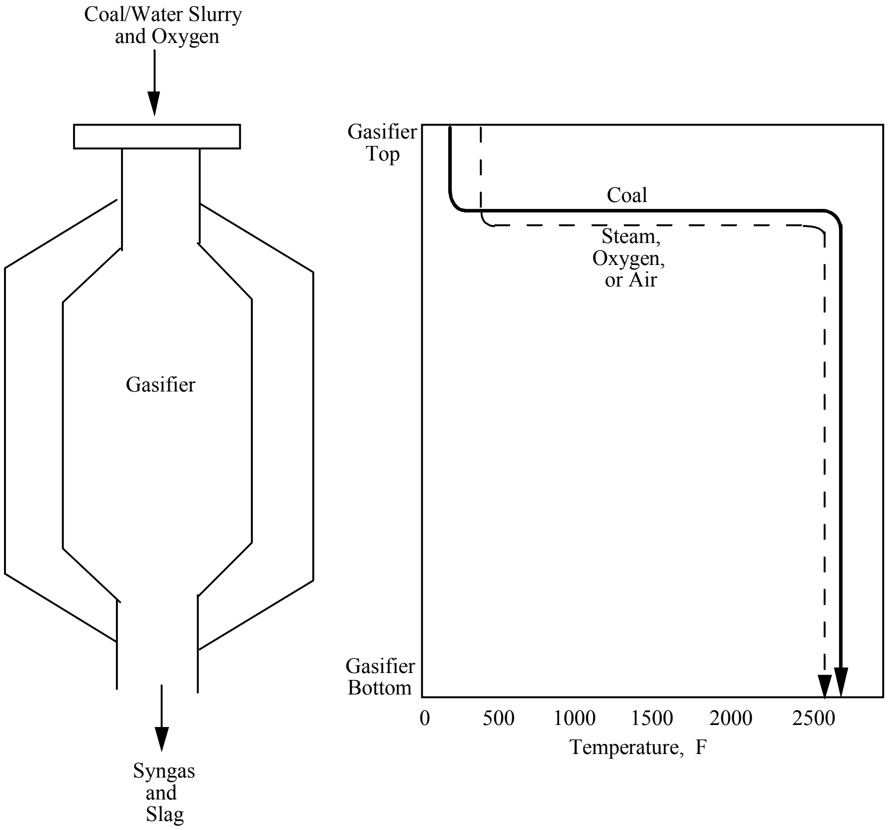


Figure 2.6: Entrained flow gasification reactors

Shell Gasifier

Unlike the other two gasifiers, coal is fed in dry form using nitrogen as the carrier. Oxygen and a small amount of steam are injected directly into the gasifier, which operates at 1,427 ^{o}C and 4.2 MPa. The high operating temperature limits the formation of CO_2. However, the H_2/CO ratio in the products is lower than what is required for FT reactions and a water gas shift reaction is required to adjust the ratio.

The Shell gasifier is another high pressure entrained flow slagging type gasifier but it operates on dry coal feed. The operating temperatures are slightly in excess of 1350^{o}C and the product gas contains principally H_2 and CO with very little CO_2. The H_2/CO ratio is of the order of 0.4 – 0.45, higher than with GE gasifier. The advantage of a Shell gasifier is its applicability to any rank of coal. However, coals with ash content in the range of 8 – 15% are recommended. The cold gas efficiency can range from 80 – 95%.

Two other gasifiers are also commercially available, though not as commonly used as the ones explained before. One is Lurgi Multi-purpose gasifier (MPG), which operates on the principle of partial oxidation. The superior advantage of this technology is its ability to handle any type of feedstock. Oxygen is mixed with steam before being fed to the burner. The operating conditions vary from 1200°C to 1450°C and 30 to 75 bar. A wide variation (0.5 – 0.8) in the H_2/CO can be obtained depending on the operating conditions.

Table 2.1: gasifier characteristics

Gasification	
Type	Features
Texaco /Chevron /GE gasifier	• Slurry-based • 1260 – 1430 °C • 41 bar • Oxygen-based • Efficiency 77 – 95% • High CO/H2 ratio • Not suitable for low-rank coals
Shell gasifier	• Dry feed • Oxygen-based • 1370 – 1600 °C • Lower CO/H2 ratio • Can be operated with any type of coal • Steam injection depends on coal type • Efficiency 80 – 94%
E-gas two-stage gasfier	• Slurry-based • Oxygen-based • 1100 °C

Conoco-Phillips E-Gas Gasifier

This is also a slurry-fed gasifier design operating in two stages. The first stage of the process is a high-temperature slagging stage into which only part of the reactants are fed in the form of a slurry and the product gas is used to drive the gasification reactions in the second stage. The efficiency of this type of gasifier is higher than single-stage gasifiers, partly because of the lower oxygen requirement here. Gasification occurs in a single stage, operating at 1,010 °C and pressure of 4.2 MPa. Here also, ash is removed in the form of molten slag.

2.5 Gas Clean-up and CO_2 Removal Technologies

The syngas from the gasifier needs to be cleaned and upgraded before it can be sent to the FT reactor. FT catalysts are extremely sensitive to sulfur compounds in syngas. The presence of CO_2 in the inlet syngas also acts as a deterrent to FT reactions. Sulfur in coal appears mostly as hydrogen sulfide (H_2S) in the syngas. Removal of CO_2 and H_2S from syngas is called acid gas removal. This can be achieved by physical absorption process like Selexol and Rectisol. The Selexol process by Dow chemicals is explained in this section. The process flow diagram for co-capturing H_2S and CO_2 is shown in Fig 2.7 [UOP, 2007].

2.5.1 Sulfur removal

In the first stage of the process, the Selexol solvent is sent through a sulfur absorber tower where it counter-currently mixes with syngas from the gasification section. H2S from syngas is absorbed into the solvent and the H2S-rich solvent is to a stripper tower where H2S is separated from the solvent.

The H2S-rich acid gas is sent to a Claus section where it is converted to elemental sulfur. The acid gas is combusted in 95% pure oxygen such that 33% of H2S is oxidized to SO2. The product gas is cooled in a waste heat recovery boiler and then sent into a Claus reactor where the H2S and SO2 in the gas react in the presence of a catalyst to form elemental sulfur and water. The sulfur-free gas is sent through more Claus reactors till almost all of H2S is converted to elemental sulfur.

Because of this clean-up step, sulfur from coal is not carried onto the FT products, making them sulfur-free liquid fuels and chemicals.

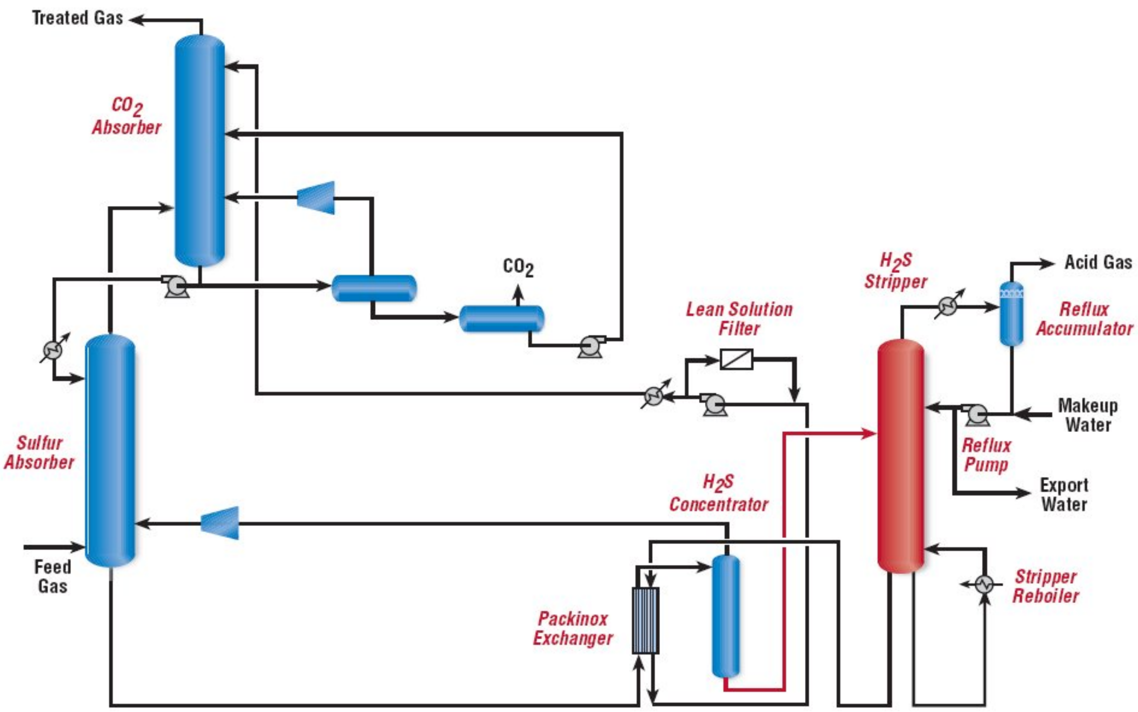


Figure 2.7: Selexol process to co-capture H_2S and CO_2 from syngas [UOP, 2007]

2.5.2 CO_2 removal

The H_2S-free syngas from the first stage of Selexol process then passes through a second absorber tower where it meets the lean solvent from H_2S-stripper tower. CO_2 in the syngas is captured by the solvent and the CO_2-rich gas is then sent to a second stripper tower where the captured CO_2 is stripped from the solvent to produce a concentrated stream of CO_2. This CO_2 is dehydrated and compressed to about 110 bar and transported via pipelines to a sequestration site. The regenerated solvent is then sent to the first stage absorber.

Rectisol technology can also be used to co-capture H_2S and CO_2 from syngas. In this, the solvent is a methanol-based material [Prelipceanu et al, 2007].

It is assumed here that the same technology can be used to capture the CO_2 produced in the FT reactor. The other technology used in Sasol for the capture of FT CO_2 is called a

Benfield unit where CO_2 is cryogenically separated from the tail gases of the FT reactor [UOP, 2009].

For CO_2 capture from the exhaust gases of a gas turbine (the co-production case), a chemical-absorption technology is used. The capture process is similar to the Selexol CO_2 capture but a chemical reaction takes place in the absorber tower where CO_2 from the flue gas reacts with MEA solvent. The CO_2-rich solvent is then thermally regenerated using steam from the steam turbine. This process requires much more regeneration energy compared to the physical absorption processes like Selexol and Rectisol.

2.6 Techno-Economic Analysis of CTL Processes

Interest in coal liquids reached its peak during the decade immediately following the first oil crisis in the mid-1970s. Relatively little new work has been done since then, mainly because of the fall in oil prices in the 1980s and the resulting decline in interest in alternative fuels. However, in recent years, with renewed interest in CTL, new studies have emerged.

Bridgwater and Anders [1991] describe a model for economic assessment of coal liquefaction. The study concluded that methanol is the most attractive fuel product in terms of capital and production costs. Neathery et al [1999] proposed a ‘pioneer plant’ concept in which a CTL plant, supplemented by natural gas firing, produces both liquid fuels and electricity. This plant was shown to be more efficient than separate integrated gasification combined cycle (IGCC) power plants producing electricity and liquid fuels being produced from the FT process using natural gas as the feedstock. A performance and cost comparison between co-production and liquids-only coal plants producing methanol was done by Larson and Tingjin [2003]. Williams et al [2006; 2009] explored carbon management options, including the usage of combined coal and biomass feedstock, in co-production CTL plants producing FT liquid fuels. The U.S. Department of Energy (DoE) published a techno-economic assessment report [NETL 2007a] of a 50,000 barrels per day liquids-only CTL plant, showing the performance and costs of a conceptual plant. A Southern States Energy Board report [SSEB, 2006] also analyses CTL plants, both liquids-only and co-production, of various capacities. Steynberg and Nel [2004] compared two co-production CTL plants, each one using different types of FT reactors, in terms of their performance and efficiency, but not in terms of their costs. Carbon constraints or CCS were not considered.

Chapter 3: Process Performance Models of CTL Plants

Mathematical modeling of a CTL process helps in predicting the mass and energy inputs required to produce a given amount of output. The main inputs to a CTL plant are coal, oxygen and water. Major outputs of the process are FT products, by-products such as electricity and emissions such as CO_2 and sulfur. Process modeling involves the calculation of mass and energy balances of individual components of the CTL plant. Aspen Plus [Aspen Technology Inc., 2007] process simulation software was used to develop the performance models. This chapter explains the details of modeling different individual components.

3.1 Modeling of Syngas Generation

Syngas generation section includes coal preparation, oxygen production in an air separation unit (ASU), gasification in a gasifier and raw gas cooling and cleanup (Fig 2.1). This section provides the modeling of these processes using Aspen Plus.

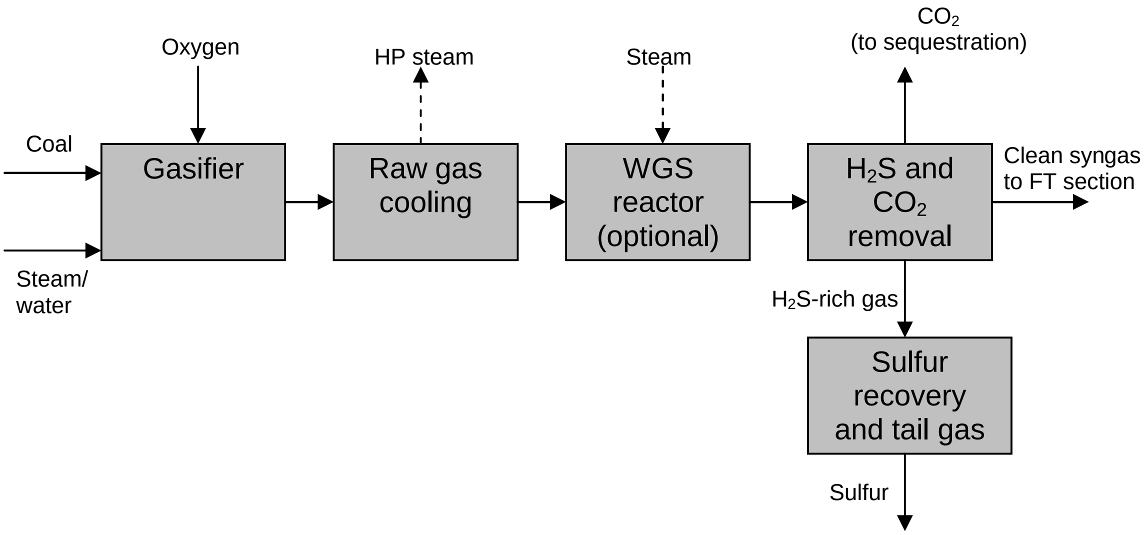


Figure 3.1: Syngas generation block flow diagram

A mathematical model for gasification should duplicate the reactions between carbon and other components in coal with oxygen and steam. Different gasifiers inject steam in different ways. In slurry-based gasifiers such as GE and E-Gas, steam comes in the form of water in the slurry used to transport coal into the gasifier. Dry-feed gasifiers (Shell) use a gas medium, usually nitrogen, to transport coal into the gasifier. Steam for such systems is fed directly into the gasifier. The other input is oxygen, which is input to the gasifier from an Air Separation Unit (ASU). Thus, though the methods of injecting all the inputs into the gasifier may differ, gasification process is essentially a reaction of coal with water/steam and oxygen to produce syngas, as shown in Fig 3.2.

3.1.1 Coal preparation model

For the purpose of modeling using Aspen Plus, coal is a non-conventional solid, in the sense that it is composed of different component elements and cannot be represented as a single chemical species. This non-conventional material has to be decomposed into conventional components which will then react in the gasifier. The elemental composition of coal is given by its ultimate analysis. The amount of moisture in coal obtained from its proximate analysis.

This non-conventional material is then ‘decomposed’ into different conventional components using a RYIELD reactor, which calculates the composition of the products based on a given yield distribution. The distribution is input using a calculator block which uses the data from ultimate and proximate analyses to calculate the mass fractions of carbon (C), hydrogen (H_2), nitrogen (N_2), chlorine (Cl_2), sulfur (S), water (H_2O), oxygen (O_2) and ash. The procedure for this calculation is shown below.

Mass fraction of every component is given by,

$$y_{component} = Component_{coal} \times \left(1 - Moisture_{coal}\right)$$

The mass fraction of each component in coal, $Component_{coal}$, is obtained from the ultimate analysis and $Moisture_{coal}$ is obtained from the proximate analysis data.

Heat released in the decomposition process is fed into the gasifier block since this process is not separate from the gasification process for practical purposes.

For this analysis, Illinois#6 bituminous coal is used as the feedstock. Coal composition in the form of its ultimate and proximate analyses is given in table 3.1.

Table 3.1: Coal properties, ultimate analyses

Coal	**Appalachian medium sulfur**	**Appalachian low sulfur**	**WPC Utah**	**Illinois#6**	**Wyoming PRB**	**ND lignite**
Rank	**Bituminous**	**Bituminous**	**Bituminous**	**Bituminous**	**Sub-bituminous**	**Lignite**
HHV(MJ/kg)	30.78	30.36	26.09	26.12	19.36	13.97
HHV (BTU/lb)	13260	13080	11240	11252	8340	6020
Ash	7.24	9.79	11.59	9.70	5.32	15.92
C	73.81	71.74	67.66	63.74	48.18	35.04
H2	4.88	4.62	4.85	4.50	3.31	2.68
N2	1.42	1.42	1.22	1.25	0.7	0.77
Cl	0.06	0.07	0.01	0.29	0.01	0.09
S	2.13	0.64	0.61	2.51	0.37	1.16
O2	5.41	6.09	6.11	6.89	11.87	11.31
Moisture	5.05	5.63	7.95	11.12	30.24	33.03

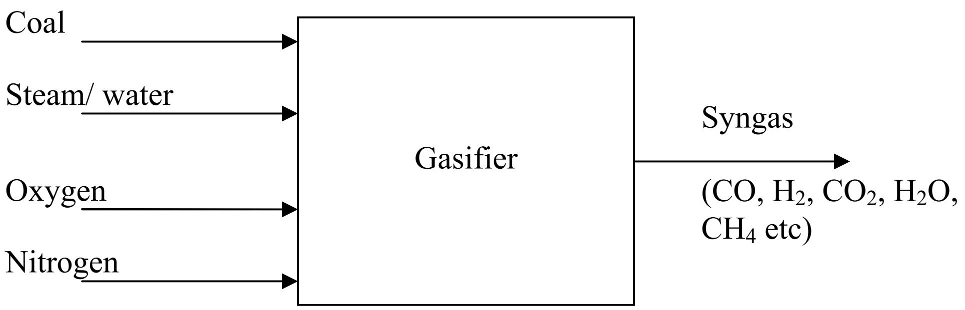


Fig 3.2: Basic flow diagram of a gasifier

3.1.2 Steam input to the gasifier

For slurry-feed gasification, the steam required for the gasification reactions comes from slurry water. In practice for slurry-feed gasifier systems, crushed coal is mixed with water and the slurry is fed to the gasifier. The concentration of solids in the slurry is fixed by a ‘slurryability’ criterion. Typical bituminous coal slurry consists of 65% solids and 35% water. The requirement for sub-bituminous coal and lignite is around 45% and 50% water by weight [Chen, 2005]. For modeling purposes, a water stream is directly input the gasifier block, instead of mixing it with coal. The flow rate of this stream is such that the slurryability criterion is met for different coals. For GE, E-Gas and Shell systems, the ratio of H2O/C in the gasifier feed is obtained from literature [NETL 2007b]. However, the effect of different water flow rates for a given amount of coal is also studied.

3.1.3 Coal drying model

Some gasification systems require drying the coal feed. A Shell gasifier has different moisture requirements for different ranks of coal. For example, the design moisture content of the coal feed is 5% for bituminous coals, 6% for sub-bituminous coals and 12% for lignite. Drying is usually done by heating the incoming coal using hot gasifier exit gases. A separator block SEP is used to model the coal drying process. The amount of drying is specified using a DesignSpec constraint. This condition is deactivated when slurry-feed gasifiers are modeled.

3.1.4 Oxygen input to the gasifier

Most of the entrained flow gasifiers use oxygen as the oxidation agent. Oxygen is separated from air typically in a cryogenic air separation unit (ASU) and the 95% pure oxygen is fed into the gasifier.

For this Aspen Plus model, ASU is not modeled explicitly. The gasifier is directly fed with 95% pure oxygen which is compressed from atmospheric pressure to the gasification pressure. The energy required for ASU and oxygen compression is modeled using equations developed for IECM. The main air compressor energy use is given by the following equation:

$$W_{MAC} = (0.0174 \times \eta_{Ox} + 0.1514) \times (m^3 / hr\ of\ oxygen)\ [kW] \tag{1}$$

The other energy use in the ASU is for compressing the 95% pure oxygen to the gasifier pressure. The compressor is modeled using the COMPR block of Aspen Plus, which calculates the energy required for compression.

Oxygen requirements to different gasifiers are also obtained from literature [NETL 2007b]. The effect of different oxygen flow rates on the product compositions is also analyzed. Typically, enough oxygen is supplied to oxidize almost all of the carbon in coal. Reactions with oxygen supply the heat required for other endothermic reactions.

3.1.5 Gasifier model

In Aspen Plus, the reactor unit RGIBBS is used to model the gasification reactions. This can be used when the possible products are known but the exact reactions that take place to produce those components are not well-known. This reactor unit calculates the composition of the products based on the minimization of Gibbs' free energy. Apart from the material flow inputs to the reactor, the pressure at which reactions take place and either the reactor temperature or the heat duty has to be specified. It is assumed that all the reactions reach chemical equilibrium. For commercial gasifiers, the operating temperature and pressure are known. These are used as inputs to the gasifier block when modeling commercial gasifiers. The effect of varying temperature and heat loss from the gasifier is also tested.

Considering the products in a typical gasifier product gas, apart from Eqns. 7 – 9 of chapter 2, the following reactions are likely to take place in the gasifier [Holt and Alpert, 2001]:

$C + 2\ H_2 \rightarrow CH_4$ (2)

$CO + H_2O \rightarrow CO_2 + H_2$ (3)

$2CO + O_2 \rightarrow 2CO_2$ (4)

$CH_4 + H_2O \rightarrow CO + 3H_2$ (5)

$S + H_2 \rightarrow H_2S$ (6)

$N_2 + 3H_2 \rightarrow 2NH_3$ (7)

$CO + H_2S \rightarrow COS + H_2$ (8)

Under practical conditions, the composition of syngas from gasifiers deviates from the values predicted by chemical equilibrium. Aspen Plus uses a parameter called “approach temperature” which can be modified for any of the reactions till the actual syngas composition is replicated. A section of Aspen Plus flowsheet is depicted in Fig 3.3.

3.1.6 Raw gas cooling and scrubbing

Different gasifier systems use different methods to cool the raw product gas. The typical raw gas cooling mechanisms are either by water quench or in a radiant syngas cooler. In a quench design, the hot raw gas and molten slag from the gasifier is sent through a high pressure water quench chamber which rapidly cools the gas/slag mixture and separates slag from the gases. The gases are then scrubbed downstream to remove any fine particulates. The other alternative is a radiant syngas cooler in which the hot raw gas is cooled by generating high pressure steam.

The quench design is a cheaper alternative but the radiant design is more efficient. In IGCC power plants employing pre-combustion CO_2 capture, the quench chamber supplies water required for the water gas shift reaction. WGS reaction is required in plants using HTFT reactors, to adjust the H_2/CO ratio of the syngas to 2:1. However, in a CTL plant using LTFT reactors, WGS is not always required prior to the FT reactor. On the other hand, the radiant syngas produces high pressure steam which can be used to generate electricity to meet the utility needs of the CTL plant. Hence, the radiant syngas cooling option is used here for all cases.

Aspen modeling of gas cooling section

The hot syngas stream from the gasifier is sent to a radiant syngas cooler to generate high pressure steam. This boiler is modeled using a HEATER block, whose inputs are the pressure drop and the outlet temperature of gases. A heat output stream calculates the amount of heat released by the cooler. This heat stream will be input to another HEATER block which generates steam.

Raw gas is also scrubbed and cleaned to separate impurities from it. The gas which exits the cooling and scrubbing section is at a temperature of about 40 ^{o}C, suitable to be cleaned in the downstream Selexol unit. This section is modeled by a FLASH2 block which separates ash/slag from the gas stream. A section of Aspen Plus flowsheet is shown in Fig 3.4.

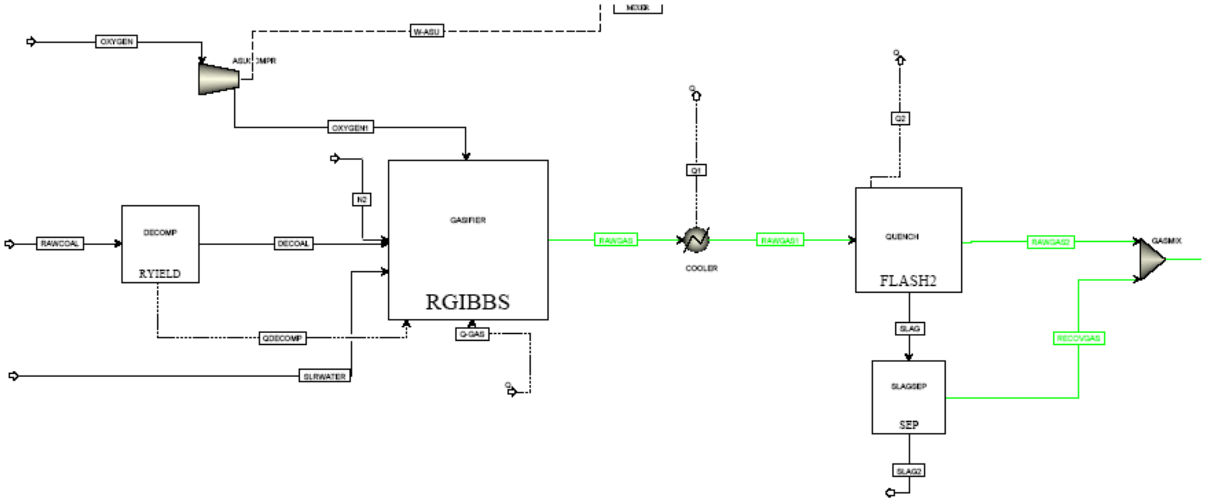


Figure 3.3: Aspen flow sheet of a gasifier model

3.1.7 Gas cleanup – sulfur and CO_2 capture

Gas clean-up section here specifically means the process used to remove sulfur compounds and CO_2 from the syngas stream. The technology used for this acid gas removal is the Selexol unit which selectively captures H_2S and CO_2 by physical absorption in a solvent. The H2S-rich gas is sent to a sulfur-recovery unit comprising of Claus/SCOT process in which H2S is converted to elemental sulfur.

The CO_2 removed from the second stage of the Selexol process is dried and compressed to 140 bar, ready to be transported via pipelines to a geological sequestration site.

Modeling of gas clean-up in Aspen Plus

The two stages of Selexol process have been modeled using the separator ‘SEP’ blocks. The first SEP block is modeled such that 99.9% of H2S is separated from the syngas (as required by the FT reactor). The H2S-rich acid gas is sent into a Claus plant. The H2S-free gas is then sent through another SEP block in which 99% of CO_2 is removed from the gas stream. The amount of Selexol solvent required for these two steps is derived from the IECM manual on IGCC plants.

In the Claus section, the H2S-rich acid gas is combusted in 95% pure oxygen such that 33% of H2S is oxidized to SO2. The product gas is cooled in a waste heat recovery boiler and then sent into a Claus reactor where the H2S and SO2 in the gas react in the presence of a catalyst to form elemental sulfur and water. Both the combustor and the Claus reactor are modeled using the stoichiometric reactor blocks ‘RSTOIC’. The product gas is condensed in a FLASH block to separate sulfur. The sulfur-free gas is sent through more Claus reactors till almost all of H_2S is converted to elemental sulfur. All the sulfur streams are collected using a MIXER block.

In co-production cases, there is an option of capturing the CO_2 present in the flue gases from gas turbine. Amine-based capture is the most relevant commercially available technology for this purpose. Since this is essentially a separation process, it has been modeled using a SEP block, similar to what was done for Selexol process. The capture efficiency for this step is 90%. Aspen Plus flowsheet of this section is shown in Fig 3.4.

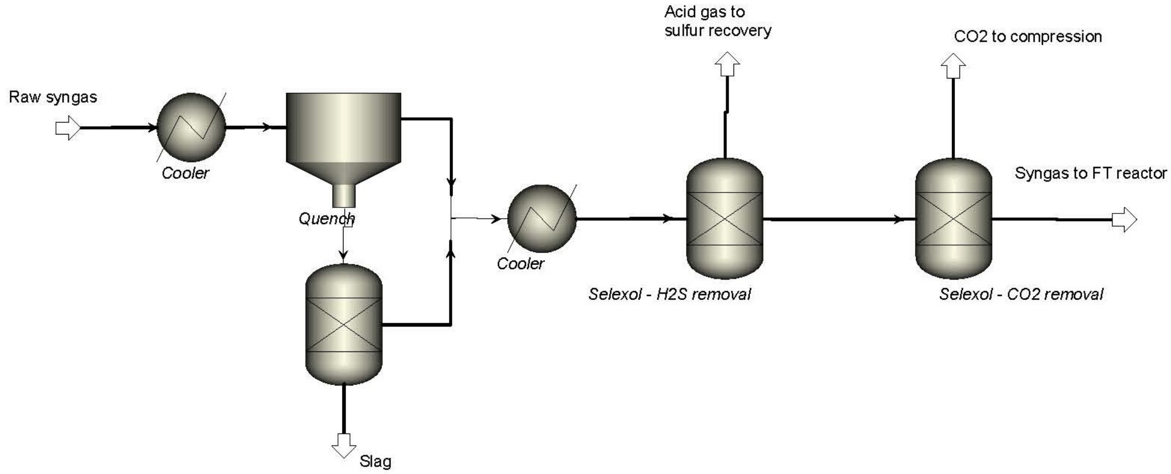


Figure 3.4: Aspen Plus flow sheet of the gas clean up section

3.1.9 Validation of the Model with GE, Conoco-Phillips and Shell Gasifiers

Three commercially available gasification technologies – GE, Conoco-Phillips and Shell gasifiers are modeled using the methodology described in the previous sections. The model was validated using the inputs and results from report published by DoE/NETL on IGCC power plants [NETL 2007b]. Syngas compositions at different places in the gasification section are shown for each case. In all the cases, 1% (by weight) of the inlet carbon was assumed to be lost in slag. This value however might be higher or lower in practical applications. In the initial step, all the gasification reactions were assumed to be in chemical equilibrium. Then the approach temperatures for individual reactions were varied to bring the syngas composition as close to the reference values as possible.

Gasifier inputs

Entrained flow gasifiers usually operate at a uniform temperature throughout the reactor. Hence, temperature can be used as an input instead of a specified heat loss. For the gasifier block (RGIBBS), temperatures and pressures for each case are shown in table 3.2.

Illinois#6 is used as the feed coal. GE and E-Gas gasifiers are slurry-fed reactors while the Shell gasifier is a dry-feed system. Using the DesignSpec option, the oxygen and steam flow rates are specified on a mol/mol of carbon in coal basis. The values for each case are shown in table #.

Table 3.2: Gasifier characteristics and inputs

	GE	E-Gas	Shell
Feed	Slurry	Slurry	Dry
Temperature (^oC)	1316	1016	1427
Pressure (MPa)	5.6	4.3	4.3
O_2/C (mol/mol)	0.47	0.43	0.42
H_2O/C (mol/mol)	0.55	0.55	0.15

Results

Composition at gasifier exit (1% carbon loss) is given in table 3.3. The numbers are close within +/- 3% of the reference values. This much error margin is allowable since the reference values are also based on models. The approach temperatures used to get these values are shown in table 3.4.

Table 3.3: Comparison of gasifier model results with reference values

	GE		E-Gas		Shell	
	NETL	Model	NETL	Model	NETL	Model
CO	34.4	33.9	38.5	36.0	57.2	57.7
H2	33.5	33.6	27.4	26.0	29.0	29.9
CO2	15.1	15.3	14.7	13.3	2.1	1.9
H2O	14.3	14.7	12.5	17.8	3.6	2.4
CH4	0.1	0.1	4.0	4.3	0.0	0.0
H2S	0.7	0.6	0.8	0.8	0.8	0.8
Others	2.9	1.8	2.1	1.8	7.3	7.3
H2/CO		0.99		0.72		0.52

Table 3.4: Approach temperatures used to obtain the syngas composition (table 3.3)

Reaction			
	GE	E-Gas	Shell
C + O2 ⇔ CO2	0	0	0
C + 0.5 O2 ⇔ CO	0	0	0
H2 + S ⇔ H2S	0	0	0
CO + H2O ⇔ CO2 + H2	- 500	0	- 250
CH4 + H2O ⇔ CO + 3 H2	- 100	- 150	0
N2 + 3 H2 ⇔ 2 NH3	0	- 500	- 890
C + CO2 ⇔ 2 CO	0	0	0
H2S + CO2 ⇔ COS + H2O	0	0	0

GE and Shell match up very close to reference but E-Gas doesn't. E-Gas is a two stage gasifier, but it is simplified to only one stage in the model. That is the cause for difference.

The H_2/CO ratio in the syngas from a Shell gasifier is 0.52 and is less than 0.67, the minimum ratio required for a low temperature FT reactor. This syngas has to be subjected to a WGS reaction to increase the H_2 content and reduce the CO content. A WGS reactor is modeled using the REQUIL reactor block which calculates the equilibrium composition based on temperature and pressure. Steam is also fed to the reactor. The mass flow rate of steam is calculated using the DesignSpec criterion such that the exit H_2/CO ratio should be 0.67.

Composition after H_2S and CO_2 removal

After H_2S and CO_2 removal, the syngas is ready to be sent to the liquefaction section. Effectively, only CO, H_2, CH_4 and inerts such as N_2 and Ar are left in the syngas. The composition for the three gasifiers are shown in table 3.5

Table 3.5: Composition of syngas that is sent to the FT synthesis section

	GE	E-Gas	Shell
CO	48.9	52.8	55.5
H2	48.4	38.1	37.2
CH4	0.2	6.3	0.0
H2O	1.2	1.5	0.0
Others	1.3	1.3	7.3
H2/CO	0.99	0.72	0.67

This ends the gasification flowsheet in Aspen Plus. The clean syngas stream results are used as input to the FT flowsheet, described in the next section.

3.2 Fischer Tropsch Synthesis Section

The clean gas stream from the gasification section which now predominantly consists of CO, H_2, small fractions of CH_4, N_2 and Ar are sent to the FT reactor section. This section comprises of the FT reactor where syngas is converted to hydrocarbons and separation of gaseous hydrocarbons (C1-C4) and unconverted syngas from liquid products. In the liquids-only cases, the gas streams are cleaned and upgraded in a gas loop before recycling to the FT reactor. In the co-production case, the gases are sent to a power block. Modeling of this section of the CTL plant is described in this section.

3.2.1 FT reactor model

The FT reactor model is divided into two parts – the actual FT reactor which converts syngas to an average hydrocarbon and a downstream reactor which splits the average hydrocarbon into compounds of different carbon numbers based on the ASF distribution.

It was discussed in the previous chapter that FT reactions are driven by reaction kinetics rather than chemical equilibrium. In order to accurately model a FT reactor, reaction kinetics have to be accounted for. Modeling of reactors based on reaction kinetics calls for the use of specific design features like the reactor dimensions and residence time. The scope of this thesis is to make it possible to evaluate the performance of the whole CTL plant under different operating conditions and plant sizes. Using reaction kinetics to model FT reactors makes it difficult to scale up or scale down the plant size. Since only a plant-level analysis is required, it was decided not to make a detailed reactor design but to make a few assumptions so as to mimic the actual reaction conditions to a fair level of accuracy. For cases where exact reaction kinetics are not known but the products are known, Aspen Plus allows the option of using a RSTOIC reactor block, which calculates the composition of products based on the fractional conversion of reactants.

Another difficulty with modeling of the FT reactor is the huge number of reactions that take place. Though FT reaction can be denoted by just one equation, it becomes very difficult to model when the carbon number varies from 1 to more than 30. A simplified model was found in literature where the whole product spectrum (C1 – C30+) is denoted by an "average hydrocarbon", whose carbon number is derived by averaging the total spectrum on a mass basis [DoE, 1992]. The average carbon number is expressed as a function of the chain growth probability. As explained in the previous chapter, the chain grown probability (α) depends on the operating conditions and catalyst.

$$x = \frac{1}{1-\alpha}$$

When for α = 0.9, as in the case of a LTFT reactor using Fe catalyst, the average carbon number becomes 10, making the average hydrocarbon $C_{10}H_{20}$ which represents the whole product spectrum. When α = 0.7, as in the case of HTFT, x = 3.33. For the sake of modeling, the average hydrocarbon is assumed to be C_3H_6.

The effective FT reaction is given by,

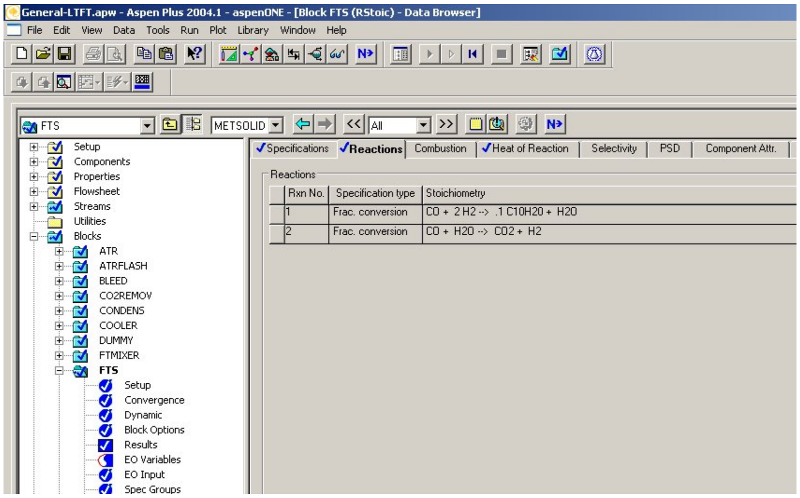
$CO + 2 H_2 \rightarrow (1/x) C_xH_{2x} + H_2O$

If the FT reactor uses a Fe-based catalyst, FT reaction is accompanied by a water-gas shift reaction:

$CO + H_2O \rightarrow CO_2 + H_2$

These two reactions are modeled in the FT reactor, using the RSTOIC block of Aspen Plus. One of the input screens of the Aspen Plus model is shown in Fig 3.5. The overall conversion of CO in a LTFT reactor is about 80% and in a HTFT reactor is close 90%. This includes the conversion in the individual FT and WGS reactions. The determination of these conversions is explained in the next subsection.

The FT products, now containing the unconverted syngas (CO and H_2), the average hydrocarbon (C_xH_{2x}), CO_2 and H_2O is input to a SEP block, where C_xH_{2x} is separated form the rest of the products. The distribution of carbon numbers in the FT products is governed by the ASF relation. The average HC has to be split into HCs of different carbon numbers following the ASF relation. The splitting is modeled using the RYIELD block, similar to the one used for decomposing coal into its components. The mass fractions of different carbon numbers are given in the form of a FORTRAN code in a CALCULATOR block.



Reactions

Rxn No.	Specification type	Stoichiometry
1	Frac. conversion	CO + 2 H2 --> .1 C10H20 + H2O
2	Frac. conversion	CO + H2O --> CO2 + H2

Figure 3.5: Aspen Plus input screen for FT reactor, modeled using the RSTOIC block

Of these products, C1 – C4 are gases and the rest are liquids. The gases are mixed with the other gas streams from the FT reactor. The RSTOIC reactor for the FT reaction, the SEP block to separate the unconverted syngas from the average hydrocarbon, the RYIELD reactor to split the average hydrocarbon into different carbon numbers and the mixer block to mix the C1-C4 gases with the rest of the gases together form the FT synthesis reactor model.

In a liquids-only configuration, the unconverted syngas is added as a recycle stream into the FT reactor after cleanup and upgrade steps in a gas loop, which will be explained in the next subsection. In a co-production configuration, unconverted syngas is burnt in a gas turbine.

There is a heat output from the FT reactor since the reaction is highly exothermic. In a commercial reactor, this heat is absorbed by water flowing through tubes within the reactor to produce medium pressure steam. In this model, this heat is removed from the FT reactor in the form of a heat stream which becomes input to a heater block that produces medium pressure steam.

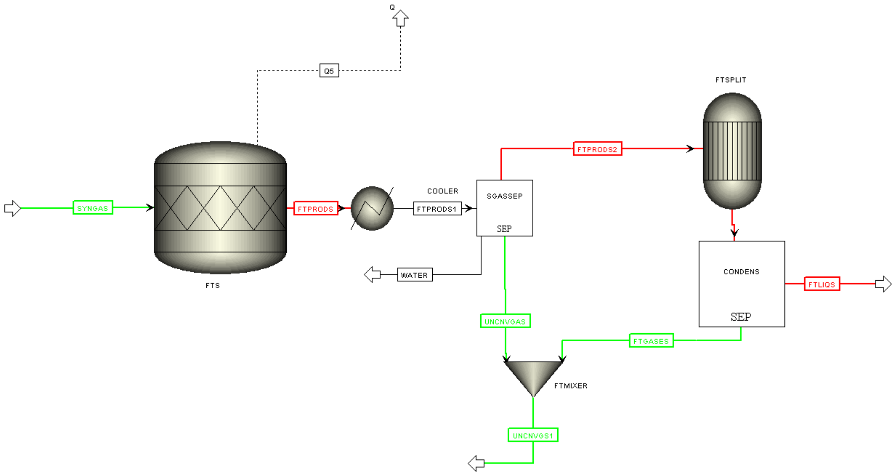


Figure 3.6: FT reactor model including the RSTOIC reactor for FT reaction, separation of the average hydrocarbon, RYIELD reactor for splitting of the average hydrocarbon and MIXER block for mixing of the gases

3.2.2 Extent of WGS reaction

The composition of products exiting the FT reactor depends on the relative extents of FT and WGS reactions. The following methodology was followed to determine the relative fractions of conversion of CO:

- For different H_2/CO ratios in the inlet syngas, CO conversion fraction in the FT reaction is varied from 0.1 – 1 in steps of 0.05, using the SENSITIVITY feature of Aspen Plus.
- For each of the above values, CO conversion in WGS reaction was varied between 0.1 – 0.9 times the fractional conversion of the FT reaction
- H_2/CO ratio in the exit syngas is monitored for all these variations
- The overall conversion of CO in the FT reactor (moles-per-hour of CO in outlet gas/ moles-per-hour of CO in inlet gas) was also monitored

- That combination of FT and WGS conversions was selected for which the outlet H_2/CO was close to the inlet H_2/CO and the overall conversion of CO was slightly more than 80%

In an ideal FT reactor, H_2 and CO are consumed in the ratio of 2:1. If the inlet syngas has a H_2/CO = 2, then the outlet unconverted syngas should also have a H_2/CO ratio of 2. Using this logic, even with the occurrence of a WGS reaction, the consumption of H2 and CO should be such that the outlet H_2/CO should be the same as that of the inlet syngas. So, the relative rates of WGS and FT are chosen so as to meet this condition.

An example of this method is shown in the following figure, where the inlet H_2/CO ratio is 0.67, which is the minimum value required for an LTFT reactor using a Fe catalyst (previous chapter). The methodology of choosing a relative WGS/FT reaction rate is as follows:

- CO conversion in FT reaction is varied from 0.1 – 0.5 and the outlet H_2/CO is plotted on the y-axis for different relative rates of WGS reaction
- For a given CO conversion in the FT reaction, as the relative extent of WGS increases, the H_2/CO ratio in the products also increases. In a WGS reaction, CO is consumed and H_2 is produced. The higher the extent of WGS reaction, higher is the fraction of H_2 in the products.
- When the relative WGS/FT rate 0.8, the exit H_2/CO ratio decreases with increasing FT reaction rate.
- For higher relative rates, the exit H_2/CO increases with increasing FT reaction rate.

- For WGS/FT = 0.8, the value is the same as the inlet H_2/CO for all values of FT rates.
- For a CO conversion of 0.45 in the FT reaction and the relative WGS/FT rate of 0.8, the overall conversion of CO is 80%. Hence this value is chosen for the case where inlet H_2/CO ratio is 0.67

Similar procedure is repeated for other syngas compositions and the relative extent of WGS rate is determined. For example, when the inlet H_2/CO ratio is 1, WGS/FT = 0.5 and FT conversion rate = 0.55. For an inlet H_2/CO ratio of 1.7, WGS/FT = 0.11 and FT conversion rate = 0.8.

For the operating conditions in HTFT reactors, WGS reaction rate is set to nearly zero since the syngas feed has a H_2/CO ratio of 2:1.

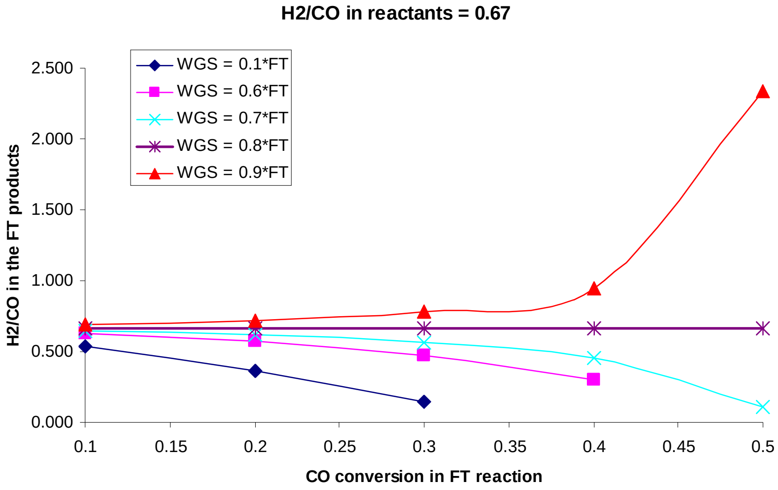


Figure 3.7: H_2/CO ratio as a function of FT reaction rate and WGS reaction rate

3.2.3 FT gas loop for liquids-only cases

The products from a FT reactor include light-end hydrocarbon gases (C1-C4), heavier hydrocarbon liquids (C5+), components of unconverted syngas (CO and H_2) and other product gases such as CO_2 and H_2O. Separation and handling of all these products forms a major portion of the FT synthesis section.

In a typical FT reactor, gases and liquids are separated by condensation. The liquid stream is sent to a refining section where it is split into different products such as naptha, diesel and wax. This part of the FT section is, however, not considered in this thesis. The liquid products (C5+) are treated as syncrude. The block flow diagram of FT loop is shown in Fig 3.8.

The first step in a generic FT gas loop is the separation of CO_2 from the gas stream. The Selexol unit downstream of the gasifier is used again in the FT section for CO_2 removal. This is followed by a cryogenic hydrocarbon recovery process which separates C2-C4 hydrocarbons from the rest of the gases. These can either be sold or used as fuel gas. These gases can also be auto-thermally reformed to produce CO and H_2, which can also be used as input to the FT reactor. Since the objective of the liquids-only plant is to maximize the liquids production, ATR is used on the light hydrocarbons. The products from ATR are mixed with the other components of the unconverted syngas, which also contains methane. For maximum effectiveness in the FT reactor, the recycled syngas should have similar composition as the fresh syngas from the gasification section. If the gas in the recycle loop has a H_2/CO ratio higher than the fresh feed, then some of the H_2 needs to be recovered to adjust the ratio. A hydrogen recovery unit separates enough H_2 from the gas stream to make the H_2/CO ratio equal to that of the fresh feed.

In the currently commercial CTL plants, mainly in South Africa, either steam reforming or auto-thermal reforming is used in the gas loop [Steynberg and Dry, 2004]. Of these two options, auto-thermal reforming is more cost-effective. So, ATR is used as the reforming process in this study.

An autothermal reactor (ATR) is a catalytic partial oxidation process of hydrocarbons to CO and H_2, under adiabatic conditions. Hydrocarbons (predominantly methane) are catalytically reacted with steam and oxygen. The ratio of H_2/CO in the products can be varied by adjusting the amount of oxygen feed. This technology is widely used when syngas is generated from natural gas, where combustion and steam-reforming of methane is done to produce CO and H_2. Heat for steam-reforming is supplied by the combustion reaction. The following are the typical reactions:

$CH_4 + 3/2\ O_2 \rightarrow CO + 2H_2O + 519$ kJ/mol

$CH_4 + H_2O \Leftrightarrow CO + 3H_2 - 206$ kJ/mol

$CO + H_2O \Leftrightarrow CO_2 + H_2 + 41$ kJ/mol

A typical ATR reactor is a pressure vessel. CH_4, steam and O_2 enter at the top. First zone is combustion zone. After this, there is catalytic zone in which unconverted CH_4 and other hydrocarbons are converted to CO and H_2. Ni-based catalyst is typically used. Because of high temperatures (> 1000 ^{o}C), inner layer of the vessel is refractory-lined.

Aspen modeling of the gas loop

The CO_2 removal is done using a separator SEP block, just like in the gasification section. 99% removal efficiency is assumed. Another SEP block is used to model the cryogenic hydrocarbon recovery unit where all the C2 – C4 hydrocarbons are separated from the gas.

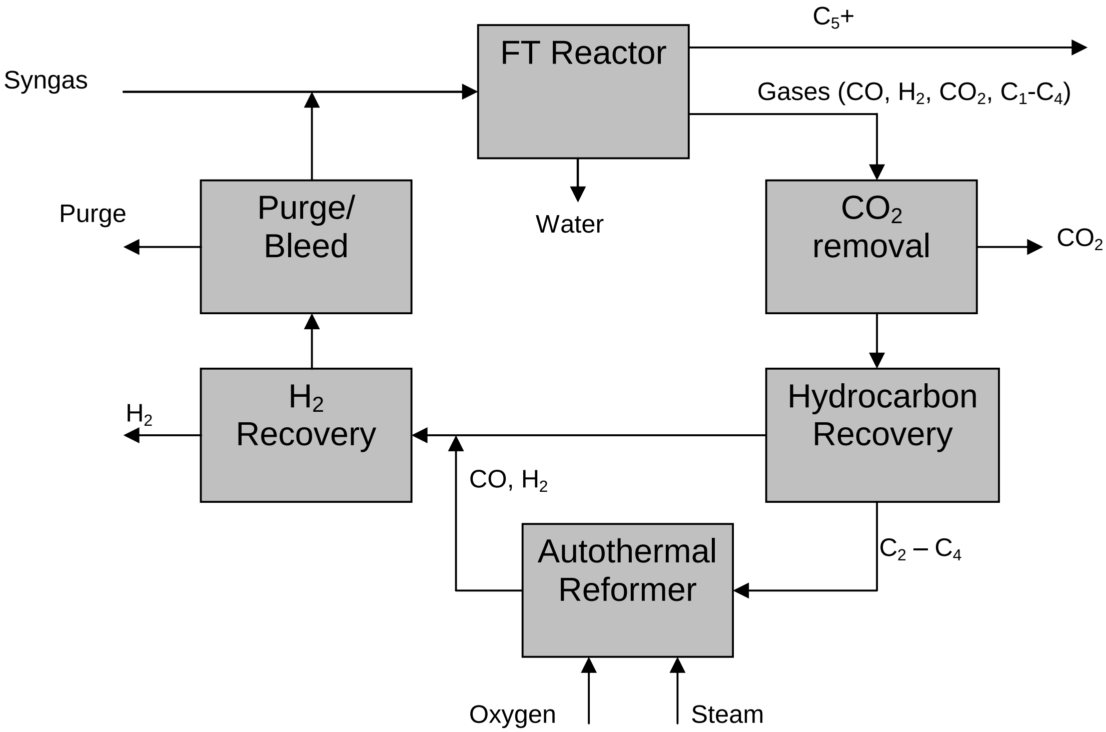
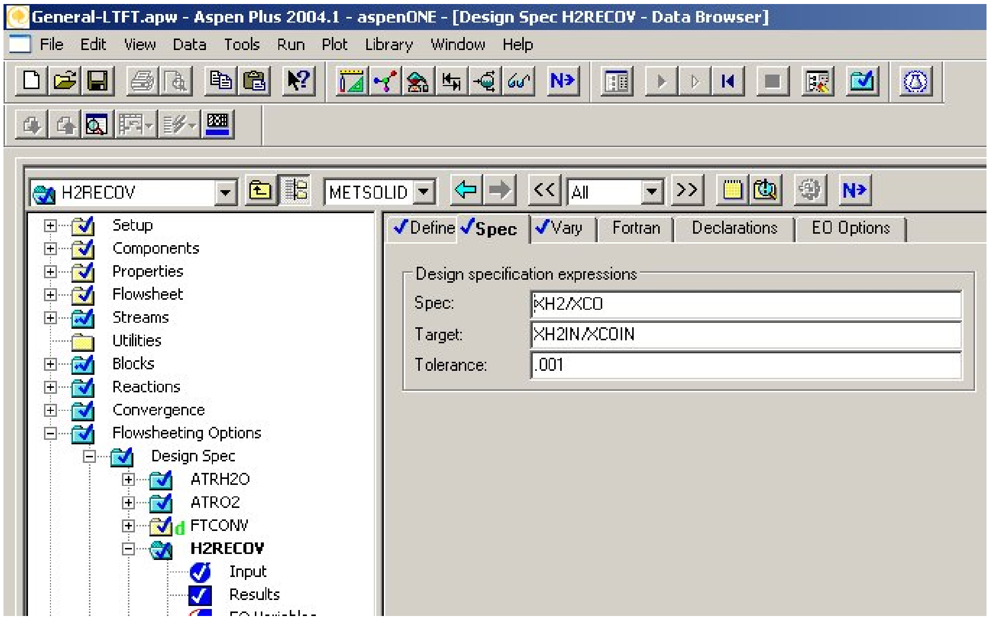


Fig 3.8: FT gas loop for liquids-only configuration. The recycled gas should have a H_2/CO close to that of fresh gas

RGIBBS reactor block is used for modeling an ATR. The pressure is set at 25 bar, a typical value for ATR and also for the FT reactor. Heat duty from the reactor is set to zero, to mimic adiabatic conditions. Typically, the amount of steam is such that the molar ratio of H_2O to carbon is about 0.6. This condition is set using the DesignSpec option such that the molar flow rate of steam is equal to 0.6 times the molar flow rate of carbon in CH_4, C_2H_4, C_3H_6 and C_4H_8. A typical O_2/C ratio is around 0.45. The actual design criteria used for calculating the ATR oxygen requirement are maximum CH_4 conversion and a temperature of around 1000 ^{o}C. It was found that these conditions are met for O_2/C molar ratio of 0.475. These conditions are input using the DesignSpec option.

Water is removed from the ATR products, which are mixed with the CH_4-rich unconverted syngas stream. The combined stream is sent to a H_2-recovery unit modeled by a SEP block. The amount of H_2 removed from the stream is set using a DesignSpec condition such that the H_2/CO ratio in the recycle gas stream should match the H_2/CO ratio of fresh feed to the FT reactor. Figure 3.9 shows the input screen of this DesignSpec block in Aspen Plus



Design specification expressions

Spec: XH2/XCO

Target: XH2IN/XCOIN

Tolerance: .001

Figure 3.9: Aspen Plus input screen for the DesignSpec block of H_2-removal block

Because of recycling of the gases, some inerts get accumulated in the gas loop. Some of the recycled gas needs to be purged to limit the accumulation. In the model, this step is achieved by using a FSPLIT block which splits one stream into multiple streams of predetermined fractions. The fraction of split stream here is determined such that the model converges to a solution. If the fraction is lower than this, the solution does not converge. In most cases, the purge fraction was found to be about 10% of the recycled gases.

Table 3.6 shows a sample of syngas composition at different places in the FT gas loop for a GE gasifier case. Fresh syngas with an inlet H_2/CO ratio of 0.99 is fed to the FT reactor. The product stream (1) from the FT reactor (RSTOIC) consists of the products of FT and

WGS reactions ($C_{10}H_{20}$, CO_2, H_2O) and unconverted syngas. The average hydrocarbon ($C_{10}H_{20}$) is separated from this stream in a SEP block and is split into FT products (stream 3) according to ASF distribution in a RYEILD reactor. The C1 – C4 gases from the FT products are mixed with the other unconverted syngas (stream 2) in a MIXER block and the mixed stream (4) is sent through the gas loop. The combination of RSTOIC, SEP, RYEILD and MIXER blocks in the Aspen model reflect the actual FT reactor, the products being liquids (C5+) and gases including the C1 – C4 FT products and the unconverted syngas. CO_2 is separated from the gas stream in a Selexol unit, modeled using a SEP block. C2 – C4 hydrocarbons are separated from the CO_2-free stream and those are subjected to autothermal reforming, converting them to CO and H_2. The ATR products are mixed with the original unconverted syngas stream and the combined stream (stream 6) is sent to a H_2-recovery unit to adjust the H_2/CO ratio equal to the fresh syngas feed. The final unconverted syngas (stream 7) is recycled to the FT reactor. In this case, there is no excess H_2 to be removed from the gas, as is evident from the same composition of streams 6 and 7.

Table 3.6: Gas compositions at different stages of gas loop

	1	2	3	4	5	6	7
CO	13.6	18.7	0.0	18.4	26.2	28.0	28.0
H_2	3.4	4.6	0.0	4.6	6.5	13.0	13.0
CO_2	22.2	30.6	0.0	30.0	0.2	0.1	0.1
H_2O	23.2	0.2	0.0	0.2	0.2	0.7	0.7
CH_4	6.0	8.2	8.7	8.6	12.2	11.9	11.9
Interts	27.3	37.7	0.0	36.9	52.7	46.8	46.8
$C_{10}H_{20}$	4.3	-	0.0	-	-	-	-
C2 – C4	-	-	24.4	1.4	2.0	0.0	0.0
C5 +	-	-	66.9	-	-	-	-

1) Products from the RSTOIC FT reactor which produces the "average hydrocarbon"
2) Separation of unconverted gases from the average hydrocarbon
3) Splitting of the average hydrocarbon according to ASF distribution
4) The C1 – C4 components from the split block are mixed with stream 1
5) After CO_2 removal
6) After separation of C2-C4 from the gases, ATR and mixing with the original stream
7) After H_2 removal to adjust for the H_2/CO ratio to fresh feed

3.2.4 FT gas loop for co-production cases

Since no recycling of syngas is required in co-production cases, there is no gas loop in the FT synthesis section. FT reactor is modeled similar to the liquids-only case. The mixed stream of C1 – C4 hydrocarbons and the unconverted syngas is sent through a Selexol SEP block to remove the CO_2 formed in the FT reactor. The CO_2-free gas is sent to the power block to be combusted in a gas-turbine combustion chamber.

Syngas has a much lower heating value compared to natural gas. As a result, the quantity of syngas required to obtain the same output is much higher than natural gas. Air flow through the turbine is limited by the choking flow limit and hence it cannot increase in proportion to fuel. High fuel volumes result in high temperatures leading to increased NOx emissions. As a result, it is required to dilute syngas to alter its heating value and increase the mass flow rate through the turbine. An additional advantage of dilution is that the mass flow through the turbine increases thereby increasing the power output. Dilution can be achieved either using steam or nitrogen from ASU. Since a large quantity of nitrogen is available from the air separation unit of a CTL plant, nitrogen is considered as the diluting medium here.

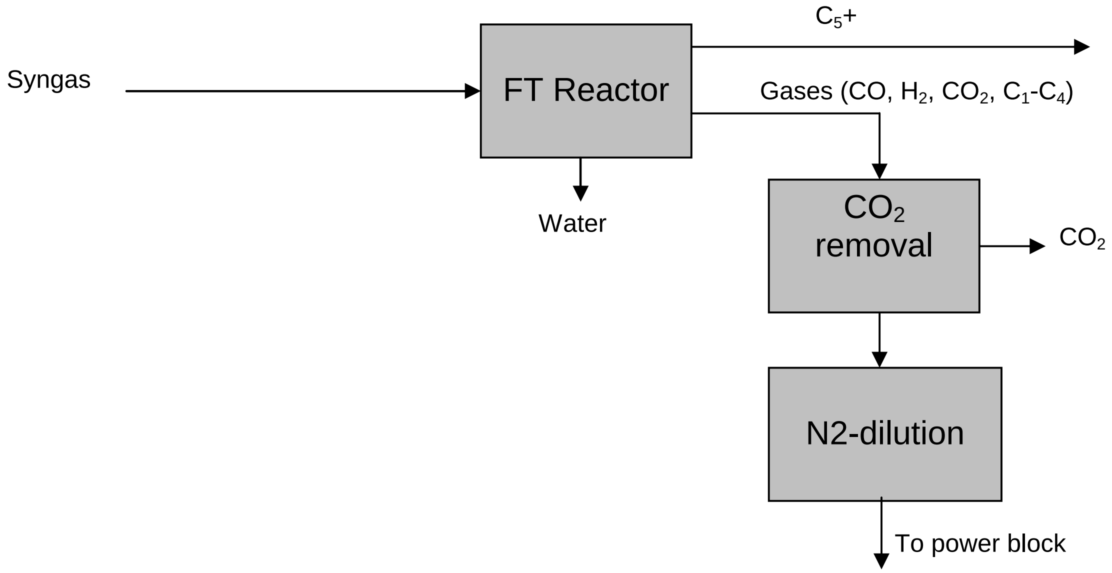


Fig 3.9: FT gas loop for co-production configuration. Unconverted syngas is diluted with N2 before being sent to the gas turbine combustion chamber

N_2-dilution

Nitrogen from ASU is mixed with the unconverted syngas from the FT section to alter the heating value. Enough nitrogen is added such that the gas entering gas turbine combustion chamber has a lower heating value between 4.5 – 4.8 MJ/m^3 [NETL 2007b]. Table # shows typical unconverted syngas composition from LTFT reactors, with the syngas generated in GE, E-Gas and Shell gasifiers using Illinois#6 coal. As was seen in the gasification section, syngas from E-Gas gasifier consists of a significant fraction of methane which comes out in the unconverted syngas. Hence, of the three cases, unconverted syngas from E-Gas gasifier has the highest heating value. Gas in the Shell case has the lowest heating value because of low percentage of H_2 and a high percentage of N_2.

Table 3.7: Typical unconverted syngas compositions from different gasifiers using Illinois#6 coal. This gas is diluted with N_2 to reduce the heating value.

	GE	E-Gas	Shell
CO	43.8	39.0	43.1
H2	43.5	29.1	29.4
CO2	0.4	0.4	0.4
C1 – C4	6.0	27.2	3.5
N2	6.0	4.2	23.6
H2O	0.4	0.2	0.1
LHV (MJ/m3)	13.97	18.85	10.9

If 4.7 MJ/m^3 is taken as the required lower heating value of the fuel gas, the volume fraction of N2 in the gas needs to be

$$x_{N2,new} = 1 - \frac{4.7}{LHV_{old}} \times \left(1 - x_{N2,old}\right)$$

The fraction of N_2 that should be in the gas turbine feed gas is roughly 68% for GE and Shell cases and 75% for the E-Gas case.

3.3 Combined Cycle Power Block

Power block consists of a gas turbine combustion chamber in which syngas is combusted in air, a gas turbine, heat recovery steam generator and a steam turbine.

The gas turbine modeled here is a GE 7FB design, which operates at a pressure ratio of 18.5 and a firing temperature of 1395 ^{o}C (2550 ^{o}F). Output from a simple cycle power plant operating on natural gas is 185 MW. Output from a combined cycle plant is 280 MW at a heat rate of 6,256 kJ/kWh (LHV).

The hot exhaust gases from the gas turbine are cooled in a heat recovery steam generator (HRSG) which generates high pressure superheated steam (9.8 MPa, 538 ^{o}C). The HRSG also reheats the intermediate pressure (2.1 MPa) steam to 538 ^{o}C.

The steam turbine operates in three stages (9.8 MPa, 2.1 MPa and 0.28 MPa). The HP steam from HRSG and that produced in the raw syngas cooling section at the gasifier exit are expanded in the first stage of steam turbine to a pressure of 2.1 MPa. This IP steam is mixed with the IP steam produced in the FT reactor and reheated in the HRSG to 538 ^{o}C before being injected to the next stage. The second stage of steam turbine expands the IP steam to 0.28 MPa which is further expanded in the LP stage to 0.005 MPa. This LP steam is sent to a condenser.

Aspen modeling of the power block

The unconverted syngas from the FT section is at a pressure close to 2.5 MPa, the operating pressure of an FT reactor. Since the gas turbine combustion chamber operates at a pressure of 1.85 MPa, syngas has to be expanded before its injection to the combustion chamber. The expander is modeled using a COMPR block with a discharge pressure of 18.5 bar. The Aspen Plus flowsheet for this section is shown in Fig 3.10.

Air at atmospheric conditions of 1 bar and 15 ^{o}C is compressed using another COMPR block. Isentropic efficiency of the compressor is determined to be 86.5% based on calibration analysis, which will be explained in the next subsection. The compressed air stream is inlet to the combustion chamber. A work stream calculates the amount of work required for compression.

The expanded syngas and compressed air streams are sent to the combustion chamber, modeled using the RSTOIC reactor block. The option of Aspen Plus generating combustion reactions is chosen. The reactor operates at 18.5 bar and 1395 ^{o}C.

The hot combustion gases are expanded in a gas turbine. The expansion involves intermediate cooling of the gases by addition of cooler compressed air so that the exhaust temperature of the gas turbine is maintained around 630 ^{o}C. But for modeling purposes, a cooler (modeled using HEATER block) is added before the gas turbine which cools the hot combustion gases enough to maintain the gas turbine exhaust temperature to 630 ^{o}C. A DesignSpec FORTRAN block calculates this temperature input to the cooler block.

Gas turbine is modeled using a COMPR block with the “turbine” option activated. The pressure ratio is set to 0.054 (1/18.5) and the isentropic efficiency is set to 87%, a value arrived at based on calibrations. A work output stream calculates the power generated in the gas turbine.

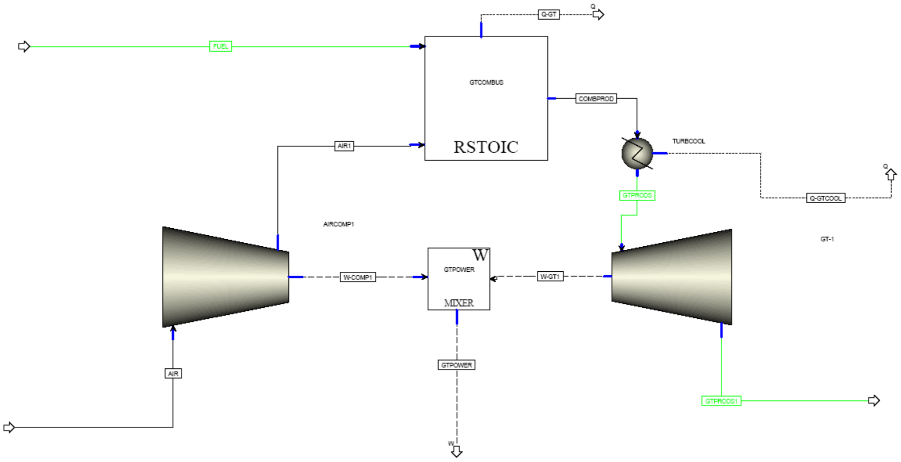


Figure 3.10: Aspen Plus block diagram of the gas turbine section

HRSG is modeled using two HEATER blocks. The first block cools the gas turbine exhaust gases to 50 ^{o}C, a temperature at which post-combustion CO_2 capture can take place. The second block heats HP feedwater to 538 ^{o}C. The two blocks are connected using a heat stream coming out of the second block into the first block. Because of this heat input, only one input parameter needs to be specified for the first block. A pressure drop of 0.1 bar is used as the input. The mass flow rate of feedwater is calculated using a DesignSpec FORTRAN block such that the exit temperature of steam is 538 ^{o}C. The feedwater at ambient pressure is pumped to 9.8 MPa using a PUMP block.

Steam turbine modeled using three COMPR blocks (in turbine mode) to replicate the HP, IP and LP sections of the actual steam turbine. HP steam from HRSG is expanded in the first turbine to 2.1 MPa. The reheater is modeled using another HEATER block with an output temperature of 538 ^{o}C. A heat output stream from this block is connected to the first HEATER block of HRSG. The IP reheated steam is expanded in the IP steam turbine to 0.28 MPa which is further expanded to 0.005 MPa in the LP steam turbine. For all three turbine sections, an isentropic efficiency of 90% is assumed. Work output streams from each COMPR block calculate the power produced by steam turbine.

The work streams from air compressor, gas turbine and the three steam turbines are added in a work MIXER block whose output work stream gives the net power produced in the power block.

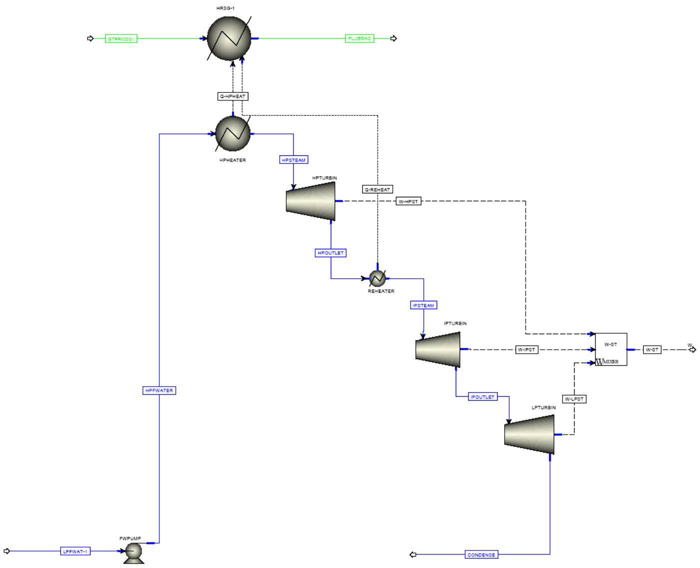


Figure 3.11: Steam cycle flowsheet in Aspen Plus.

Calibration of gas turbine model

The gas turbine model was calibrated using the GE specifications. The calibration procedure for a 7FA turbine is shown here and a similar procedure was used for the calibration of the 7FB model too.

Table 3.8 shows the design details available of a GE 7FA and 7FB turbine operating with natural gas as the fuel [Eldrid et al, 2004].

Table 3.8: Characteristics of GE 7FA and 7FB gas turbines [Eldrid et al, 2004]

	7FA	7FB
Pressure ratio	15.5	18.5
Simple cycle output (MW)	171.7	185
Combined cycle output (MW)	262.6	280.3
Simple cycle heat rate (kJ/kWh, LHV)	9,873	9,469*
Combined cycle heat rate (kJ/kWh, LHV)	6,425	6,256
Mass flow rate (kg/s)	445	448
* By calculation		

The natural gas composition and properties used for calibration are shown in table 3.9.

Table 3.9: Properties of natural gas used for gas turbine model calibration

CH4	93.9
C2H6	3.2
C3H8	0.7
C4H10	0.4
CO2	1.0
N2	0.8
LHV	47.76 MJ/kg (35 MJ/Nm3)
HHV	52.97 MJ/kg (39 MJ/Nm3)

The calibration procedure used is as follows:

- Gas turbine and air compressor are modeled in Aspen as explained before
- Fuel flow rate fixed to match the heat rate. The values are 35,500 kg/hr and 36,777 kg/hr for 7FA and 7FB respectively
- Air flow rate is varied to make the total flow of 445 kg/s for 7FA and 448 kg/s for 7FB, using the DesignSpec criterion
- Combustion products are cooled to make the gas turbine exhaust temperature 602 °C for 7FA and 631 °C for 7FB
- Compressor and turbine efficiencies are varied to match the design output and heat rate, as shown in Figs 3.12 and 3.13. Based on the figures, 86.5% and 87% are used as the values for isentropic efficiencies of compressor and turbine respectively

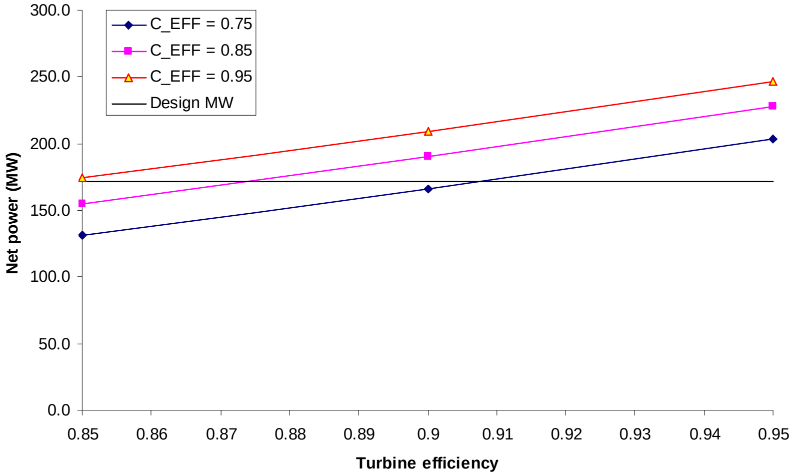


Figure 3.12: Variation of net power output with isentropic turbine efficiency in the gas turbine calibration model

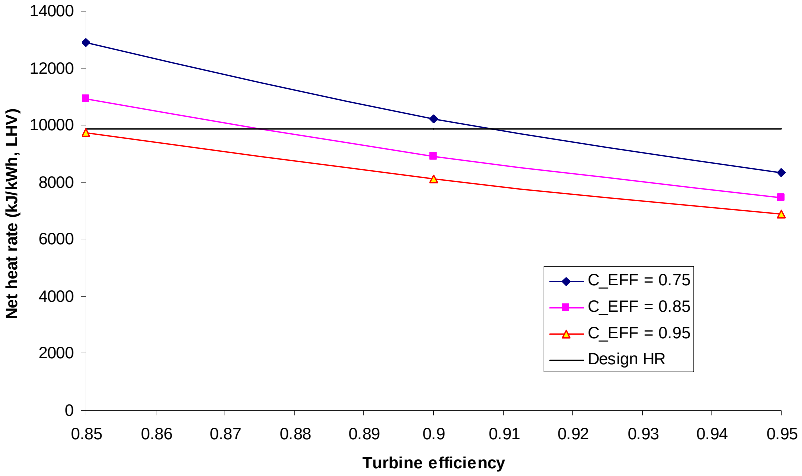


Figure 3.13: Variation of net plant heat rate (LHV) with isentropic turbine efficiency in the gas turbine calibration model

These efficiencies are used for the syngas case too. However, fuel and air flow rates in the syngas case are different. As explained before, the LHV of syngas is set to 4.7 MJ/m3 by N2-dilution. NETL baseline study [NETL 2007b] suggests that the gas turbine output should be maintained at 232 MW. The air/fuel ratio for this combination of fuel and output was found to be close to 4, on a mass basis.

In the co-production CTL case, fuel flow rate is determined by the design output of liquids. Air flow rate is specified using a DesignSpec criterion to be 4 times the fuel flow rate on a mass basis. Using the turbine and compressor efficiencies described above, the net power output of a CTL plant is calculated.

3.4 Auxiliary Power Requirement of a CTL Plant

Different components in the whole CTL plant require some amount of power input. The methodology of calculating the auxiliary power requirements of the plant is explained here. The bulk of auxiliary power is required for the air separation unit, CO_2 compression and FT block. Most of the equations are obtained from IECM documentation for IGCC power plants [IECM, 2009]. The FT plant requirements are obtained from recent literature [NETL 2007a; SSEB, 2006]. Since not all the equipment in a CTL plant has been accounted for, the actual overall auxiliary load will be higher than what is calculated here. To adjust for that, the calculated value is increased by 15%, a value consistent with similar studies.

Air Separation Unit

The auxiliary power requirement for an ASU unit has two components – main air compressor (MAC) and oxygen compression. The MAC power requirement is given by

$$W_{MAC} = (0.00174 \times \eta_{O2} + 0.1514) \times V_{O2} \text{ (kW)}$$

where, η_{O2} is the purity of oxygen stream (95% here) and V_{O2} is the volumetric flow rate of oxygen in m^3/hr.

The power required for oxygen compression is obtained as a work stream from the oxygen compressor COMPR block in the Aspen flow sheet.

Selexol CO_2 separation

The Selexol process which separates CO_2 from the syngas requires power to run components such as the recycle compressors. This includes the Selexol processes of both the gasification and FT sections. The auxiliary load is given by:

$$W_{Selexol} = 3.1742 \times \frac{\alpha^{0.745536}}{(1-\alpha)^{0.05724}} \times \frac{x_{CO2}}{p_{Syngas}^{0.49097}} \times f_{Syngas}^{0.990122} \text{ (kW)}$$

where, α is the amount of CO_2 removed (99% here), x_{CO2} is the mole fraction of CO_2 in the inlet syngas to Selexol process, p_{Syngas} is the pressure of inlet syngas (bar) and f_{Syngas} is the molar flow rate of inlet syngas (kmol/hr).

The captured CO_2 is also compressed to 140 bar. The required compression work is given by:

$$W_{Compr} = 0.26419 \times (f_{CO2} \times \alpha)^{1.001821} \times p_{final}^{0.499753} \text{ (kW)}$$

where, f_{CO2} is the molar flow rate of the CO_2 stream to be compressed (kmol/hr) and p_{final} is the final pressure (140 bar, in this case).

Fischer-Tropsch section

The cryogenic gas separation unit used to separate C2-C4 components and the syngas recycle compressors require energy input. Since a detailed process model for those two components is not done in this study, the energy requirement is estimated from literature using similar a similar gas loop [NETL 2007a]. The overall FT energy requirement is estimated on the basis of the amount of liquids produced to be 9.219 kWh/barrel.

MEA post-combustion capture

In cogeneration cases, MEA post-combustion carbon capture is used to capture CO2 from the exhaust gases of gas turbine. This technology requires a considerable amount of energy for solvent regeneration. This is calculated using the methodology described in IECM documentation and is not repeated here.

Balance of Plant

As explained before, the sum of auxiliary power requirements in the gasification and FT sections is increased by 15% to account for the equipment not modeled in this study.

Aspen Plus modeling of auxiliary power requirement

All the auxiliary power requirements are modeled using separate work streams and their values are calculated using CALCULATOR fortran blocks. All the streams are added together in a work MIXER block along with the work streams of power produced in the gasification, FT and power block sections. The output of the MIXER block is the net power output from the whole CTL plant.

3.5 Calculation Procedure and Results

The performance model developed in Aspen Plus is divided into three flowsheets for the three process sections:

- Gasification and gas cleanup section
- Fischer-Tropsch synthesis section
- Combined cycle power block

The objective of the model is to calculate the material and energy inputs and outputs of a CTL plant producing a specified quantity of liquids. For different coal types and gasifier technologies, the gasification flowsheet calculates the quantity and composition of syngas going into the FT synthesis section, power generation capacity of steam from gas cooling section, auxiliary power requirements of the gasification island, CO_2 emissions and other mass and energy balances. Using that syngas and a choice of FT reactor, the FT synthesis section flowsheet calculates the quantity of liquids produced, auxiliary power requirements of the FT section, CO_2 emissions from the FT section, power generation capacity of steam produced in the FT reactor, by-products and other mass and energy balances. For co-production cases, the FT flowsheet also calculates the composition and quantity of unconverted syngas (with N2-dilution) that can be sent to the combined cycle power block. The power block flowsheet then calculates the power produced using unconverted syngas. The results of the three flowsheets show the inputs and outputs of the overall CTL plant. The sequence of calculations has been designed as follows:

- The type of coal, gasifier technology, FT technology and plant configuration (liquids-only or co-production) are specified
- Capacity of the CTL plant is specified, ex: 50,000 barrels/day
- Using a DesignSpec criterion, the FT section flowsheet calculates the amount of syngas needed. The amount of syngas needed depends mainly on its composition.
- This quantity of syngas is used as a design criterion for the gasification flowsheet. Using a DesignSpec option, the flowsheet calculates the amount of coal required
- For co-production cases, one of the outputs of the FT flowsheet is the composition and quantity of unconverted syngas. This is input to the power block flowsheet which calculates the amount of power produced
- The results from the three flowsheets are added together to get the overall plant performance results

This section details the important mass and energy results calculated using the process performance model. The plant size considered here 50,000 barrels/day. The results are organized according to the type of Fischer-Tropsch reactor technology. Results for LTFT case are shown in table 3.10.

Table 3.10: Results from LTFT process performance model

Coal, CO2 – tonnes/day Power – MW		E-Gas		GE		Shell	
		Liq-only	Co-gem	Liq-only	Co-gen	Liq-only	Co-gen
Appalachian Medium S	Coal	19,009	25,676	16,497	20,558	15,493	19,813
	CO2 (no CCS)	28,874	49,655	24,472	35,904	22,394	34,790
	CO2 (with CCS)	43	1,717	16	875	16	1,113
	Net power (no CCS)	-	2,192	-	856	-	1,258
	Net power (with CCS)	-	1,923	-	692	-	1,113
	Efficiency(no CCS)	47.7	55.5	55.0	51.1	58.5	58.7
	Efficiency (CCS)	47.7	52.6	55.0	48.9	58.5	56.4
Illinois#6	Coal	21,658	28,812	19,049	23,571	17,980	22,986
	CO2 (no CCS)	28,364	47,609	24,420	35,392	22,533	34,942
	CO2 (with CCS)	41	1,560	14	801	16	1,111
	Net power (no CCS)	-	1,748	-	1,045	-	1,196
	Net power (with CCS)	-	1,493	-	887	-	1,030
	Efficiency (no CCS)	49.3	53.2	56.1	55.2	59.4	58.8
	Efficiency (CCS)	49.3	50.3	56.1	53.0	59.4	56.4
Wyoming PRB	Coal	28,919	37,491	26,803	32,803	25,551	32,649
	CO2 (no CCS)	29,555	46,462	27,302	38,227	25,655	38,898
	CO2 (with CCS)	32	1,254	13	671	16	1,107
	Net power (no CCS)	-	1,534	-	786	-	979
	Net power (with CCS)	-	1,295	-	627	-	802
	Efficiency (no CCS)	49.8	52.6	53.8	50.0	56.4	52.8
	Efficiency (CCS)	49.8	49.8	53.8	47.8	56.4	50.4
ND lignite	Coal	37,155	46,335	37,273	44,105	35,697	45,610
	CO2 (no CCS)	27,033	39,826	27,944	36,948	26,382	39,816
	CO2 (with CCS)	23	825	12	454	16	1,106
	Net power (no CCS)	-	1,402	-	652.4	-	982
	Net power (with CCS)	-	1,211	-	506	-	803
	Efficiency (no CCS)	53.7	57.2	53.6	49.6	55.9	52.4
	Efficiency (CCS)	53.7	54.7	53.6	47.6	55.9	50.0

Chapter 4: Process Cost Model of CTL Plants

The performance models described in the previous chapter calculate the mass and energy flows within the CTL plant. Those results can be used to estimate the fixed and variable costs of the whole plant. Estimation of costs is important in order to make a decision about whether a plant is economically feasible under a given set of circumstances. This chapter describes the methodology followed for estimating the cost of a CTL plant. A code is written using MATLAB to calculate the costs.

4.1 Cost Estimation Methodology

The procedure used here follows the EPRI TAG guidelines for cost estimation of power plants [EPRI, 1986]. Fixed and variable costs are estimated at a component level and then added together to get the overall cost of the plant. For example, in a CTL plant, fixed and variable costs are estimated for major components such as gasifier, syngas cooling, and FT reactor and so on and then all of these are added to get the cost of the whole CTL plant. The terms used are explained below.

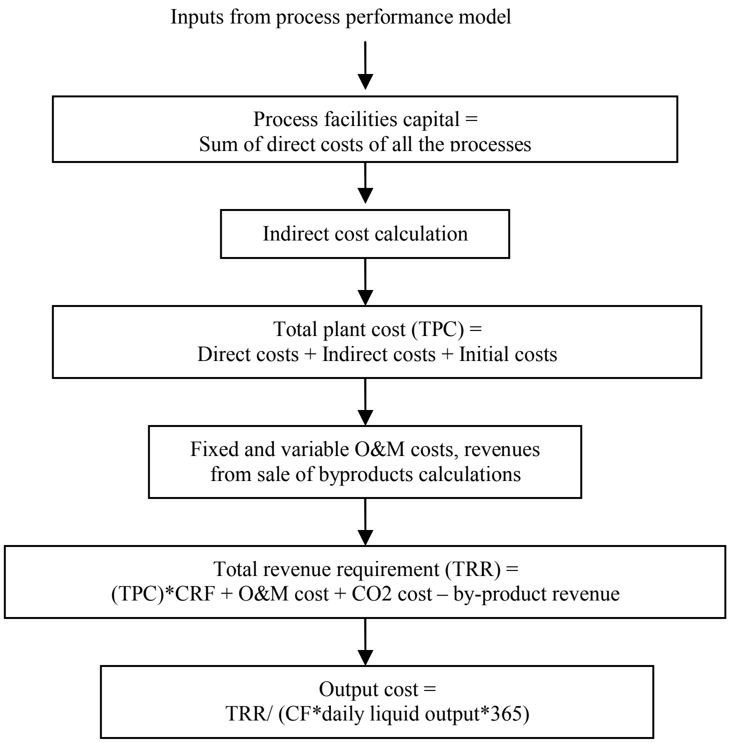


Fig 4.1: Methodology of cost assessment [EPRI, 1986]

4.1.1 Direct Capital Cost (DC)

The direct cost of a component is the capital required to build that component and install it in the plant. Ideally, these costs are known from the equipment manufacturer but since most of the data is confidential, it is difficult to obtain these values for academic analyses. Therefore, in most cases, direct costs are estimated from data available in open literature.

4.1.2 Process Facilities Capital (PFC)

Process facilities capital is the sum of direct costs of all the components in a process plant. This gives the direct capital cost required to build the overall plant.

4.1.3 Indirect Capital Cost (IC)

Besides the construction cost of each component, there are also indirect costs that need to be applied. Usually, these are applied as percentages of PFC. Indirect costs are divided into the following five categories

- General facilities capital (GFC)
- Engineering and home office overhead (EHO)
- Project contingency
- Process contingency
- Royalty fees

General facilities capital (GFC) is the capital required for the construction of general facilities like buildings, roads, shops etc. This cost is usually between 5 – 20% of PFC.

Engineering and home office overhead is typically between 7 – 15% of PFC

Project contingency costs are intended to factor in the uncertainty involved in the cost estimates and process contingency costs cover the uncertainty associated with the technical performance of the process. When a project is designed, all the equipment that is required is not immediately clear. Additional equipment will be necessary when the actual plant is built. To cover for this kind of uncertainty, a project contingency factor is used. The more simplified a cost estimate is, the higher the project contingency should be. When new technologies are operated, there is an uncertainty associated with its technical performance because of lack of prior experience. A process contingency factor is used to accommodate this uncertainty. The newer a technology, higher is the process contingency.

Royalty charges are sometimes included in the indirect capital costs and sometimes as different from capital costs. Here, they are used along with other indirect costs.

4.1.4 Total Plant Cost (TPC)

The sum of direct and indirect capital costs is called as the total plant cost.

4.1.5 Total Capital Requirement (TCR)

Total capital requirement includes all the capital necessary for a particular project. It consists of the following components, besides the total plant cost:

- Total plant investment including the allowance for funds used during construction or interest during construction
- Owner costs including preproduction costs, inventory capital and initial cost of catalysts and chemicals

In this study, all the capital costs are assumed to be overnight capital costs. Hence, interest during construction is neglected. Wherever possible, owner costs are included.

Pre-production costs are those which account for operator training and costs accrued during start-up of the plant. Typically, these are taken as equivalent to one month of fixed operating costs. Post-production cost is taken as equivalent to one month of variable operating costs.

Inventory capital is the cost of inventories such as fuels and other consumables. This is taken as 0.5% of TPC.

Initial costs of catalysts and chemicals are to account for the initial loading of catalysts and chemicals in certain equipment. For example, a certain quantity of Selexol solvent is loaded into the absorber vessel prior to its start-up. Wherever possible, these costs are estimated from open literature.

4.1.6 Operating and Maintenance Costs (O&M)

Operating and maintenance costs are usually estimated for a year of operation. These can be divided into fixed O&M and variable O&M costs.

Fixed O&M costs include operating labor, annual maintenance costs and administrative costs. Operating labor costs are calculated by multiplying the labor charge ($33/day) with the number of operating labor present on the site in a year. Annual maintenance cost is usually specified as a percentage (usually 2%) of TPC. Administrative costs include operating labor costs and maintenance labor costs. Maintenance labor costs are specified as a percentage of annual maintenance cost. Administrative costs are typically specified as 30% of operating labor and maintenance labor costs.

Variable O&M costs cover the cost of consumables such as coal, solvents, chemicals, catalysts and electricity. Wherever the requirement of consumables is not estimated by the process model, these costs are estimated from open literature.

4.1.7 By-Product Credits

The by-products from the plant such as sulfur, slag and electricity can be sold at market prices to get additional revenues. In this study, electricity from a co-production plant is assumed to be sold at market prices to the grid. In a liquids-only configuration, it is assumed that there is no excess electricity to be sold. Sulfur and slag are not given any value.

4.1.8 CO_2 Constraints

Depending on the existence of regulations, CO_2 emissions from the plant can be taxed. A carbon price is given to every ton of CO_2 emitted and acts as additional operating cost of the plant. Cases with and without CO_2 constraints are considered here.

4.1.9 Total Revenue Requirement (TRR)

To calculate the total revenue requirement of the plant, capital costs need to be levelized for the entire life of plant. The levelization factor is called a capital recovery factor (CRF), which depends on the discount rate used and the plant life. Multiplying the capital cost with CRF annualizes the capital cost. This can then be added to annual O&M and CO_2 costs to get the annualized costs. When by-product credits are subtracted from this number, the total revenue requirement of the plant is obtained.

4.1.10 Capacity Factor

The capacity factor (CF) of a plant denotes the equivalent amount of time a year when the plant operates at its full capacity. For example, if CF is 80%, that means that the plant effectively operates at its full capacity for 80% of 365 days. This factor is used to calculate the annual production of output which is liquids in the case of a CTL plant.

4.1.11 Cost of Liquid Product

Cost of product liquid is obtained by dividing TRR by the annual production of output liquids. This is expressed in the units of $/barrel. If this cost is lower than the market price of crude oil, then the CTL plant will be economically viable.

4.2 CTL Component Costs

The following equations were used to calculate direct costs of components in the gasification and power islands. All costs are reported in constant 2007 1,000 US dollars. In all the equations, $N_{O,i}$ means number of operating trains and $N_{T,i}$ means the total number of trains for component 'i'.

4.2.1 Coal Handling

Coal handling costs depend on the mass flow of coal.

$$DC_{CH} = N_{T,CH} \times 11.995 \times \left(\frac{m_{coal\,input}}{N_{O,CH}} \right)$$

Maximum train size for coal handling section is 22,750 tonnes/day. No spare trains are assumed for coal handling.

4.2.2 Air Separation Unit

The capital cost of ASU depends on the flow rate of product oxygen and the purity of that stream.

$$DC_{ASU} = \frac{41.43 \times N_{T,ASU} \times (T_a)^{0.067}}{(1-\eta_{ASU})^{0.073}} \times \left[\frac{M_{Oxygen}}{N_{O,ASU}} \right]^{0.852}$$

In this study, 95% is assumed to be the purity of oxygen in all cases. Maximum train size of an ASU is 7,730 kmol/hr. Since ASU is a high-capital equipment, no spare trains are assumed.

4.2.3 Gasification Section

The cost of a gasification section involves that of the gasifier vessel as well as the hot syngas radiant cooler vessel. The costs are estimated differently for different gasifier technologies, from recent literature. The scaling variable is the as-received coal flow rate. For quench gasifiers,

$$DC_G = N_{T,G} \times 21.12 \times \left(\frac{m_{coal\,input}}{N_{O.G}} \right)^{0.943}$$

For GE radiant gasifier,

$$DC_G = N_{T,G} \times 43.00 \times \left(\frac{m_{coal\,input}}{N_{O.G}} \right)^{0.943}$$

For E-Gas gasifier,

$$DC_G = N_{T,G} \times 40.07 \times \left(\frac{m_{coal\,input}}{N_{O.G}} \right)^{0.943}$$

For Shell gasifier,

$$DC_G = N_{T,G} \times 55.23 \times \left(\frac{m_{coal\,input}}{N_{O.G}} \right)^{0.943}$$

The maximum train size for the quench, GE and E-Gas cases is 2,903 tonnes/day while it is 2,772 tonnes/day for Shell. Since this is very important equipment in the whole plant, one spare train is assumed.

4.2.4 Low Temperature Gas Cooling

After the gases from the gasifier are cooled first in a radiant cooler, they are further cooled in a low temperature gas cooling section, which includes a series of heat exchangers. The cost depends on the mass flow rate of syngas flowing through it.

$$DC_{LT} = 0.0496 \times N_{O,LT} \times \left[\frac{m_{syngas,in}}{N_{O,LT}} \right]^{1.0}$$

The maximum train size is 590,900 kg/hr of syngas. One spare train is assumed for this section.

4.2.5 First-stage Selexol – H_2S removal

The first stage of a Selexol process removes H2S from the syngas stream. Its cost depends on the flow rate of syngas and H2S-removal efficiency.

$$DC_{SXL} = \frac{0.876 \times N_{T,S}}{\left(1-\eta_S\right)^{0.059}} \times \left[\frac{M_{Syngas,in}}{N_{O,S}} \right]^{0.980}$$

The maximum train size is 30,590 kmol/hr of syngas.

Initial solvent loading (kg) in the Selexol process is estimated as

$$m_{Selexol} = N_{T,S} \times \left(-11455 + 15.77 \times \frac{M_{H2S} \big/ N_{O,S}}{x_{H2S}^{1.04}} \right)$$

Annual make-up solvent (kg/yr) is given by

$$m_{Selexol} = N_{O,S} \times \left(-159.1 + 1.58 \times \frac{M_{Syngas,in}}{N_{O,S}} \right)$$

For operating cost calculations, this equation is multiplied by the plant capacity factor. The price of Selexol solvent is \$3.3/kg [NETL baseline].

4.2.6 Second-stage Selexol – CO_2 removal

The cost model for the second-stage Selexol removal is more detailed, including components such as absorber tower, slump tank, power recovery turbine and recycle compressor.

The overall methodology is explained elsewhere [Chen, 2005] and is not repeated here. The cost equations are given below:

Absorption column (atm, kmol/hr)

$$DC_{absorber} = N_{T,Abs} \times 1.33 \times \left[-1375.356 + 16.536 \times p_{abs,i} + 0.1404 \times \left(M_{solvent} + M_{syngas} \right) \right]$$

Power recovery turbine

$$DC_{turb} = 1.33 \times (219.086 + 0.1085 \times (kW)_{tur} + 0.0201 \times p_{tur,o}^{2})$$

Slump tank

$$DC_{slumpt} = 2.667 \times N_{T,Slump} \times \left[\frac{m_{solvent,in}}{N_{O,Slump}} \right]^{0.7446}$$

Recycle compressor

$$DC_{rec} = 5.598 \times \left(kW \right)_{RC}^{0.7784}$$

Flash tank (kg/s)

$$DC_{flash} = 1.3077 \times N_{T,flash} \times \left[\frac{m_{solvent,in}}{N_{O,flash}} \right]^{0.8005}$$

Selexol pump

$$DC_{pump} = 2.016 \times \left(kW \right)_{pump}^{0.7164}$$

Refrigeration

$$DC_{ref} = 1.3325 \times N_{T,refg} \times \left[16.4796 \left(\frac{m_{solvent}}{N_{O,refg}} \right)^{0.3618} \times \left(\Delta T_{solvent} \right)^{0.4064} \right]$$

4.2.6 Sulfur Recovery – Claus plant

The capital cost depends on the mass flow of sulfur.

$$DC_{Claus} = 15.681 \times N_{T,C} \times \left[\frac{m_{Sulfur,out}}{N_{O,S}} \right]^{0.668}$$

Initial loading of catalyst (kg) is given by

$$m_{claus} = N_{T,C} \times 0.0111 \times \left[\frac{M_{Sulfur,out}}{N_{O,S}} \right]$$

Make-up catalyst (kg/year) is given by

$$m_{claus} = N_{O,C} \times 0.0211 \times \left[\frac{M_{Sulfur,out}}{N_{O,S}} \right]$$

For operating cost calculations, this equation is multiplied by the plant capacity factor. The price of Claus catalyst is \$603.9/tonne.

4.2.7 Tail gas treatment – Beavon Stretford

This cost also depends on the amount of sulfur produced.

$$DC_{BS} = 84.80 + 161.67 \times N_{T,BS} \times \left[\frac{M_{Sulfur,out}}{N_{O,BS}} \right]^{0.645}$$

Initial loading cost (\$) of B-S chemical is given by

$$C_{BS} = 188.76 \times m_{Sulfur,BS}$$

Make-up cost (\$/year) of B-S chemical is

$$C_{BS} = 374 \times m_{Sulfur,BS}$$

4.2.8 CO_2-Compression

CO_2 compression costs are estimated based on the power requirements of compressors.

$$DC_{CO2} = 21.014 \times (kW)^{0.64}$$

4.2.9 Gas Turbine

Capital cost of a GE 7FB gas turbine is estimated from recent literature [NETL 2007b] based on the power output of the whole gas turbine section.

$$DC_{GT} = 194.393 \times MW_{GT}$$

4.2.10 Heat Recovery Steam Generator

HRSG costs depend on the pressure level of high pressure steam and the steam flow rate.

$$1057307 \times \left[\frac{P_{HP\,steam}}{1500} \right]^{1.526} \times \left[m_{HP\,steam} / 600000 \right]^{0.242}$$

4.2.11 Steam Turbine

Cost of steam turbine is also scaled based on the power output.

$$DC_{ST} = 211.071 \times MW_{ST}$$

4.2.12 CO_2 Transport and Storage

For this study, the pipeline infrastructure for CO_2 transport and the geological sequestration site are considered to be beyond the plant boundary. It is assumed that the compressed CO_2 can be disposed by paying for its transport and storage. Hence, CO_2 transport and storage costs occur as variable O&M in the cost calculations. The pricing used is \$5/tonne CO_2 each for transport and storage and a fee of \$0.25/tonne CO_2 for storage monitoring.

4.2.13 Fischer-Tropsch Section

The cost data for FT processes are not as widely available as for other technologies. Here, cost data are taken predominantly from four sources (Mitre, 1990; Bechtel, 1993; NETL, 2006; SSEB, 2006). SSEB report also contains FT cost data for co-production cases. Two reports include detailed cost information for all the components in a FT process, including the recycle loop and refining. The NETL report cites Bechtel report as the original source of the process model. But the cost data do not match when adjusted to 2007 dollars, as will be shown below. For comparison, cost data for the whole FT process is shown in table 4.1.

Table 4.1: Capital costs of FT sections reported in various sources

Source	Liquids output (bbl/day)	Capital cost ($M, 2007)
Gray and Tomlinson, 1990	71,384	1,541
Bechtel, 1990	20,000	174
DoE, 1998	48,629	731
NETL, 2007a	49,992	439
SSEB, 2006	10,000	100
SSEB, 2006	30,000	273
SSEB, 2006	60,000	493

The best fit linear regression for liquids-only cases was obtained when the Gray and Tomlinson (1990) and DoE (1998) values were removed. The linear regression is shown in Fig 4.2. The cost-estimation equation is given in terms of barrels/day of liquids output and includes all components of the FT gas loop such as the FT reactor, hydrocarbon recovery unit, hydrogen recovery, auto thermal reactors and recycle gas compressors.

$$DC_{FT} = 8.6 \times (barrels / day)$$

The FT section cost for co-production cases is estimated from two data points contained in the SSEB report (2006) and is given by

$$DC_{FT} = 9.2 \times (barrels / day)$$

The FT section cost of liquids-only cases is lower than the co-production case because of the higher efficiency that can be obtained by recycling of unconverted syngas.

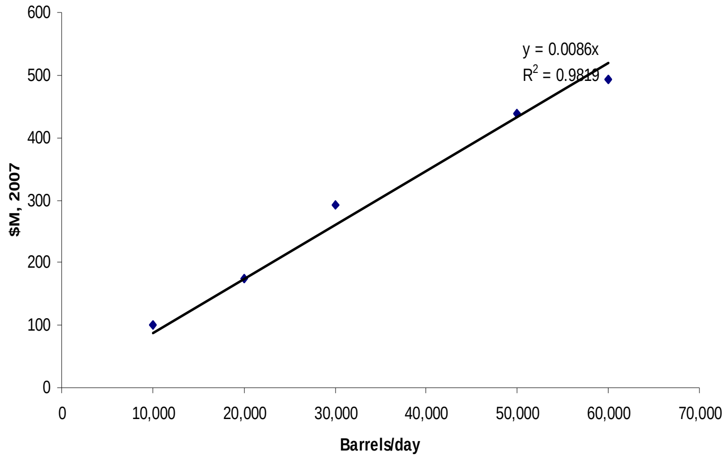


Figure 4.2: Cost estimation for FT synthesis section

It is difficult to obtain cost data for HTFT reactors from open literature. It is assumed here that the same equations can be used for HTFT cases too. If there is any cost advantage for HTFT reactors owing to their higher conversion efficiencies, it will be shown on the cost of rest of the CTL plant, because lesser amount of syngas is needed to produce the same amount of liquids.

FT catalyst costs

Only one study could be found which contained details about the initial loading of FT catalyst and annual make-up catalyst required [Bectel, 1990]. The plant capacity is 20,000 barrels/day, uses 6 reactors with 51,907.5 kg of catalyst/reactor. Catalyst life was assumed to be 60 days. Annual variable cost for FT catalyst was reported as \$8.6 million in 1990 values. When inflated to 2007 values, this cost would be \$13.48 million/year. By similar calculation, the initial catalyst loading would be \$2.4 million (2007). The following relations can be derived for initial loading and annual make-up catalyst

Initial loading (\$)

$$C_{FT,initial} = 120 \times (barrels / day)$$

Make-up catalyst cost ($/year)

$$C_{FT,makeup} = 674 \times (barrels / day)$$

4.3 Uncertainty Analysis

The cost models are equipped with probabilistic uncertainty analysis capability. All the cost-estimation equations shown above give a deterministic value of the total plant costs. However, there is inherent uncertainty and/or variability involved in almost all the cost parameters, which has to be captured to get a comprehensive picture of the costs. In this study, uncertainty is modeled using Monte Carlo simulation technique [Morgan and Henrion, 1990]. The Matlab code generates random numbers between 0 and 1 to denote a cumulative probability. Each parameter is given a range of values and a probability distribution such as triangular or uniform. Using the random number as the probability, costs are calculated using the inverse cumulative distribution function for that particular distribution. The cost model performs 20,000 simulations for each case by generating 20,000 random numbers for probability.

The ranges and probability distributions given to each cost parameter are shown in Table #. The assumptions and data leading to these ranges are as follows:

- Data about the variability or uncertainty in direct capital costs are unavailable. So a range of +/- 25% of the deterministic value was used. This amount of uncertainty is common in cost estimation [NETL 2007b]
- For indirect capital cost components, standard ranges are used [Chen, 2005]. Process contingency is used to cover up for the lack of experience in the technology in

question. Since this is a relatively new technology with no operational experience, at least in the US, process contingency was varied over a wider range of 10 – 40 %.

- A range of 5 – 20% for CRF covers a range of discount rates, from as low as 3% to as high as 15%, and plant life of 10 to 50 years. Since it is most likely to have private investment in this kind of a facility, for which CRF is usually about 15%, a triangular distribution with most likely probability of 15% is used.
- Coal prices since 1950 [EIA, 2009] show a very wide variation ranging from \$20 to \$100/tonne for bituminous coals. For sub-bituminous coal and lignite, the prices have been fairly stable. The range for low quality coals is assumed to be between \$10 - \$20/tonne. Since there was no set pattern in the change of coal price, a uniform distribution is used. The current price of coal is about \$60/tonne for Illinois#6 and \$15/tonne for low quality coals, which has been used for base-case calculations.
- A CTL plant is a combination of a process plant using coal and a petroleum refinery. The capacity factor of petroleum refineries in US has been very high (about 90%) over the past two decades [EIA, 2009]. Since there are other components like gasifiers etc in the plant, unlike a petroleum refinery, a slightly low capacity factor of 85% is used for base case. The uncertainty in capacity factor is denoted by a triangular distribution with minimum, most likely and maximum values of 75%, 85% and 95% respectively.
- Operating costs of CCS vary over a wide range depending on the amount of CO_2, size of pipelines used, distance transported and the type of storage site. The ranges are shown in table 4.2 [IPCC, 2005]. The values used for deterministic calculations are approximate averages of these costs.

Table 4.2: Ranges used for uncertainty analysis

Input	Base case value	Uncertainty/Sensitivity range	
Direct capital cost (DC)	Calculated by substituting the outputs of performance model into the equations shown in section 4.2	+/- 25% of base case, ***Triangular [-25%, base case, 25%]***	
General facilities capital (GFC)	15% of DC	10 – 20%	Indirect capital cost – ***Triangular*** ***[40, 75, 100***]
Engg & home office (EHO)	10% of DC	7 – 12%	
Process contingency	25% of DC	10 – 40%	
Project contingency	15% of DC	10 – 20%	
Royalty charges	10% of DC	7 – 12%	
Capital recovery factor (CRF) used to annualize capital costs	0.15	5% - 20% (depending on discount rate and plant life) ***Triangular [0.05, 0.15, 0.2]***	
Coal price	\$60/tonne – Ill#6 \$15/tonne – PRB, lignite	\$20 – 100 /tonne Ill#6, \$10-20, PRB, lignite ***Uniform [20, 60]***	
Capacity factor (fraction of maximum operation per year)	0.85	0.75 – 0.95 ***Triangular [0.75, 0.85, 0.95]***	
CO_2 transport cost	\$ 5 /tonne CO_2	\$1.3 – 10.4 /tonne CO_2 ***Uniform [1.3, 10.4]***	CCS O&M costs, from IPCC report [ref 27]
CO_2 storage cost	\$ 5 / tonne CO_2	\$ 0.65 – 10.4 /tonne CO_2 ***Uniform [0.65, 10.4]***	
Sequestration monitoring cost	\$ 0.25 /tonne CO_2	\$ 0.13 – 0.39 / tonne CO_2 ***Uniform [0.13, 0.39]***	

4.4 Results from Process Cost Model

The values of variables required for calculating costs of individual components are obtained from the process performance model. Those form inputs to the cost model which calculates the capital and O&M costs and the cost of liquid product. Table 4.3 shows important cost results for different combinations of coal type and gasifier technologies. The capacity of the plant is 50,000 barrels/day. The Matlab code used for these calculations is shown in Appendix A2 for liquids-only, co-production and uncertainty analysis.

Table 4.3: Cost results for a 50,000 barrels/day CTL plant

Cap cost - $/barrel/day Liq. prod. cost - $/barrel CO2 price - $25/tonne			E-Gas		GE		Shell	
			Liq-only	Co-gen	Liq-only	Co-gen	Liq-only	Co-gen
Appalachian Medium S	No CCS	Cap cost	93,078	119,668	86,652	144,604	81,309	114,357
		Liq. prod cost (no CO2 price)	91.8	76	83.3	48.0	78.4	56.1
		Liq.prod cost (CO2 price)	106.2	93.8	95.6	72.8	89.6	73.4
	CCS	Cap cost	94,376	133,099	87,821	177,020	82,391	130,409
		Liq. prod cost (no CO2 price)	98.4	98	89.0	89.4	83.6	80.1
		Liq.prod cost (CO2 price)	98.4	98.8	89.0	90.2	83.6	80.7
Illinois#6	No CCS	Cap cost	98,001	126,205	91,897	149,903	86,127	121,918
		Liq. prod cost (no CO2 price)	82.5	59	76.1	50.8	71.6	50.2
		Liq.prod cost (CO2 price)	96.6	76.7	88.3	74.6	82.9	67.7
	CCS	Cap cost	99,284	138,354	93,064	179,729	87,211	137,953
		Liq. prod cost (no CO2 price)	89.0	80	81.7	89.6	76.9	74.3
		Liq.prod cost (CO2 price)	89.0	80.8	81.7	90.4	76.9	74.8
Wyoming PRB	No CCS	Cap cost	110,209	145,558	106,643	164,425	101,082	143,866
		Liq. prod cost (no CO2 price)	71.7	62	69.2	44.8	65.8	53.6
		Liq.prod cost (CO2 price)	86.5	81.0	82.8	68.0	78.6	73.0
	CCS	Cap cost	111,529	155,816	107,900	188,801	102,265	160,003
		Liq. prod cost (no CO2 price)	78.5	83	75.5	79.3	71.7	78.9
		Liq.prod cost (CO2 price)	78.5	83.1	75.5	79.9	71.7	79.5
ND lignite	No CCS	Cap cost	127,224	172,085	129,022	180,584	122,296	175,050
		Liq. prod cost (no CO2 price)	83.4	84	84.5	60.4	80.4	73.4
		Liq.prod cost (CO2 price)	96.9	102.5	98.4	80.3	93.5	93.3
	CCS	Cap cost	128,472	179,474	130,299	196,706	123,499	191,192
		Liq. prod cost (no CO2 price)	89.6	102	90.9	86.5	86.4	99.0
		Liq.prod cost (CO2 price)	89.6	102.4	90.9	87.0	86.4	99.6

Chapter 5: Large Scale Impact Assessment Model

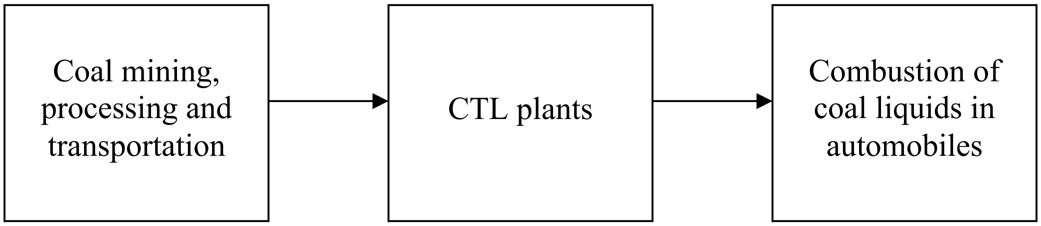
Using coal liquids in place of conventional liquid fuels helps in reducing petroleum imports and thereby increases the energy security of the country. However, when a large number of CTL plants are built, there will be associated impacts on the country's coal consumption, CO_2 emissions and land use. Before devising policies about the use of coal liquids, it is important to understand the magnitude of those impacts. This chapter describes simple methodologies to estimate the increase in coal consumption, life cycle CO_2 emissions, water use and land use of large-scale implementation of CTL.

5.1 Estimation of Life Cycle CO_2 Emissions

Coal liquids are ultra clean in terms of criteria air pollutants. When utilized as mother fuels, there is evidence that FT liquids, particularly FT diesel, burn more efficiently than conventional diesel, in terms of brake specific fuel consumption (g/kWh). This may result in lower CO_2 emissions from FT diesel compared to conventional diesel, when combusted in an automobile [Norton et al, 1998]. However, when the life cycle is considered, coal liquids will have a much higher footprint because of the CO_2 emissions from the CTL plant. Hence, it is important to understand the magnitude of life cycle CO_2 emissions.

Here, a simplified life cycle assessment of coal liquids is done. The life cycle of coal liquids involve the following stages:

- Pre-production – coal mining, processing and transportation
- Production – CTL plants
- Post-production – combustion of liquids in automobiles



Data for pre-production and post-production stages is obtained from literature (Jaramillo, 2007). The values and their basis are explained below.

5.1.1 Pre-production stage

The pre-production stage consists of the mining and processing of coal and its transport to the plant site. Coal mining and processing requires combustion of fossil fuels and hence there are greenhouse gas emissions associated with it. Coal transportation to the plant site may take place through trains, barges or trucks, which require further burning of fossil fuels. The GHG emissions associated with all these processes are estimated to be in the range of 8.2 – 16.4 lb CO_2 equivalent/million BTU of coal. The national weighted average heat content of coal used for this calculation was 10,520 BTU/lb. Based on these numbers, the CO_2 equivalent emissions of the pre-production stage can be estimated to be in the range of 0.086 – 0.173 kg CO_2/kg coal.

For this analysis, the average of the range (0.129 kg CO_2/kg coal) is used. since this number was arrived at based on US average values, it is assumed to be the same for all the coal types.

Table 5.1 shows the quantity of coal required per barrel of liquid output from CTL plants of liquids-only and co-production configurations using different gasifier types. These values are multiplied by 0.129 to give the pre-production CO2 emissions per barrel of liquid (shown in table 5.2)

Table 5.1: Specific coal requirements for different coals and technologies (kg/barrel)

	GE		EGas		Shell	
	Liq-only	Co-prod	Liq-only	Co-prod	Liq-only	Co-prod
Illinois#6	381	471	433	576	360	460
Wyoming PRB	536	656	578	750	511	653
ND Lignite	745	882	743	927	714	912

Table 5.2: Specific pre-production stage CO2 emissions from different coal and technology combinations (kg/barrel)

	GE		EGas		Shell	
	Liq-only	Co-prod	Liq-only	Co-prod	Liq-only	Co-prod
Illinois#6	49	61	56	75	47	59
Wyoming PRB	69	85	75	97	66	84
ND Lignite	96	114	96	120	92	118

5.1.2 Production stage

Table 5.3 shows the CO_2 emissions associated with different coal types and gasifier technologies at the CTL plant level. These values, obtained from the performance model described in chapter 3, are taken to be the CO_2 emissions during the production stage of coal liquids. Emissions because of the fossil energy used in construction of the plant are not taken into account.

Table 5.3: Production stage CO_2 emission factors (kg/barrel)

		GE		EGas		Shell	
		Liq-only	Co-prod	Liq-only	Co-prod	Liq-only	Co-prod
Illinois#6	No CCS	494	708	583	952	457	699
	CCS	6	16	16	31	6	22
Wyoming PRB	No CCS	551	765	603	929	519	778
	CCS	5	13	13	25	6	22
ND Lignite	No CCS	563	739	549	797	534	796
	CCS	5	9	9	478	6	22

5.1.2 Post-production stage

In this study, the liquid product from the FT reactor was modeled as containing only olefins, whereas in reality there are other types of hydrocarbons, as explained in chapter 2. The refined product which goes into automobiles has a different composition, estimating which is beyond the scope of this thesis. But literature suggests that FT liquids produced from coal have a carbon content of 44.2 lb carbon/million BTU and a heat content of 0.11 million BTU/gallon [Marano and Ciferno, 2001; Jaramillo, 2007]. Using these values, the downstream emissions of coal liquids can be estimated to be 341 kg CO_2/barrel. Emissions associated with transportation of liquids from the CTL plant to fuel stations are neglected.

5.1.4 Life Cycle Emissions

CO_2 emissions from coal liquids over their life can be obtained by adding the emissions from different stages of the life cycle. The results for different coals and gasifier technologies are shown in table 5.4. These factors are used when assessing the large scale impacts of coal liquids.

Table 5.4: Life cycle emissions of CO_2 (kg/barrel)

		GE		EGas		Shell	
		Liq-only	Co-prod	Liq-only	Co-prod	Liq-only	Co-prod
Illinois#6	No CCS	884	1110	980	1368	844	1099
	CCS	396	418	414	447	394	423
Wyoming PRB	No CCS	962	1191	1019	1367	926	1204
	CCS	416	439	429	463	414	448
ND Lignite	No CCS	1000	1194	987	1258	967	1256
	CCS	442	463	446	478	440	481

5.2 Land Use Assessment

With popular opposition to the building of new coal power plants, land use assessment is an important factor in the implementation of large scale CTL plants. There have been few studies estimating the land required by CTL plants. NETL report on CTL plants [NETL, 2007a] assumes a site of 300 acres for a 50,000 barrels/day plant utilizing approximately 24 kilo tonnes/day of coal. However, this number is misleading because another NETL study on baseline coal power plants [NETL, 2007b] assumes the same land use for a 600 MW IGCC plant using 5 kilo tonnes/day of coal. Since data is rare, in this thesis, a rough estimation of land use is obtained by extrapolating data from coal power plants.

It is likely that the physical size of a plant is proportional to the quantity of coal consumed. However, data from a utility company holding coal fired power plants of different capacities does not provide any correlation between the electrical capacity of the plant and its physical size [Tri-state, 2009]. For example, a 1274 MW power plant takes up 1,120 acres while a 1,800 MW plant takes up only 521 acres.

A DoE document suggests a size of 19 acres per MW for coal power plants [EERE, 2006]. Another study on life-cycle land-use assessment estimates that a 1000MW plant in the US requires between 330 and 1000 acres of land. On an average, a 1000 MW power plant has a direct land transformation of 500 acres [Fthenakis and Kim, 2009]. It can be assumed that IGCC and PC power plants of similar gross sizes and pollution control devices require the same amount of land. A CTL plant can be considered as an extension of IGCC power plant but CTL requires additional land because of the FT and refinery sections. If allocation is made on the basis of cost distribution, gasification and gas clean up section accounts for about 60% of the plant capital cost. So, a rough estimate of land use for a CTL plant is to multiply the land use of IGCC by 1.5. Scaling can be done based on coal flow rate. For a thermal efficiency of 35%, using the US average coal heat content of 24.5 MJ/kg (10,520 BTU/lb), the coal flow rate for a 1000 MW plant would be roughly 10,000 tonnes/day. So, direct land use of a power plant can be scaled as 0.05 acres/tonnes/day of coal and for a CTL plant would be 0.075 acres/tonnes/day. Based on this, table 5.5 shows the size of land per daily barrel of liquids output for different coals and gasification technologies.

Table 5.5: Land use factors for different coal types and technologies (acres/daily barrel)

	GE		EGas		Shell	
	Liq-only	Co-prod	Liq-only	Co-prod	Liq-only	Co-prod
Illinois#6	0.029	0.035	0.032	0.043	0.027	0.034
Wyoming PRB	0.040	0.049	0.043	0.056	0.038	0.049
ND Lignite	0.056	0.066	0.056	0.070	0.054	0.068

5.3 Water Use Assessment

In a typical power plant, daily fresh water is required for cooling tower usage. Water used in other process areas is usually recycled. 85% of fresh water usage is for cooling tower usage. The main parameter which determines the water requirement is steam flow rate, which in turn is linked to steam turbine output. For IGCC power plants, based on data from literature, the average water consumption per unit of steam power output can be estimated as 2.90 m^3/MWh [NETL 2007b]. This value can be used for a CTL plant also, since most of the process areas are similar to IGCC power plants. Water is a product in the FT reactions. It is estimated that about 1.3 tonnes of water is produced per tonne of hydrocarbon output. This roughly translates to 0.16 m^3 of water per barrel of liquids output. With suitable cleaning, this water can be used as boiler feedwater for steam generation [Steynberg and Dry, 2004]. The net water usage of CTL plant will be the difference between that used in the cooling tower and that produced in the FT reactor. From the process performance models, water usage was estimated and the values per unit output are shown in table 5.6. These values are used for large scale water usage assessment.

Table 5.6: Water use factors for different coals and technologies (m^3/barrel)

	GE		EGas		Shell	
	Liq-only	Co-prod	Liq-only	Co-prod	Liq-only	Co-prod
Illinois#6	0.593	0.994	0.539	1.313	0.388	0.864
Wyoming PRB	0.678	1.046	0.601	1.278	0.396	0.889
ND Lignite	0.805	1.114	0.710	1.224	0.413	0.936

5.4 Large Scale Impacts

Large scale impacts of CTL are estimated by using the values determined in the previous sections. The US petroleum consumption in 2008 was 19.4 million barrels/day [EIA]. The fraction of liquid fuel demand supplied by coal liquids determines the large scale impacts of using CTL plants. The type of coal and choice of technology also affect the impacts. The effect on overall coal consumption, CO_2 emissions, water and land use are estimated as function of the transportation fuel demand met by coal liquids. All the comparisons are made using 2008 figures as the base values. Since co-production plants are capable of producing electricity at a large scale, the option of co-production plants displacing conventional coal power plants is considered. A comparative assessment of having co-production plants supply both liquids and electricity as opposed to separate production of liquids in a liquids-only CTL plant and electricity in a conventional coal power plant is made.

5.4.1 Separate and co-production of liquids and electricity

The following assumptions are made while comparing co-production with separate production:

- CTL plants and power plants use the same coal
- Implementation of CCS applies to both CTL and power plants
- Power plants are assumed to be using sub-critical pulverized coal technology

The calculation procedure is as follows:

- Liquids-only plant capacity is assumed to be 50,000 barrels/day
- For a co-production plant of this capacity, net electrical output is calculated
- Coal fired power plant produces the same net electrical output using the same coal as the CTL plant. Performance of power plants is obtained using IECM
- Coal consumption comparison of separate production and co-production is given by:

$$\Delta_{Coal} = \left(1 - \frac{Coal_{co-production}}{Coal_{liquids-only} + Coal_{power\ plant}}\right) \times 100\%$$

- CO_2 emissions comparison is given by

$$\Delta_{CO2} = \left(1 - \frac{CO2_{co-production}}{CO2_{liquids-only} + CO2_{power\ plant}}\right) \times 100\%$$

Net plant efficiencies (HHV) of a typical sub-critical PC power plant with all the pollution control technologies are 36.1%, 34.4% and 32.8% for Illinois#6, Wyoming PRB and ND lignite respectively, without CCS. With CCS, the efficiencies drop to 20.9%, 18.7% and 17% respectively. Similarly, coal consumption and CO_2 emissions are calculated using IECM.

From the results of the process performance model described in chapter 3, the comparative coal consumption and CO_2 savings of co-production are shown in table 5.7. These values are used while estimating large scale impacts of CTL under different conditions.

Table 5.7: Comparative coal and CO_2 reductions form co-production of liquids and electricity against separate production

		Illinois#6		Wyoming PRB		ND lignite	
		No CCS	CCS	No CCS	CCS	No CCS	CCS
PC + GE	Coal	17%	28%	11%	21%	11%	33%
	CO_2	24%	77%	16%	77%	16%	89%
PC + E-Gas	Coal	22%	17%	23%	18%	15%	23%
	CO_2	27%	95%	28%	96%	19%	97%
PC + Shell	Coal	19%	15%	15%	9%	16%	10%
	CO_2	26%	95%	19%	94%	21%	94%

5.4.2 Scenarios of CTL deployment

Large scale implementation is evaluated under the following scenarios:

1) Liquids-only CTL plants are built and the conventional coal-fired power plants continue
2) Co-production plants are built and conventional coal-fired power plants continue
3) Co-production plants are built and conventional coal-fired power plants are displaced

In scenarios 1 and 2, the overall (national) coal consumption is obtained by adding the coal required for CTL plants to the 2008 value, since the coal used for power plants will not change. In scenario 3, the overall coal consumption is the coal required for CTL plants minus the coal that would have been used in the displaced power plants.

If x is the fraction of petroleum consumption provided by coal liquids, the overall coal consumption, CO_2 emissions and land use for a particular technology would be calculated as:

$$Coal\,(million\,tonnes\,/\,day) = x \times 19.5 \times (tonnes\,Coal\,/\,barrel)_{\text{technology}}$$

$$CO2\,(million\,tonnes\,/\,day) = x \times 19.5 \times (tonnes\,CO2\,/\,barrel)_{\text{technology}}$$

$$Land\,(million\,acres) = x \times 19.5 \times (acres\,/\,barrel\,/\,day)_{\text{technology}}$$

CO_2 emissions in 2008 because of energy consumption are close to 5.8 billion tonnes. Coal consumption in 2008 was 1,020 million tonnes, 93% of which was used for power generation. Demonstrated reserve base was 446 billion tonnes.

Chapter 6: Techno-Economic Evaluation of a 50,000 barrels/day Coal-to-Liquids Plant

This chapter describes the application the comprehensive techno-economic assessment models of CTL plants described in the previous chapters. A schematic of the models is shown in Fig 6.1. Both liquids-only and co-production configurations are modeled for a plant producing 50,000 barrels/day of liquids from Illinois#6 bituminous coal. The plant uses GE gasification and low temperature FT reactor technologies. Plants with and without CCS are considered. Through an uncertainty and sensitivity analysis, the important factors that affect the cost of liquid fuel production from coal, including the plant size, price of coal, economic assumptions, technical factors and carbon constraints are studied. All costs are reported in constant 2007 USD.

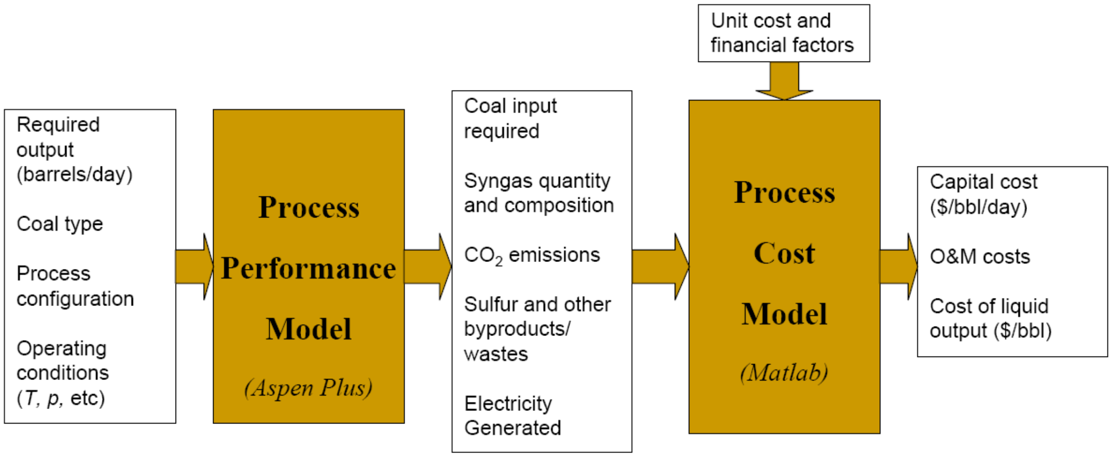


Figure 6.1: The techno-economic model consisting of process performance models developed in Aspen Plus and process cost models developed using Matlab

6.1 Analysis of the Liquids-Only Configuration

The process performance and cost models were applied to the liquids-only configuration. Table 6.1 shows the main results for performance and cost of the plant, both with and without CCS.

6.1.1 Liquids-only plant without CCS

The amount of coal needed to produce 50,000 barrels/day of liquid fuel output is about 19 kilo tonnes/day and the emissions of CO_2 are close to 24.7 kilo tonnes/day. The overall plant efficiency calculated as the energy content of liquid products per unit input energy (based on higher heating value), is about 56%.

For this plant without, capital cost comes out to be close to $91,900 per daily barrel and the cost of product liquid is about $76/barrel.

Table 6.1: Performance and cost results from the techno-economic models, for liquids-only and co-production configurations, with and without CCS

	Liquids-only		Co-production	
	No CCS	With CCS	No CCS	With CCS
Coal consumption (tonnes per day)	19,049	19,049	23,571	23,571
CO_2 emissions (tonnes per day)	24,693	288	35,392	801
Net power output (MW)	-	-	1,045	887
Efficiency (%, higher heating value)	56.1	56.1	55.2	53.0
Specific capital cost ($ per daily barrel)	91,897	93,064	117,196	129,345
Cost of liquid product ($/barrel, $0/tonne CO_2)	76.1	81.8	54.1	75.5
Cost of liquid product ($/barrel, $25/tonne CO_2)	88.4	81.8	71.8	75.5

Distribution of capital and O&M costs

Figure 6.2 shows the break-down of capital cost among the major sections of the plant. Syngas production contributes to more than 60% of the capital cost, followed by the FT process (about 20%) and the other sections of the plant.

The contribution of capital and operating cost components to the liquid product cost is depicted in Fig 6.3. It is clear that capital cost component is the biggest contributor, accounting for 60% of the total cost. Operating costs occur in the form of consumables like coal and are the next major contributor to cost.

Effect of a carbon price on the cost of liquid products

In the future, it is likely that there will be an implicit or explicit cost associated with every ton of CO_2 emitted into the atmosphere. To see the effect of carbon price on the output cost, a price of \$25/tonne CO_2 was considered and the results are also shown in table 6.1. The cost of liquid product increases to \$88.4/barrel with a carbon price.

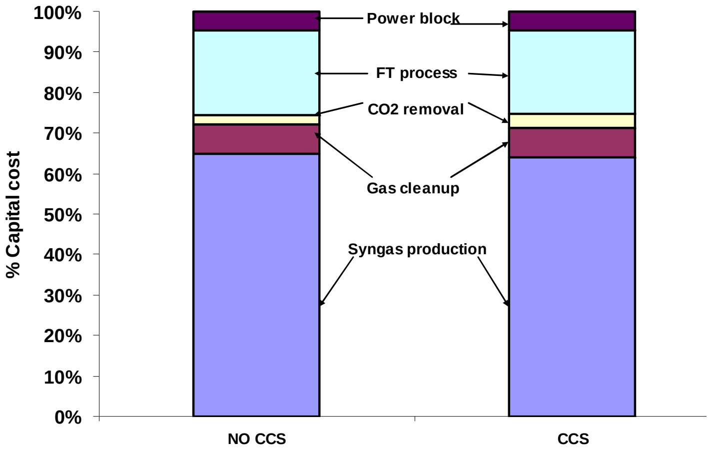


Figure 6.2: Distribution of capital cost for a liquids-only plant. Syngas production section accounts for close to 60% of the capital cost, followed by the FT section

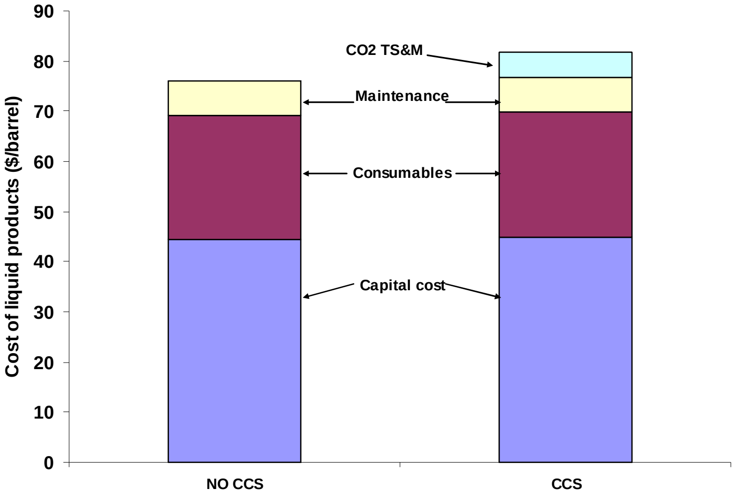


Figure 6.3: Distribution of liquid product cost for a liquids-only plant. Capital cost component accounts for close to 50% of the total cost.

6.1.2 Liquids-only plant with CCS

As mentioned earlier, CO_2 is captured during the CTL process and the plant level CO_2 emissions can be controlled by geological sequestration. In a CTL plant which is designed for CCS, additional capital costs occur in the form of compressors which compress the CO_2 separated in the Selexol process to a pressure of close to 150 bar so that it is easier to transport CO_2 in supercritical state. Additional operating expenses occur in the form of pipeline transportation costs, geological sequestration and monitoring costs.

With the addition of CCS, almost all the CO_2 emissions can be eliminated. Carbon containing components from the purge gases of FT loop account for the remaining CO_2. As explained in chapter 3, the additional energy required for CO_2 compression is assumed to be produced by waste heat recovery. Hence, the efficiency of the plant does not change with the addition of CCS. Capital cost increases to about $93,065 per daily barrel (Table 6.1), an increase of 1.3% and the output cost increases to about $82/barrel, an increase of 7.5% from the plant without CCS. Thus, operating costs of CCS affect the output cost of product liquids more than the increase in capital costs. Because of the extremely low CO_2 emissions, CO_2 price does not affect the output cost much

As in the plant without CCS, Fig 6.2 shows the break-down of capital costs among process section and Fig 6.3 shows the break-down of output cost in terms of the capital and operating costs.

It can be seen from Table 1 that the cost of liquid product from a plant with CCS is less than paying a carbon price of \$25/tonne CO_2.

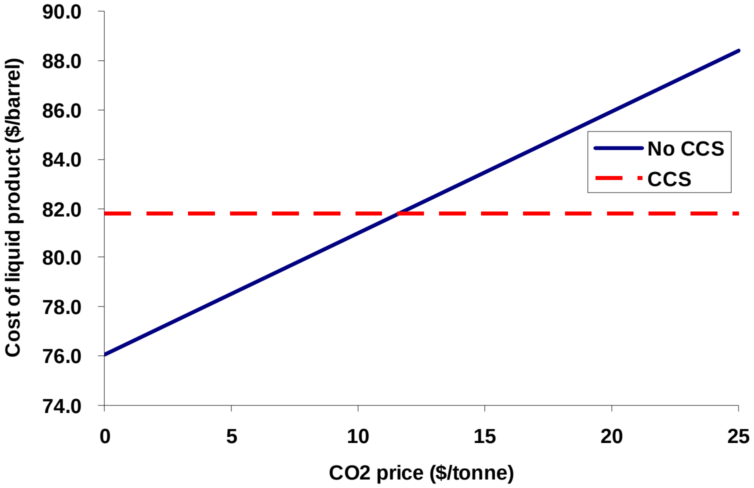


Figure 6.4: Effect of carbon price on cost of liquid product

Figure 6.4 shows the effect of increasing CO_2 price on the cost of liquid product. It can be seen that, for a CO_2 price over \$12/tonne, a plant with CCS would be more economical than paying carbon tax.

6.1.3 Uncertainty Analysis

Figure 6.5 shows the effect of uncertainties in economic and non-economic parameters on the product cost for case without CCS. The ranges of uncertainties are shown in chapter 3 and are not repeated here. Uncertainties in capital cost parameters, particularly the wide variation in CRF, are the cause of much of the variation in output cost. Figure

6.6 compares only the output costs for plants without and with CCS and the effect of CO_2 price on the product cost from a plant without CCS. The 90% confidence interval of output cost is \$56 - \$97/barrel for a plant without CCS and \$62 - \$104/barrel for a plant with CCS.

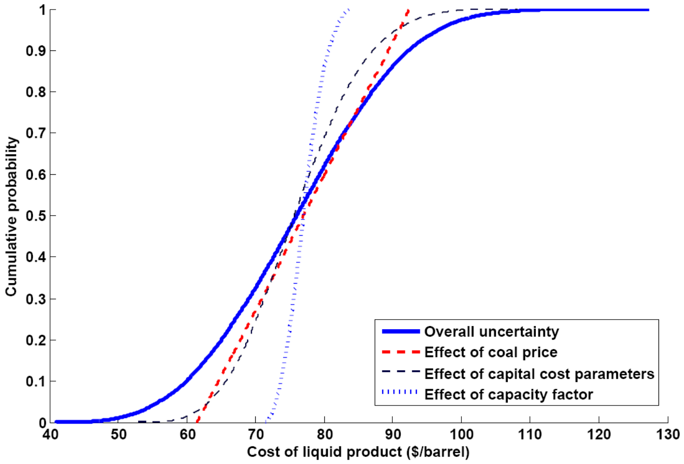


Figure 6.5: Cumulative probability distributions of cost of liquid product (\$/barrel) for plant without CCS. Capital cost assumptions, particularly the capital recovery factor, cause the maximum uncertainty in the output cost

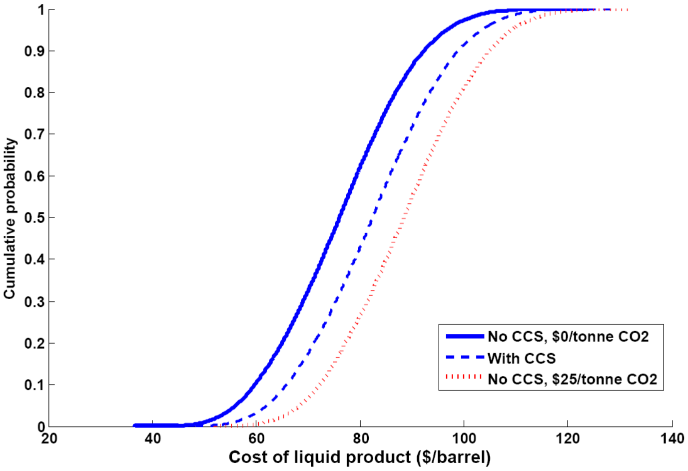


Figure 6.6: Comparison of costs of liquid products from plants without and with CCS, including the effect of uncertainty. Arrows indicate deterministic values.

6.1.4 Sensitivity to plant output capacity

The effect of plant capacity on the capital cost and cost of product liquid was also analyzed. Plant capacity was varied from 25,000 barrels per day to 125,000 barrels per day. The variation in specific capital cost is depicted in Fig 6.7. The specific capital cost of a 125,000 barrels/day plant is 10% less than that of a 25,000 barrels/day plant. The economy of scale of CTL plants is evident from the decreasing trend of capital cost with plant capacity. Figure 6.8 shows the cost of product liquids for different plant capacities. As is the case with the capital cost, cost of product liquid also shows a slight trend of economy of scale.

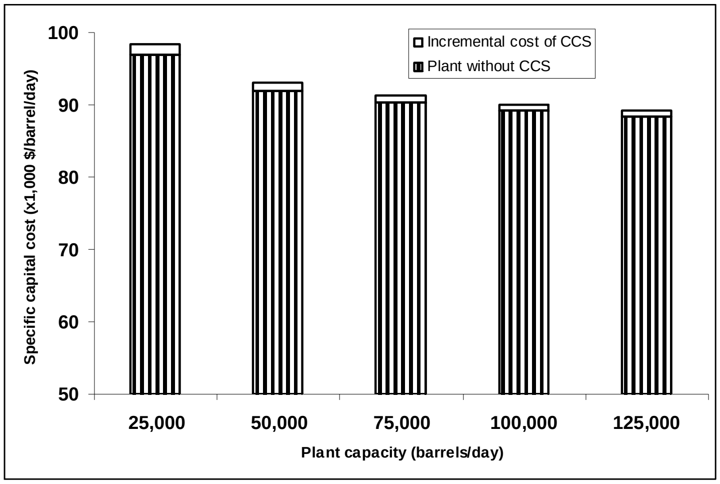


Figure 6.7: Specific capital costs ($/barrel/day) of plants with different capacities. Economy of scale is evident.

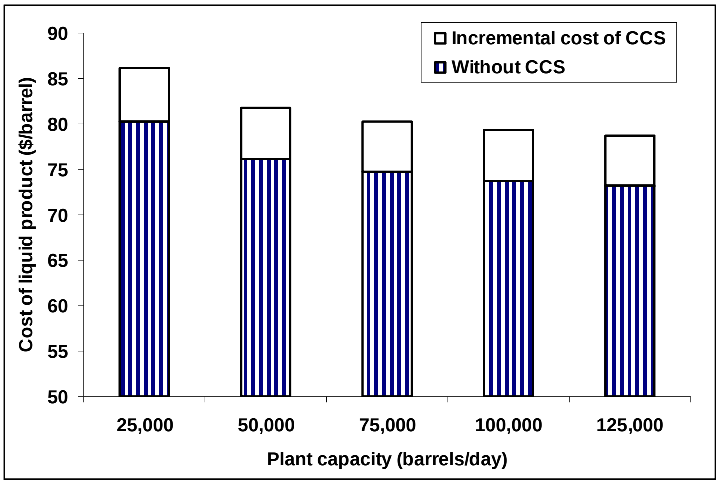


Figure 6.8: Cost of liquid product ($/barrel) of plants with different capacities. As with the capital costs, economy of scale is evident here also.

6.2 Analysis of the Co-production Configuration

The models were also applied to a CTL plant with co-production configuration in which the unconverted syngas and the FT product gases are combusted in a combined cycle power plant to generate electricity. The performance and cost results are also shown in table 6.1.

6.2.1 Co-production plant without CCS

The amount of coal needed to produce 50,000 barrels/day of liquid fuel output is about 23.6 kilo tonnes/day, 24% more than that of the liquids-only case and the emissions of CO_2 are close to 35.4 kilo tonnes/day, 43% higher than in the liquids-only case. Besides the liquids output, a co-production plant without CCS produces more than 1,000 MW of electricity which can sold to the grid for additional revenue. However, the overall plant efficiency is slightly less than the liquids-only case.

The capital cost of this plant is close to 27% higher than the liquids-only plant without CCS. However, when the by-product electricity is sold to the grid at \$80/MWh, the cost of liquid product is \$54.1/barrel without a CO_2 price and \$71.8/barrel with a CO_2 price of \$25/tonne CO_2. In both cases, the cost of liquid product is lower than in the corresponding liquids-only cases. Despite the increase in capital cost, because of the revenue generated by electricity, co-production plants can produce cheaper liquid fuels than liquids-only plants.

6.2.2 Co-production plant with CCS

CCS in a co-production plant applies to the Selexol CO_2 capture in the gasification and FT sections as well as post-combustion CO_2 capture in the power block. With the addition of CCS, CO_2 emissions can be reduced to 800 tonnes/day. There is an energy penalty for CO_2 capture and compression and hence the net electricity output is reduced to 887 MW and the efficiency of the plant decreases by 2 percentage points.

Capital cost increases by about 10% compared to a co-production plant without CCS. The output cost is \$75.5/barrel without CO_2 price and \$75.9/barrel with a CO_2 price of \$25/tonne, when electricity is sold at \$80/MWh. Unlike the liquids-only case, a CO_2 price of \$25/tonne is not enough to make CCS a cost-effective option, when electricity is sold at \$80/MWh. The revenue generated by electricity dominates the cost of CO_2 emissions.

6.2.3 Effect of electricity selling price and CO_2 price

The cost of product liquids from a co-production plant depends strongly on the revenue generated from electricity sales. Figure 6.9 shows the effect of electricity selling price on the cost of product liquids for cases where there is no CCS and with CCS (without and with a carbon price of \$25/tonne of CO_2). The electricity prices at which co-production breaks even with liquids-only plant (based on the cost of liquid products) are shown with arrows. For all the cases, co-production plants become cheaper than liquids-only plants when the selling price of electricity is in the range of \$35 – 70/MWh. This price range corresponds with the current market prices of electricity, which can be expected to grow when there are carbon constraints. In effect, the results show that co-production plants can produce liquid fuels which are cheaper than those produced from liquids-only plants.

Figure 4 also shows that CCS becomes more costly than paying a CO_2 price of \$25/tonne, if the electricity selling price were to exceed \$20/MWh. Without CCS, the CO_2 emissions are very high from a CTL plant. In order to encourage CCS, the CO_2 price should have to be higher than \$25/tonne. By varying CO_2 price, it was found that CCS will be the cheaper option at these ranges of electricity selling prices, for CO_2 price exceeding $35/tonne.

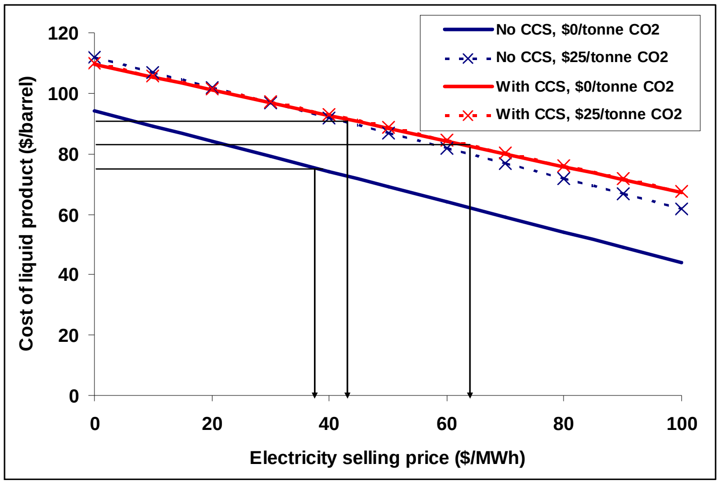


Figure 6.9: Effect of selling price of electricity (cents/kWh) on the cost of liquid product from a co-production CTL plant. Arrows show the prices at which co-production breaks even with liquids-only plants in terms of cost of liquid products.

6.3 Discussion

From the performance and cost results presented above, it is clear for the input assumptions, that liquids can be produced from coal with a relatively high overall thermal efficiency. The efficiency of a co-production plant is slightly lower than the liquids-only configuration despite the large electricity production. This shows that recycling of unconverted syngas to the FT reactor avoids an increase in coal consumption, thereby leading to higher thermal efficiencies for the entire plant.

The costs of liquid product from both liquids-only and co-production plants are comparable to the crude oil prices seen in the past 2-3 years. From the cost breakdown, it can be inferred that CTL plants are highly capital intensive, with the capital cost component accounting for about half the total product cost. The capital requirement for a 50,000 barrels/day liquids-only CTL plant is on the order of $5 billion. It was also seen that when all the uncertainties were considered, the cost of liquid product can vary by a factor of 2. Thus, if coal liquids are not competitive in the market, CTL plants cause a significant financial risk. Though co-production plants are much costlier than liquids-only configurations in terms of capital cost, because of the high electricity revenues, the cost of liquid product is lower than that of the liquids-only case, at market prices of electricity. It was also seen that the liquid product cost from a co-production plant decreases rapidly with increasing electricity prices. With future carbon constraints, electricity prices can be expected to grow. Thus, co-production plants can be effective in reducing the financial risk of a CTL plant.

Plant-level CO_2 emissions can be greatly reduced by using the CCS technology. The incremental capital costs of CCS are minimal because CO_2 capture is already included in the base plant. Even with CCS, the liquid product costs are comparable to recent crude oil prices. For a liquids-only configuration, CCS is a cheaper option when the CO_2 price exceeds $12/tonne. However, for a co-production plant, electricity revenues balance out the cost because of carbon price. The CO_2 price has to be more than $35/tonne to make CCS cost-effective, when the electricity prices are in the range of $0 - $100/MWh. Without CCS, there will be a huge increase in CO_2 emissions. Thus, even though co-production plants mitigate financial risk, they also cause environmental risk in the form of increased CO_2 emissions, unless there is a sufficiently high price on CO_2 emissions.

Chapter 7: CTL Plants with Different Gasification Technologies

In the previous chapter, the techno-economic model was applied to a CTL plant using GE gasification technology. This chapter describes the application of the models to two other gasification technologies – Conoco Phillips E-Gas and Shell. The characteristics of the gasifiers are explained in chapter 2 and model modifications to suit different gasifier technologies are explained in chapter 3. Table 7.1 summarizes the operating conditions and syngas compositions from these gasifiers. Illinois#6 coal is used as the feedstock. Both liquids-only and co-production configurations are modeled for a plant producing 50,000 barrels/day of liquids, using LTFT reactor technology. Plants with and without CCS are considered. Through an uncertainty and sensitivity analysis, the important factors that affect the cost of liquid fuel production from coal, including the plant size, price of coal, economic assumptions, technical factors and carbon constraints are studied. All costs are reported in constant 2007 USD.

Table 7.1: Operating conditions and syngas compositions of the gasifiers

	GE	E-Gas	Shell
Feed	Slurry	Slurry	Dry
Temperature (^{o}C)	1316	1016	1427
Pressure (MPa)	5.6	4.3	4.3
O_2/C (mol/mol)	0.47	0.43	0.42
H_2O/C (mol/mol)	0.55	0.55	0.15
Syngas composition			
CO	0.345	0.365	0.571
H_2	0.335	0.259	0.300
CO_2	0.151	0.133	0.022
H_2O	0.142	0.174	0.027
CH_4	0.001	0.044	0.001

GE/Texaco Gasifier

GE gasifier (earlier Texaco/Chevron Texaco) is a cylindrical pressure vessel in which coal is fed in the form of water slurry and the oxidant is pure oxygen (95% purity, in this case). The operating temperature is 1,316 ^{o}C and pressure is 5.6 MPa. Ash is removed in the form of molten slag. The gasifier uses a radiant cooling technology to cool the raw syngas.

Conoco-Phillips E-Gas Gasifier

This is also a slurry-fed gasifier design operating in two stages. However, for modeling purposes, it is assumed that gasification occurs in a single stage, operating at 1,010 ^{o}C and pressure of 4.2 MPa. Here also, ash is removed in the form of molten slag.

Shell Gasifier

Unlike the other two gasifiers, coal is fed in dry form using nitrogen as the carrier. Oxygen and a small amount of steam are injected directly into the gasifier, which operates at 1,427 ^{o}C and 4.2 MPa. The high operating temperature limits the formation of CO_2. However, the H_2/CO ratio in the products is lower than what is required for FT reactions and a water gas shift reaction is required to adjust the ratio.

7.1 Analysis of the Liquids-Only Configuration

The process performance and cost models were applied to the liquids-only configuration. Table 7.2 shows the main results for performance and cost of the plant, both with and without CCS.

Table 7.2: Performance and cost results for liquids-only plants with different gasifiers

	GE	EGas	Shell
Output (barrels/day)	50,000	50,000	50,000
Coal (tonnes/day)	19,049	21,648	17,980
CO_2 without CCS (tonnes/day)	24,693	29,139	22,829
CO_2 with CCS (tonnes/day)	288	816	312
Efficiency (% HHV)	56.1	49.3	59.4
Capital cost (without CCS \$/barrel/day)	91,897	96,476	84,837
Capital cost (with CCS \$/barrel/day)	93,064	97,758	85,921
Cost of liquid (without CCS, \$/barrel, \$0/tonne CO_2)	76.1	81.6	71.0
Cost of liquid (without CCS, \$/barrel, \$25/tonne CO_2)	88.4	96.2	82.4
Cost of liquid (with CCS, \$/barrel)	81.8	49.3	76.2

7.1.1 GE case

Using a GE gasifier system, 19 kilo tonnes/day of coal is required to produce 50,000 bbl/day of liquids. The overall plant efficiency, calculated as the energy content of liquid products divided by the coal energy input (based on higher heating value), is close to 56%. Without CCS, this system emits about 24.7 kilo tonnes/day of CO_2. Capital cost of such a plant is estimated to be \$91,987/barrel/day and the cost of product liquid is \$76.1/barrel, when there is no CO_2 price. For a CO_2 price of \$25/tonne, the product cost increased to nearly \$88.5/barrel, an increase of \$12/barrel. On the other hand, addition of CCS (including CO_2 compression, transport and storage), increased the capital cost to \$93,064/barrel/day, an increase of 1.3% from the case without CCS, while the product cost increased to \$82/barrel. This shows that employing CCS is more cost-effective than paying a carbon price of \$25/tonne CO_2.

7.1.2 E-Gas case

Compared to the GE case, the system using E-Gas gasifier consumes higher amount of coal (21,648 tonnes/day) and emits about 29.1 kilo tonnes/day less CO_2, about 18% more than in the GE case. The purge gas from the FT section of E-Gas also contains more CO_2

than the corresponding GE case. This is evident from the higher CO_2 emissions from the E-Gas case with CCS.

The capital cost of a liquids-only plant using E-Gas gasification system is about \$96,476/barrel/day without CCS and \$97,758/barrel/day with CCS, about 4.5% more than the corresponding GE cases. Similarly, the cost of product liquids is \$82/barrel without CCS and \$88 with CCS. As with the GE case, CCS is more cost-effective than paying a carbon price of \$25/tonne CO_2, which increases the liquid product cost to \$96/barrel.

7.1.3 Shell case

A 50,000 barrel/day CTL plant using Shell gasifier uses about 6% less coal (18 kilo tonnes/day) and emits about 8% less CO_2 (23 kilo tonnes/day) compared to the GE case and 20% less coal and 27% less CO_2 compared to the E-Gas case, without CCS. As a result, this system has the highest efficiency of around 59%. The capital cost without CCS is \$84,837/barrel/day and \$85,921/barrel/day with CCS. The cost of product liquid is estimated to be \$71/barrel without CCS, which increases to \$82/barrel when CCS is added. The increase is less than the other two cases because of the lesser CO_2 needed to be captured. A carbon price of \$25/tonne CO_2 makes the cost of product liquid \$76/barrel.

The main reason for better performance and economics of a Shell system is the low amount of CO_2 produced in the gasifier, which translates into lower coal requirement for the production of same amount of syngas (CO and H_2), compared to the other two systems. As shown in Table 1, the combined volume fraction of CO and H_2 in the syngas from a Shell gasifier is about 85%, compared to only around 60% in the GE and EGas gasifiers.

7.1.4 Uncertainty Analysis

Figure 7.1 shows the effect of uncertainties in economic and non-economic parameters on the product cost for all the gasifier cases, with CCS. The ranges of uncertainties are shown in chapter 3 and are not repeated here. The costs vary over a large range ($50 - $100/barrel), when all the uncertainties are taken into account. Since CTL plants are high-capital projects, it is important to understand the financial risks involved because of uncertainties.

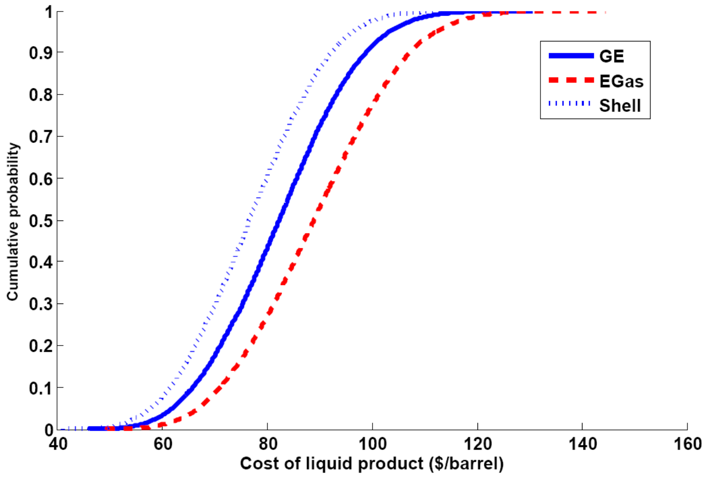


Figure 7.1: Uncertainty analysis for a liquids-only plant with CCS for the three gasifier cases. Dry-feed Shell gasifier costs less than the other two

7.2 Analysis of the Co-production Configuration

Table 7.3 shows the results for co-production CTL plants which co-produce electricity along with 50,000 barrel/day of liquids.

Table 7.3: Performance and cost results for co-production plants with different gasifiers

Gasifier	GE	EGas	Shell
Output (barrels/day)	50,000	50,000	50,000
Coal (tonnes/day)	23,571	28,812	22,986
CO_2 (without CCS, tonnes/day)	35,392	47,609	34,986
CO_2 (with CCS, tonnes/day)	801	1560	1,110
Net power output (without CCS, MW)	1,045	1,749	1,196
Net power output (with CCS, MW)	887	1,560	1,030
Efficiency (without CCS, % HHV)	55.2	53.2	58.8
Efficiency (with CCS, % HHV)	53.0	50.3	56.4
Capital cost (without CCS, $/barrel/day)	117,196	137,119	111,516
Capital cost (with CCS, $/barrel/day)	129,345	166,946	127,551
For electricity selling price of $80/MWh:			
Cost of liquid (without CCS, $/barrel, $0/tonne CO_2)	54.1	43.9	44.6
Cost of liquid (without CCS, $/barrel, $25/tonne CO_2)	71.8	67.7	62.1
Cost of liquid (with CCS, $/barrel)	75.5	82.7	68.7
Cost of liquid (with CCS, $25/barrel)	75.9	83.5	69.2

7.2.1 GE case

A co-production CTL plant with GE gasifier consumes 23.6 kilo tonnes/day of coal. Without CCS, 35.4 tonnes/day of CO_2 is emitted and about 1,045 MW of electricity is co-produced. With CCS, CO_2 emissions reduce to 800 tonnes/day and the co-product electricity decreases to 890 MW. The overall efficiency of this plant is 55.2% without CCS and 53% with CCS, which is lower than the corresponding liquids-only case. The capital cost of the plant without CCS is $117,196/barrel/day and $129,345/barrel/day with CCS, about 30% higher than the corresponding liquids-only plants.

7.2.2 E-Gas case

With E-Gas gasifier, coal consumption is 28.8 kilo tonnes/day, which is 22% higher than in the GE case. CO_2 emissions without CCS are estimated to be 47.6 kilo tonnes/day, which came down to 1,590 tonnes/day with CCS. The electricity produced is much higher than in the GE case – 1,749 MW without CCS and 1,493 MW with CCS. The unconverted syngas which is burnt in the combined cycle power plant contains a higher amount of methane, thereby having a higher overall heating value than compared to the gas in the GE case. More N2 has to be added to adjust the heating value. Also, the quantity of unconverted syngas is higher in this case because of the higher fraction of methane. This is the reason for the higher net power output as well as higher CO_2 emissions. The capital cost of the plant without CCS is $137,119/barrel/day and $166,946/barrel/day with CCS, about 40% higher than the corresponding liquids-only plants.

7.2.3 Shell case

As in the liquids-only plants, a co-production CTL plant with a Shell gasifier consumes the least amount of coal (23 kilo tonnes/day) and emits 34.9 kilo tonnes/day of CO_2 without CCS. The electricity production is higher than the GE case but lower than the E-Gas case – 1,196 MW without CCS and 1,110 MW with CCS. The overall efficiency of the plant is higher than both GE and E-Gas cases but lower compared to the corresponding liquids-only plant using a Shell gasifier. This shows that the relative efficiencies of co-production and liquids-only configurations depend heavily on the gasifier technology used.

The cost of product liquids from a co-production plant depends on the revenue generated from electricity sales. Table 3 also compares the cost of liquid product in all three cases for an electricity selling price of $80/MWh. When there is no CCS and no CO_2 price, the E-Gas case has the lowest liquid product cost but when there is either CCS or CO_2 price or both, CTL plant with a Shell gasifier produces the cheapest liquid fuels.

7.2.4 Effect of electricity selling price and CO_2 price

Figures 7.2 – 7.4 show the effect of the electricity selling price on the cost of product liquids for the GE, E-Gas and Shell cases, respectively. For all cases, co-production plants become cheaper than liquids-only plants when the selling price of electricity is in the range of $30 – 70/MWh. This price range corresponds approximately to current market prices of U.S. electricity. In effect, the results show that co-production plants can produce liquid fuels which are cheaper than those produced from liquids-only plants.

These figures also show that CCS becomes more costly than paying a CO_2 price of $25/tonne, if the electricity selling price were to exceed $20/MWh. Without CCS, the CO_2 emissions are very high from a CTL plant. In order to encourage CCS, the CO_2 price should have to be higher than $25/tonne. By varying CO_2 price, it was found that CCS will be the cheaper option at these ranges of electricity selling prices, for CO_2 price exceeding $35/tonne for GE and Shell cases and $45/tonne for the E-Gas case.

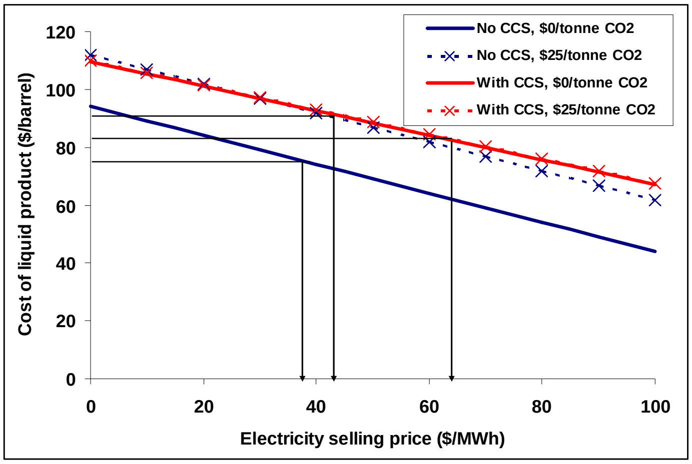


Figure 7.2: Effect of electricity selling price on the cost of liquid product for a co-production CTL plant using GE gasifier. $25/tonne CO_2 is not enough to make CCS cost-effective

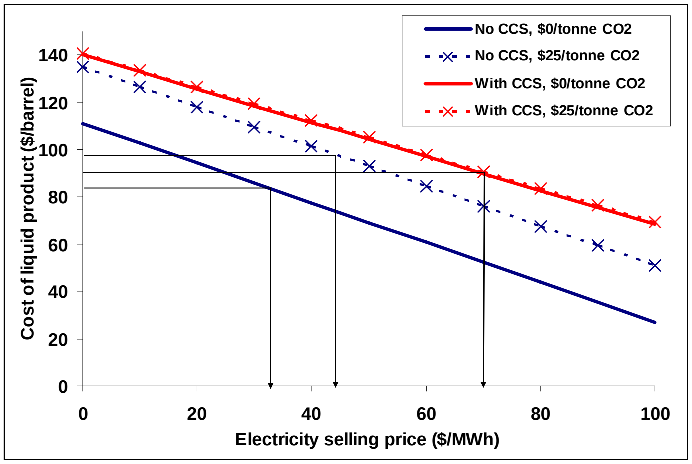


Figure 7.3: Effect of electricity selling price on the cost of liquid product for a co-production CTL plant using E-Gas gasifier. $25/tonne CO_2 is not enough to make CCS cost-effective

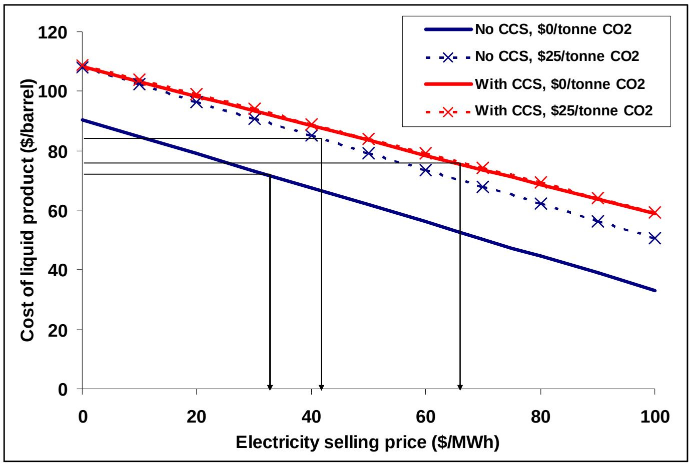


Figure 7.4: Effect of electricity selling price on the cost of liquid product for a co-production CTL plant using Shell gasifier. $25/tonne CO_2 is not enough to make CCS cost-effective

7.3. Discussion

The process using a dry-feed Shell gasification has the lowest capital and product cost of the three. Coal consumption for a Shell-based CTL process is much lower than the other two options, as are the CO_2 emissions without CCS are also significantly lower. The main reason for better performance and economics of a Shell system is the low amount of CO_2 produced in the gasifier, which translates into lower coal requirement for the production of same amount of syngas (CO and H_2), compared to the other two systems. The combined volume fraction of CO and H_2 in the syngas from a Shell gasifier is about 85%, compared to only around 60% in the GE and EGas gasifiers. It is clear that dry-feed systems have a definite cost advantage over slurry systems. Within the two slurry systems, the one operating at a higher temperature has performance and cost advantages.

The costs of liquid product from both liquids-only and co-production plants are comparable to the crude oil prices seen in the past 2-3 years. From the cost breakdown, it can be inferred that CTL plants are highly capital intensive, with the capital cost component accounting for about half the total product cost. The capital requirement for a 50,000 barrels/day liquids-only CTL plant is on the order of $5 billion. It was also seen that when all the uncertainties were considered, the cost of liquid product can vary by a factor of 2. Thus, if coal liquids are not competitive in the market, CTL plants cause a significant financial risk. Though co-production plants are much costlier than liquids-only configurations in terms of capital cost, because of the high electricity revenues, the cost of liquid product is lower than that of the liquids-only case, at market prices of electricity. It was also seen that the liquid product cost from a co-production plant decreases rapidly with increasing electricity prices. With future carbon constraints, electricity prices can be expected to grow. Thus, co-production plants can be effective in reducing the financial risk of a CTL plant.

Plant-level CO_2 emissions can be greatly reduced by using the CCS technology. The incremental capital costs of CCS are minimal because CO_2 capture is already included in the base plant. Even with CCS, the liquid product costs are comparable to recent crude oil prices. For a liquids-only configuration, CCS is a cheaper option when the CO_2 price exceeds \$12/tonne. However, for a co-production plant, electricity revenues balance out the cost because of carbon price. The CO_2 price has to be more than \$35/tonne to make CCS cost-effective, when the electricity prices are in the range of \$0 - \$100/MWh. Without CCS, there will be a huge increase in CO_2 emissions. Thus, even though co-production plants mitigate financial risk, they also cause environmental risk in the form of increased CO_2 emissions, unless there is a sufficiently high price on CO_2 emissions.

Chapter 8: CTL Plants with Different Types of Coal

In the previous two chapters, the techno-economic model was applied to a CTL plant using Illinois#6 as the feed coal. This chapter analyses the effect of different coal types on the plant performance and cost. The coals modeled additionally are the sub-bituminous Wyoming Powder River Basin and North Dakota lignite. Results of the plant with Illinois#6 are also shown. Table 8.1 shows the ultimate analyses and properties of these coals. Both liquids-only and co-production configurations are modeled for a plant producing 50,000 barrels/day of liquids, using LTFT reactor technology. Plants with and without CCS are considered. Through an uncertainty and sensitivity analysis, the important factors that affect the cost of liquid fuel production from coal, including the plant size, price of coal, economic assumptions, technical factors and carbon constraints are studied. All costs are reported in constant 2007 USD.

Table 8.1: Properties of coals used for this analysis

Coal	**Illinois#6**	**Wyoming PRB**	**ND lignite**
Rank	**Bituminous**	**Sub-bituminous**	**Lignite**
Component	Mass percentage		
Ash	9.70	5.32	15.92
C	63.74	48.18	35.04
H2	4.50	3.31	2.68
N2	1.25	0.7	0.77
Cl	0.29	0.01	0.09
S	2.51	0.37	1.16
O2	6.89	11.87	11.31
Moisture	11.12	30.24	33.03
HHV(MJ/kg)	26.12	19.36	13.97

Table 8.2: Compositions of syngas that goes to FT synthesis section, for different coal types and technologies

Coal	Illinois #6			Wyoming PRB			ND lignite		
Gasifier	**GE**	**E-Gas**	**Shell**	**GE**	**E-Gas**	**Shell**	**GE**	**E-Gas**	**Shell**
CO	0.489	0.528	0.561	0.435	0.499	0.549	0.347	0.412	0.532
H2	0.484	0.381	0.376	0.530	0.425	0.368	0.600	0.513	0.356
CO2	0.002	0.002	0.001	0.003	0.003	0.001	0.004	0.003	0.001
CH4	0.002	0.063	0.001	0.001	0.042	0.000	0.000	0.022	0.000
Others	0.023	0.026	0.061	0.031	0.031	0.082	0.049	0.050	0.111
H2/CO	0.990	0.722	0.670	1.218	0.852	0.670	1.729	1.245	0.669

8.1 Effect of Coal Type on Syngas Composition

The composition of syngas depends on the type of coal and the technology used to gasify it. Table 8.2 shows the composition of syngas that goes into the FT reactor, for different coals and gasification technologies. For slurry-based GE and E-Gas gasifiers, concentration of solids in coal slurry was fixed at 63% for bituminous coals, 56% for sub-bituminous and 50% for lignite. These values are obtained based on slurriability criteria for different coals [Chen, 2005]. For dry-feed Shell gasifier, bituminous coals were dried to 5% moisture levels, sub-bituminous to 6% and lignite to 12%.

Based on the values in table 8.2, the following observations can be made:

- For all coals, CO content increases with increasing gasification temperature, in the ascending order of E-Gas, GE and Shell gasifiers
- For all coals, H_2 content decreases with increasing temperature. In other words, H_2/CO reduces with increasing gasification temperature
- For all coals, syngas from GE gasifier has the highest H_2/CO ratio, followed by E-Gas and Shell

- For GE and E-Gas gasifiers, H_2/CO ratio increases with decreasing coal quality. This is because of the increasing moisture content in the gasifier feed coal as coal quality decreases. For Shell gasifiers, the ratio doesn't change because the raw gas from gasifier is shifted to bring up the H2/CO ratio to 0.67, the minimum required for LTFT synthesis
- For all coals, syngas from E-Gas gasifier has the highest methane content. This is because of the lower gasification temperature and also the two-stage gasification process.
- For E-Gas gasifier, methane content decreases with decreasing coal quality

8.2 Analysis of Liquids-Only Configuration

The performance and cost results of using different coals in different gasifiers are given in tables 8.3 – 8.5.

8.2.1 Illinois#6 Case

This case is the same as was described in the previous chapter. The results are repeated here for the sake of continuity. The results are shown in table 8.3.

GE Gasifier

Using a GE gasifier system, 19 kilo tonnes/day of coal is required to produce 50,000 bbl/day of liquids. The overall plant efficiency, calculated as the energy content of liquid products divided by the coal energy input (based on higher heating value), is close to 56%. Without CCS, this system emits about 24.7 kilo tonnes/day of CO_2. Capital cost of such a plant is estimated to be \$91,987/barrel/day and the cost of product liquid is \$76.1/barrel, when there is no CO_2 price. For a CO_2 price of \$25/tonne, the product cost increased to nearly \$88.5/barrel, an increase of \$12/barrel. On the other hand, addition of CCS (including CO_2 compression, transport and storage), increased the capital cost to \$93,064/barrel/day, an increase of 1.3% from the case without CCS, while the product cost increased to \$82/barrel. This shows that employing CCS is more cost-effective than paying a carbon price of \$25/tonne CO_2.

Table 8.3: Performance and cost results for Illinois#6, different gasifier technologies

Gasifier	GE	EGas	Shell
Output (barrels/day)	50,000	50,000	50,000
Coal (tonnes/day)	19,049	21,648	17,980
CO_2 without CCS (tonnes/day)	24,693	29,139	22,829
CO_2 with CCS (tonnes/day)	288	816	312
Efficiency (% HHV)	56.1	49.3	59.4
Capital cost (without CCS \$/barrel/day)	91,897	96,476	84,837
Capital cost (with CCS \$/barrel/day)	93,064	97,758	85,921
Cost of liquid (without CCS, \$/barrel, \$0/tonne CO_2)	76.1	81.6	71.0
Cost of liquid (without CCS, \$/barrel, \$25/tonne CO_2)	88.4	96.2	82.4
Cost of liquid (with CCS, \$/barrel)	81.8	49.3	76.2

E-Gas Gasifier

Compared to the GE case, the system using E-Gas gasifier consumes higher amount of coal (21,648 tonnes/day) and emits about 29.1 kilo tonnes/day less CO_2, about 18% more than in the GE case. The purge gas from the FT section of E-Gas also contains more CO_2 than the corresponding GE case. This is evident from the higher CO_2 emissions from the E-Gas case with CCS.

The capital cost of a liquids-only plant using E-Gas gasification system is about \$96,476/barrel/day without CCS and \$97,758/barrel/day with CCS, about 4.5% more than the corresponding GE cases. Similarly, the cost of product liquids is \$82/barrel without CCS and \$88 with CCS. As with the GE case, CCS is more cost-effective than paying a carbon price of \$25/tonne CO_2, which increases the liquid product cost to \$96/barrel.

Shell Gasifier

A 50,000 barrel/day CTL plant using Shell gasifier uses about 6% less coal (18 kilo tonnes/day) and emits about 8% less CO_2 (23 kilo tonnes/day) compared to the GE case and 20% less coal and 27% less CO_2 compared to the E-Gas case, without CCS. As a result, this system has the highest efficiency of around 59%. The capital cost without CCS is $84,837/barrel/day and $85,921/barrel/day with CCS. The cost of product liquid is estimated to be $71/barrel without CCS, which increases to $82/barrel when CCS is added. The increase is less than the other two cases because of the lesser CO_2 needed to be captured. A carbon price of $25/tonne CO_2 makes the cost of product liquid $76/barrel.

The main reason for better performance and economics of a Shell system is the low amount of CO_2 produced in the gasifier, which translates into lower coal requirement for the production of same amount of syngas (CO and H_2), compared to the other two systems. As shown in Table 1, the combined volume fraction of CO and H_2 in the syngas from a Shell gasifier is about 85%, compared to only around 60% in the GE and EGas gasifiers.

8.2.2 Wyoming PRB Case

Wyoming PRB is a sub-bituminous coal. The results for a 50,000 barrels/day liquids-only plant are shown in table 8.4.

GE Gasifier

Compared to the bituminous case, coal consumption of the CTL plant using a GE gasifier increases by 40%. But interestingly, CO_2 emissions without CCS increase only by 12%. This is because of the lower carbon content of a sub-bituminous coal. With CCS, CO_2

emissions in this case are lower than with a bituminous coal. The overall plant efficiency is 53.8%, which is lower than when bituminous coal is used.

Capital cost with and without CCS are 16% higher than with bituminous coal. Capital cost directly varies with coal flow rate. The cost of liquid product is lower than with bituminous coal despite an increase in coal flow rate. This is because of the lower price of PRB coal (\$15/tonne) compared to Illinois#6 coal (\$60/tonne). Even here, CCS is more cost-effective than a CO_2 price of \$25/tonne.

Table 8.4: Performance and cost results for Wyoming PRB, different gasifier technologies

Gasifier	GE	EGas	Shell
Output (barrels/day)	50,000	50,000	50,000
Coal (tonnes/day)	26,803	28,919	25,551
CO_2 without CCS (tonnes/day)	27,553	30,171	25,952
CO_2 with CCS (tonnes/day)	264	648	312
Efficiency (% HHV)	53.8	49.8	56.4
Capital cost (without CCS \$/barrel/day)	106,643	108,225	99,310
Capital cost (with CCS \$/barrel/day)	107,900	109,545	100,492
Cost of liquid (without CCS, \$/barrel, \$0/tonne CO_2)	69.2	70.7	64.8
Cost of liquid (without CCS, \$/barrel, \$25/tonne CO_2)	83.0	85.8	77.8
Cost of liquid (with CCS, \$/barrel)	75.5	77.6	70.8

E-Gas Gasifier

Compared to the GE case, the system using E-Gas gasifier consumes 8% more coal and emits about 10% more CO_2. Compared to the bituminous case, 33% more sub-bituminous coal is required to produce the same amount of liquids. Even though syngas has lesser methane content than from a bituminous coal, because of higher moisture content, coal flow rate increases. The purge gas from the FT section of E-Gas also contains more CO_2 than the corresponding GE case, but lower when compared to bituminous coal with E-Gas gasifier. The overall plant efficiency is marginally more than the bituminous case.

Capital cost is 12% more than the corresponding bituminous coal cases. This increase is less than what was seen in the GE case. As with the GE case, cost of liquid product is less than the bituminous case and CCS is more cost-effective than paying a carbon price of \$25/tonne CO_2.

Shell Gasifier

Similar to the bituminous coal cases, Shell gasifier uses less coal and emits less CO_2 compared to the other two. As a result, the capital cost is also lower in this case. However, when compared to the bituminous case, the coal consumption is 42% more and CO_2 emissions are 14% higher and the overall plant efficiency is lower by 3 percentage points. Again, the main reason for better performance and economics of a Shell system is the low amount of CO_2 produced in the gasifier which translates into lower coal requirement for the production of same amount of syngas (CO and H_2), compared to the other two systems. The moisture content in the gasifier feed coal is also much lower compared to the slurry-based systems.

8.2.3 ND lignite case

Compared to other coals, lignite has the highest ash and moisture contents. Ratio of solids in the coal slurry is also lower and the moisture content in the dried coal to Shell gasifier is higher. the results for this are shown in table 8.5

GE Gasifier

Lignite coal consumption is 50% higher than bituminous coal and 40% higher than sub-bituminous coal for a GE gasifier. But CO_2 emissions without CCS increase only by 2% compared to PRB. This is again because of the lower carbon content of lignite. With CCS, CO_2 emissions in this case are lower than the other cases. The overall plant efficiency decreases marginally compared to sub-bituminous coal case.

Both capital cost and the cost of liquid product are much higher compared to the higher quality coals. CCS is still more cost-effective than the case with CO_2 price.

Table 8.5: Performance and cost results for ND Lignite, different gasifier technologies

Gasifier	GE	EGas	Shell
Output (barrels/day)	50,000	50,000	50,000
Coal (tonnes/day)	37,273	37,155	35,697
CO_2 without CCS (tonnes/day)	28,172	27,466	26,679
CO_2 with CCS (tonnes/day)	240	456	312
Efficiency (% HHV)	53.6	53.7	55.9
Capital cost (without CCS $/barrel/day)	129,022	124,727	119,891
Capital cost (with CCS $/barrel/day)	130,299	125,975	121,094
Cost of liquid (without CCS, $/barrel, $0/tonne CO_2)	84.5	82.1	79.1
Cost of liquid (without CCS, $/barrel, $25/tonne CO_2)	98.5	95.8	92.4
Cost of liquid (with CCS, $/barrel)	90.9	88.4	85.2

E-Gas Gasifier

With lignite as feedstock, E-Gas gasifier has better performance and cost characteristics compared to the GE case. Coal consumption and CO_2 emissions are lower than when a GE gasifier is used. Capital cost is 3% lower than the GE case and the liquid product cost is cheaper by about $2/MWh. This shows that for very low quality coals, E-Gas is a better choice than GE, in terms of both performance and cost.

Shell Gasifier

The Shell gasifier is still the best in terms of performance and costs. Coal consumption, CO_2 emissions, capital costs and liquid product costs are all lower compared to the other gasifier cases. But the coal consumption is about 40% higher than the corresponding PRB case.

8.2.4 Uncertainty Analysis

Figure 8.1 shows the effect of uncertainties in economic and non-economic parameters on the product cost for a Shell gasifier case with all the coals, with CCS. The ranges of uncertainties are shown in chapter 3 and are not repeated here, except for the price range of sub-bituminous and lignite coals is chosen as between \$10 - \$20/tonne. The costs vary over a large range (\$50 - \$110/barrel), when all the uncertainties are taken into account. The figure shows the importance of feedstock on the cost of liquid product. Though Illinois#6 coal case has the highest efficiency, Wyoming PRB produces cheaper fuels. Liquids from ND lignite are the costliest over the range.

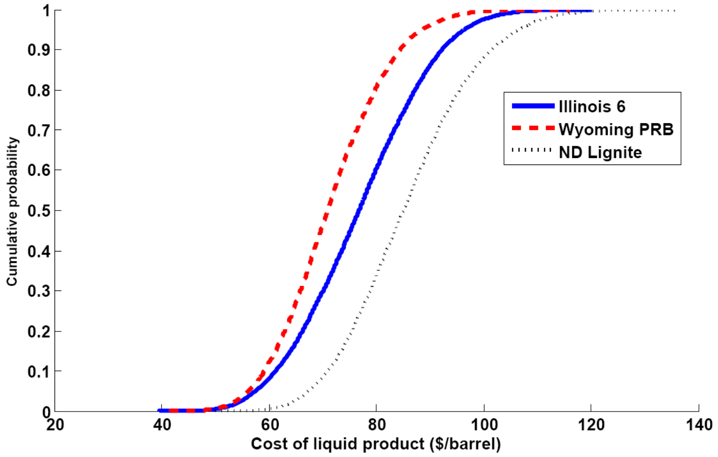


Figure 8.1: Uncertainty analysis for a liquids-only plant with CCS for the Shell case, with all the coals. Wyoming PRB has the lowest cost

8.3 Analysis of the Co-production Configuration

Tables 8.6 – 8.8 show results of co-production configurations using Illinois#6, PRB and ND lignite coals respectively.

Table 8.6: Performance and cost results for Illinois#6, different gasifier technologies, for a co-production configuration

Gasifier	GE	EGas	Shell
Output (barrels/day)	50,000	50,000	50,000
Coal (tonnes/day)	23,571	28,812	22,986
CO_2 (without CCS, tonnes/day)	35,392	47,609	34,986
CO_2 (with CCS, tonnes/day)	801	1560	1,110
Net power output (without CCS, MW)	1,045	1,749	1,196
Net power output (with CCS, MW)	887	1,560	1,030
Efficiency (without CCS, % HHV)	55.2	53.2	58.8
Efficiency (with CCS, % HHV)	53.0	50.3	56.4
Capital cost (without CCS, \$/barrel/day)	117,196	137,119	111,516
Capital cost (with CCS, \$/barrel/day)	129,345	166,946	127,551
For electricity selling price of \$80/MWh:			
Cost of liquid (without CCS, \$/barrel, \$0/tonne CO_2)	54.1	43.9	44.6
Cost of liquid (without CCS, \$/barrel, \$25/tonne CO_2)	71.8	67.7	62.1
Cost of liquid (with CCS, \$/barrel)	75.5	82.7	68.7
Cost of liquid (with CCS, \$25/barrel)	75.9	83.5	69.2

8.3.1 Illinois#6 case

These results are the same as in the previous chapter.

GE Gasifier

A co-production CTL plant with GE gasifier consumes 23.6 kilo tonnes/day of coal. Without CCS, 35.4 tonnes/day of CO_2 is emitted and about 1,045 MW of electricity is co-produced. With CCS, CO_2 emissions reduce to 800 tonnes/day and the co-product electricity decreases to 890 MW. The overall efficiency of this plant is 55.2% without CCS and 53% with CCS, which is lower than the corresponding liquids-only case. The capital cost of the plant without CCS is $117,196/barrel/day and $129,345/barrel/day with CCS, about 30% higher than the corresponding liquids-only plants.

E-Gas Gasifier

With E-Gas gasifier, coal consumption is 28.8 kilo tonnes/day, which is 22% higher than in the GE case. CO_2 emissions without CCS are estimated to be 47.6 kilo tonnes/day, which came down to 1,590 tonnes/day with CCS. The electricity produced is much higher than in the GE case – 1,749 MW without CCS and 1,493 MW with CCS. The unconverted syngas which is burnt in the combined cycle power plant contains a higher amount of methane, thereby having a higher overall heating value than compared to the gas in the GE case. More N2 has to be added to adjust the heating value. Also, the quantity of unconverted syngas is higher in this case because of the higher fraction of methane. This is the reason for the higher net power output as well as higher CO_2 emissions. The capital cost of the plant without CCS is \$137,119/barrel/day and \$166,946/barrel/day with CCS, about 40% higher than the corresponding liquids-only plants.

Shell Gasifier

As in the liquids-only plants, a co-production CTL plant with a Shell gasifier consumes the least amount of coal (23 kilo tonnes/day) and emits 34.9 kilo tonnes/day of CO_2 without CCS. The electricity production is higher than the GE case but lower than the E-Gas case – 1,196 MW without CCS and 1,110 MW with CCS. The overall efficiency of the plant is higher than both GE and E-Gas cases but lower compared to the corresponding liquids-only plant using a Shell gasifier. This shows that the relative efficiencies of co-production and liquids-only configurations depend heavily on the gasifier technology used.

The cost of product liquids from a co-production plant depends on the revenue generated from electricity sales. Table 3 also compares the cost of liquid product in all three cases for an electricity selling price of \$80/MWh. When there is no CCS and no CO_2 price, the E-Gas case has the lowest liquid product cost but when there is either CCS or CO_2 price or both, CTL plant with a Shell gasifier produces the cheapest liquid fuels.

8.3.2 Wyoming PRB case

The results for this case are shown in table 8.7

GE Gasifier

A co-production CTL plant using sub-bituminous coal uses 60% more coal and emits 6% less CO_2 compared to bituminous coal. The net power output without CCS is 786 MW, which is much smaller than the bituminous case. With CCS, CO_2 emissions reduce to 671 tonnes/day and the co-product electricity decreases to 627 MW. The overall efficiency of this plant is 50% without CCS and 47.8% with CCS, which is lower than the corresponding liquids-only case as well as the bituminous case. The capital cost of the plant without CCS is $133,380/barrel/day, 25% higher than the corresponding liquids-only case. With CCS, the capital cost increase further by 8%. The cost of liquid product is lower than the corresponding liquids-only cases when electricity is sold at $80/MWh. As in the bituminous case, CCS is not cost-effective compared to a CO_2 price of $25/tonne.

Table 8.7: Performance and cost results for Wyoming PRB, different gasifier technologies, for a co-production configuration

Gasifier	GE	EGas	Shell
Output (barrels/day)	50,000	50,000	50,000
Coal (tonnes/day)	32,803	37,491	32,649
CO_2 (without CCS, tonnes/day)	38,227	46,462	38,898
CO_2 (with CCS, tonnes/day)	671	1,254	1,107
Net power output (without CCS, MW)	786	1,534	979
Net power output (with CCS, MW)	627	1,295	802
Efficiency (without CCS, % HHV)	50.0	52.6	52.8
Efficiency (with CCS, % HHV)	47.8	49.8	50.4
Capital cost (without CCS, $/barrel/day)	133,381	148,109	129,512
Capital cost (with CCS, $/barrel/day)	143,639	172,485	145,649
For electricity selling price of $80/MWh:			
Cost of liquid (without CCS, $/barrel, $0/tonne CO_2)	55.3	36.0	45.8
Cost of liquid (without CCS, $/barrel, $25/tonne CO_2)	74.4	59.2	65.3
Cost of liquid (with CCS, $/barrel)	76.1	70.5	71.2
Cost of liquid (with CCS, $25/barrel)	76.5	71.1	71.7

E-Gas Gasifier

The CTL co-production plant with EGas gasifier is more efficient than the corresponding GE case, mainly because of the huge difference in net power output. The plant without CCS produces 1,535 MW of electricity and with CCS, this reduces to 1,295 MW. This is reflected in the cost of liquid product which is much lower than the corresponding GE case and liquids-only cases. This is lower than even the Shell case, unlike in the previous cases where a plant with Shell gasifier produced the cheapest liquids.

Shell Gasifier

The CTL co-production plant with Shell gasifier is more efficient than the other two cases. Capital cost is also lower than GE and E-Gas cases. However, since the net power generated is lower than in the E-Gas case, the cost of liquid product is higher.

In terms of performance, dry-feed gasifier still has the best characteristics.

8.3.3 ND lignite case

The results for this case are shown in table 8.8. The behavior of different gasifiers is similar to the PRB case. However, here E-Gas case is the most efficient, despite its coal consumption being the highest. The high net electricity output balances the increase in coal flow rate. As a result, despite E-Gas being the costliest in terms of capital cost, the cost of liquid product is the cheapest under all carbon constraints.

Table 8.8: Performance and cost results for ND lignite, different gasifier technologies, for a co-production configuration

Gasifier	GE	EGas	Shell
Output (barrels/day)	50,000	50,000	50,000
Coal (tonnes/day)	44,105	46,335	45,610
CO_2 (without CCS, tonnes/day)	36,947	39,826	39,816
CO_2 (with CCS, tonnes/day)	454	825	1,106
Net power output (without CCS, MW)	652	1,402	982
Net power output (with CCS, MW)	506	1,210	803
Efficiency (without CCS, % HHV)	49.6	57.2	52.4
Efficiency (with CCS, % HHV)	47.6	56.4	50.0
Capital cost (without CCS, $/barrel/day)	156,012	160,673	155,435
Capital cost (with CCS, $/barrel/day)	163,402	176,795	171,577
For electricity selling price of $80/MWh:			
Cost of liquid (without CCS, $/barrel, $0/tonne CO_2)	75.3	49.7	62.8
Cost of liquid (without CCS, $/barrel, $25/tonne CO_2)	93.8	69.6	82.7
Cost of liquid (with CCS, $/barrel)	93.5	75.8	88.4
Cost of liquid (with CCS, $25/barrel)	93.7	76.2	89.0

8.3.4 Effect of electricity selling price and CO_2 price

To illustrate the effect of electricity selling price and CO_2 price on the cost of liquid product, the combination of ND lignite and E-Gas gasifier is chosen. Figure 8.2 shows the effect of the electricity selling price on the cost of product liquids. Co-production plant becomes cheaper than liquids-only plants when the selling price of electricity is in the range of $30 – 60/MWh. Like in all the other cases studies previously, the results show that co-production plants can produce liquid fuels which are cheaper than those produced from liquids-only plants. The CO_2 price needs to be about $40/tonne to make CCS the cost-effective carbon mitigation option.

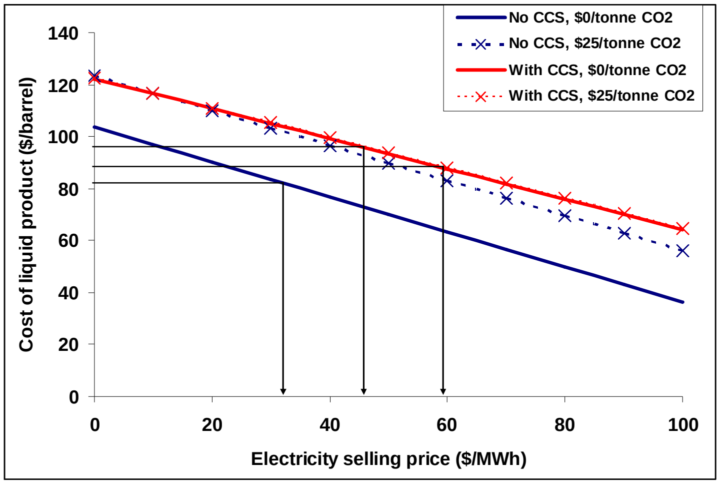


Figure 8.2: Effect of electricity selling price on the cost of liquid product for a co-production CTL plant using GE gasifier. $25/tonne CO_2 is not enough to make CCS cost-effective

7.3. Discussion

The results show that in general, bituminous CTL plants are more thermally efficient, consume less coal and emit less CO_2 than lower quality coals. In low quality coals, there is a lot of moisture and/or ash, which have to be removed to get syngas of useful composition. Since the amount of components which have to be removed is less in bituminous coals, coal consumption also is lower in bituminous cases.

Even though performance-wise bituminous coals are better, in terms of cost of liquid product, sub-bituminous and lignite are more cost-effective, mainly because of their low prices.

The most important point that comes out of this analysis is that both performance and cost depend a lot on the type of technology and feedstock used.

Chapter 9: Large Scale Impacts of CTL

In this chapter, the magnitude of emissions and resource consumption impacts of large scale implementation of CTL plants is estimated. For a base case, it is assumed that 20% of US petroleum demand is met by coal liquids.

9.1 Coal Consumption Factors

Specific coal consumption factors for different coals and different gasifier technologies were obtained from the performance model. The values in tonnes of coal required per barrel of liquid output are shown in Fig 9.1. As seen in the previous chapters, the figure also shows that the dry-feed Shell gasifier technology has the lowest coal consumption for all the coals, followed by GE and then E-Gas. For liquids-only cases, GE gasifier with ND lignite coal feed has the highest coal consumption factor. In co-production cases, E-Gas with ND lignite has the highest factor.

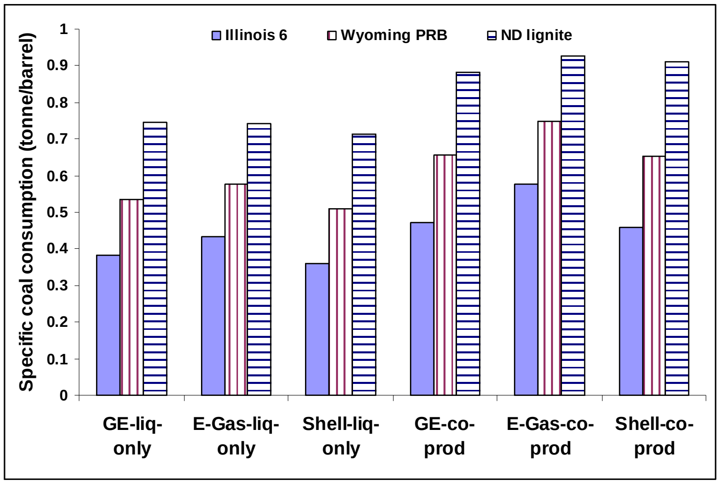


Figure 9.1: Specific coal consumption factors for different coals and technologies, for liquids-only and co-production configurations

9.2 Life Cycle CO_2 Emission Factors

Specific life cycle CO_2 emission factors are obtained using the methodology explained in chapter 5. The values in tonnes of CO_2/barrel of liquid are shown in Fig 9.2 for cases without CCS and in Fig 9.3 for cases with CCS. With CCS at the plant level, life cycle CO_2 emissions can be reduced by more than half in all the cases.

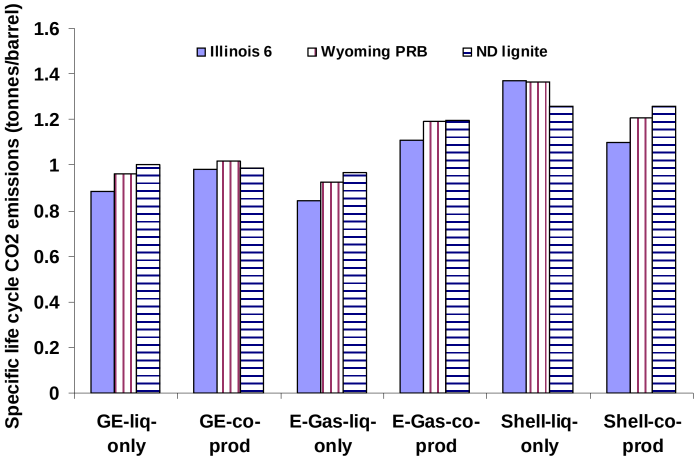


Figure 9.2: Specific CO_2 emission factors for different coals and technologies, for liquids-only and co-production configurations, without CCS

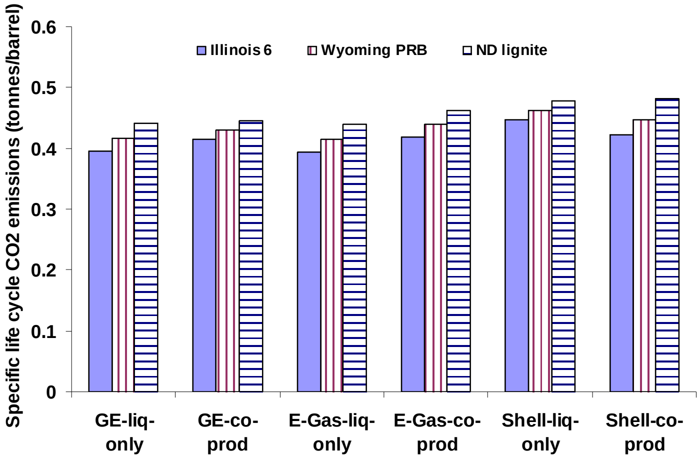


Figure 9.3: Specific CO_2 emission factors for different coals and technologies, for liquids-only and co-production configurations, with CCS

9.3 Land Use Factors

Land use factors calculated in chapter 5 are shown here in Fig 9.4. Since land use was scaled directly with coal flow rate, co-production plants with lignite have the highest land use impact.

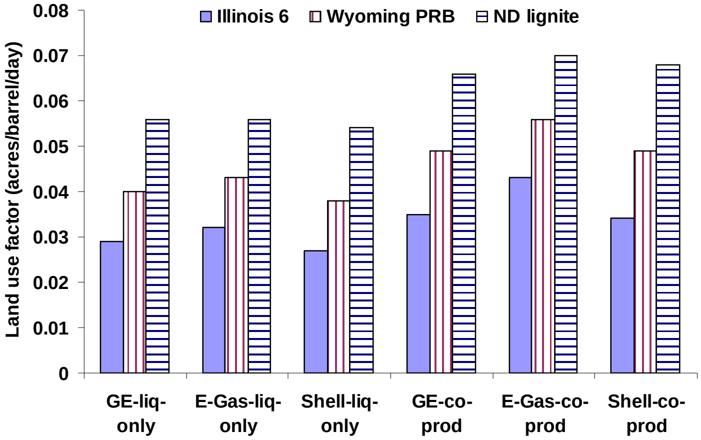


Figure 9.4: Specific land-use estimation factors for different coals and technologies, for liquids-only and co-production configurations

9.4 Water Use Factors

Calculation procedure for water use factors was explained in chapter 5. Figure 9.5 shows the factors used for impact assessment.

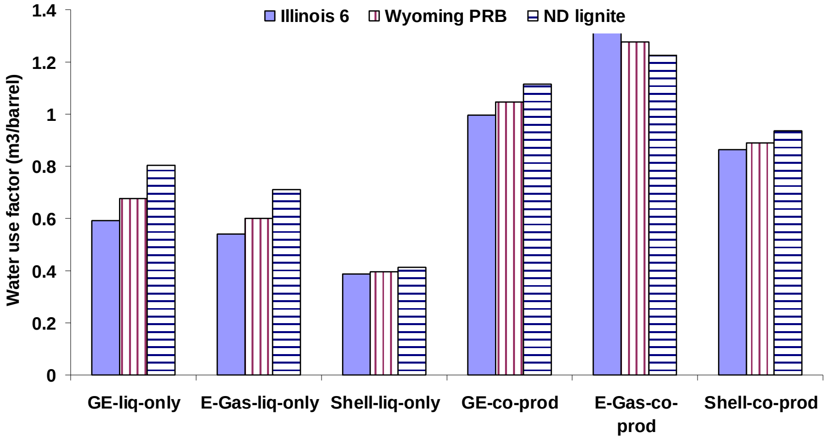


Figure 9.5: Specific water-use estimation factors for different coals and technologies, for liquids-only and co-production configurations

9.5 Estimation of Large Scale Impacts

To estimate the impacts of coal liquids substituting 20% of 2008 US petroleum demand, the choice of technology and coal type need to be known. Though CTL plants using dry-feed gasification system and bituminous coal have the lowest coal consumption, CO_2 and land use impacts, it is unrealistic to expect all the coal liquids being produced using that combination. Here, weighting factors are used to determine weighted average values for coal consumption, life cycle CO_2 emissions and land use factors.

In 2008, US coal production was 47.5% bituminous, 46.1% sub-bituminous and 6.5% lignite, by mass [EIA, 2009, coal production statistics]. Anthracite production is excluded in calculating these percentages. Since 2008 is taken as the base year, it will be assumed that coal liquids will be produced by a coal feedstock comprising of these percentages of different coal types.

Since any technology can be used with equal probability, equal weights are given to each of the gasifier technologies.

Using these weighting percentages, the calculated weighted average impact factors are shown in table 9.1.

Table 9.1: Weighted average impact assessment factors

Coal (tonnes/barrel)	0.483 for liquids-only 0.613 for co-production
CO2, no CCS (tonnes/barrel)	0.939 for liquids-only 1.225 for co-production
CO2, with CCS (tonnes/barrel)	0.412 for liquids-only 0.442 for co-production
Land use (acres/barrel/day)	0.036 for liquids-only 0.046 for co-production
Water use (m3/barrel)	0.539 for liquids-only 1.066 for co-production

9.6 Estimation of Impacts for 20% Substitution

Large-scale impact assessment is done for the case of 20% of the petroleum demand substituted by coal liquids. In this scenario, 3.88 million barrels/day of liquids would have to be produced by CTL technology. The impacts will differ with the configuration of the plant. Results of coal consumption for this purpose, CO_2 emissions associated, land and water requirements are shown in table 9.2. Increase in quantities over 2008 values are also shown in within parentheses. In 2008, US coal consumption was 1,020 million tonnes and CO_2 emissions associated with energy were 5.8 billion tonnes. Since conventional petroleum is displaced, the use phase CO_2 emissions associated with that has to be subtracted from the life cycle emissions of coal liquids to calculate the net increase in CO_2 emissions from 2008 values. The emission factor for conventional petroleum is taken as 0.381 tonnes CO_2/barrel (20 lb/gallon).

Table 9.2: Quantities for 20% replacement of US petroleum demand by coal liquids. Net increase in values from 2008 levels are shown in parentheses

	Liquids-only	Co-production
Coal consumption (million tonnes/day)	1.873 (67%)	2.380 (85%)
CO2 without CCS (million tonnes/day)	3.642 (14%)	4.747 (21%)
CO2 with CCS (million tonnes/day)	1.600 (0.8%)	1.714 (1.5%)
Land requirement (million acres)	0.140	0.178
Water use (million m3/day)	2.091	4.135

If only liquids-only plants are built, the coal consumption associated with coal liquids will be 3.642 million tonnes/day, which will greatly increase the US coal consumption (by 67%). If co-production plants are built, the overall coal consumption will be go up by 85%. These are significant increases in coal consumption.

Life cycle CO_2 emissions of coal liquids in this case are 1.6 million tonnes/day. In 2008, the proven reserve base of coal was 446 billion tonnes. The net increase in CO_2 emissions without plant level CCS is 14%. With CCS, the increase will be marginal, about 0.8%. If co-production plants are built, the overall CO_2 emissions without CCS will be 21% higher and with CCS, the increase will be only 1.5%. The land use for liquids-only plants will be 0.14 million acres and for co-production 0.178 million acres, roughly one-third of Allegheny county. Fresh water requirements range from 2 million m3/day to 4 million m3/day. In 2004, fresh water withdrawal from rivers was nearly 500 million m3/day [DoE, 2006]. Compared to this number, water requirement will increase only marginally because of large scale CTL implementation.

The analysis above shows that large scale implementation of CTL will have adverse impacts on resources and environment. Even though CO_2 emissions do not increase by much if CCS were used, the coal consumption will still go up by a huge extent. CTL plants also require significant amount of land. If mitigation measures are not taken in other sectors, using CTL on a large-scale leads to environmental risk.

9.7 CO_2 Reduction Potential of CTL

It was seen in chapter co-production of liquids and electricity is more efficient and emits less CO_2 compared to separate production. Here, potential of co-production in reducing the overall CO_2 emissions is discussed, first at the plant level and then at a large scale.

9.7.1 Plant level comparison

A 50,000 barrels/day co-production plant can produce net electricity ranging from 650 MW – 1750 MW without CCS and between 500 MW – 1,500 MW with CCS, depending on the gasifier and coal combinations. As mentioned in chapter 5, pulverized coal plants without CCS have efficiencies in the range of 32 – 36% (HHV) and 17 – 21% with CCS, depending on the quality of coal. A comparison is made here of co-production of liquids and power in a co-production CTL plant and separate generation of liquids in a liquids-only CTL plant and power in conventional coal power plants. Figure 9.5 shows the coal consumption values for different gasification and coal combinations, with and without CCS. Generally, as coal quality decreases, coal consumption increases for separate production, both for capture and non-capture cases. Coal consumption does not change with the addition of CCS for co-production plants because some amount of output power is used to supply the CCS energy requirements. However, addition of CCS increases the coal consumption in separate generation. Though coal consumption in liquids-only CTL plants does not change with CCS, power plants consume more coal to meet the requirements of CCS and to maintain constant power output. For the lignite-E-Gas case, coal consumption increases by as much as 66% with the addition of CCS. In all cases, co-production plants consume less coal than separate production of liquids and power. When there is no CCS, co-production plants consume 10 – 35% less coal than separate production. With CCS, the savings with co-production are much higher, ranging between 30 – 100%. Thus it is clear that co-production is more efficient than separate production of liquids and power. The marginal efficiency increases with the addition of CCS.

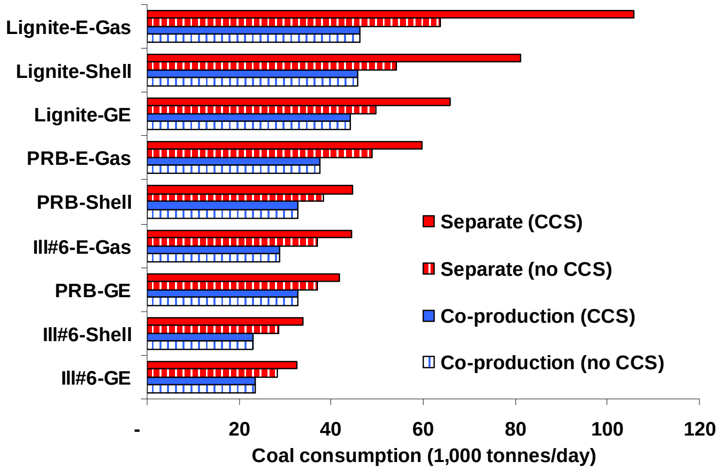


Figure 9.6: Comparison of coal consumption for co-production and separate production liquids and power. The liquids output capacity of CTL plants is 50,000 barrels/day.

Figure 9.6 makes a similar comparison of CO_2 emissions. Again it is clear that CO_2 emissions are also lower for co-production than separate production. Even with the addition of CCS, co-production plants have way lower CO_2 emissions compared to separate production.

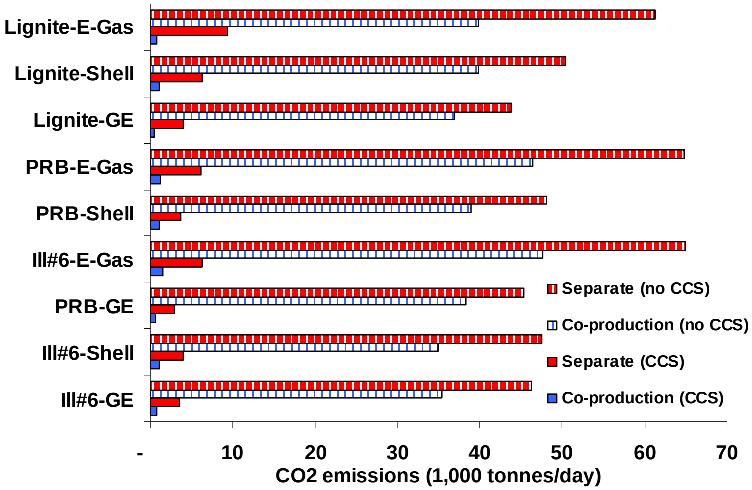


Figure 9.7: Comparison of CO_2 for co-production and separate production liquids and power. The liquids output capacity of CTL plants is 50,000 barrels/day.

From the preceding discussion, it can be ascertained that co-production of liquids and power is significantly more efficient and leads to much lower CO_2 emissions than separate production. If co-production plants can displace conventional coal power plants, the increase in coal consumption can be lower as compared to CTL plants being built with conventional coal power plants continuing to produce power. With the implementation of large scale CCS, displacing conventional coal power plants with co-production CTL plants can actually lead to lowering the overall CO_2 emissions.

9.7.2 Large scale comparison

For 20% petroleum displacement, co-production plants are capable of replacing about 93 GW of net electrical capacity without CCS and 78 GW with CCS. For the assumed 85% base case capacity factor, this means that co-production plants can supply 693,370 GWh and 577,810 GWh respectively. In 2008, total coal based electricity consumption was 1,994,385 GWh. This means that CTL co-production plants can displace up to 35% of conventional coal power without CCS and 29% with CCS, at the same time supplying 20% of the country's liquid fuel demand.

To meet these requirements using separate production of liquids in liquids-only CTL plants and power in conventional coal plants, the overall coal consumption is 23% more than co-production without CCS and 50% more with CCS. Similarly, the overall life cycle CO_2 emissions from co-production are about 23% lower than with separate production. These comparisons are depicted in Fig 9.8.

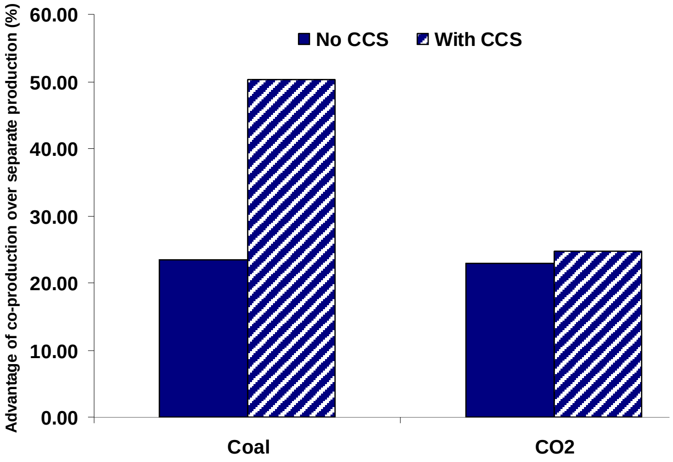


Figure 9.8: Advantage of co-production of liquids and power compared to separate production, in terms of coal consumption and life cycle CO_2 emissions. Co-production has significant advantages over separate generation

9.7.3 Co-production plants displacing conventional coal power plants

Table 9.2 shows that using co-production plants will increase the overall life cycle CO_2 emissions from 2008 levels by 21% without CCS and by 1.5% with CCS, for 20% substitution of liquid fuel demand by coal liquids. Here, the option of co-production plants displacing conventional coal power plants is explored for the following scenarios:

- Co-production plants without CCS displace power plants without CCS

- Co-production plants with CCS displace power plants without CCS (none of the power plants in 2008 included CCS)
- Co-production plants with CCS displace power plants with CCS

A comparison of coal consumption and life cycle CO_2 emissions for each of these scenarios is shown in table 9.3. The values show the percentage increase over 2008 US coal consumption (1,020 million tonnes) and energy related CO_2 emissions (5,800 million tonnes). For this calculation, capacity factors were assumed as 85% for CTL plants and 75% for coal power plants. Since 20% of conventional petroleum is displaced, their emissions are also deducted from these life cycle CO_2 calculations.

Table 9.3: Increase over 2008 US coal consumption and CO_2 emissions caused because of displacing conventional coal power plants with co-production CTL plants, for 20% substitution of liquid fuel demand by coal liquids

Scenario	Increase over 2008 values	
	Coal	CO_2
Co-production plants without CCS displace power plants without CCS	44%	6%
Co-production plants with CCS displace power plants without CCS	49%	– 9%
Co-production plants with CCS displace power plants with CCS	27%	– 3%

If co-production plants without CCS displace conventional coal power plants without CCS, the overall annual coal consumption will be 1,470 million tonnes, an increase of 44% over 2008 values and annual life cycle CO_2 emissions will be 6,130 million tonnes, an increase of 6%. If co-production plants with CCS replace power plants without CCS, then the overall coal consumption will significantly increase by.49%. But the overall CO_2 emissions will be reduced by 9% from the 2008 values. When both co-production and power plants have CCS, there is still a decrease of 3%, but smaller than the case when power plants did not have CCS. Since no power plants had CCS in 2008, the second scenario is more realistic.

The above calculations show that co-production CTL plants with CCS, supplying 20% of petroleum demand, can meet around 30% of US electricity demand (energy basis) and by displacing conventional coal power plants, have the potential of reducing the US CO_2 emissions by 9% from the 2008 emissions.

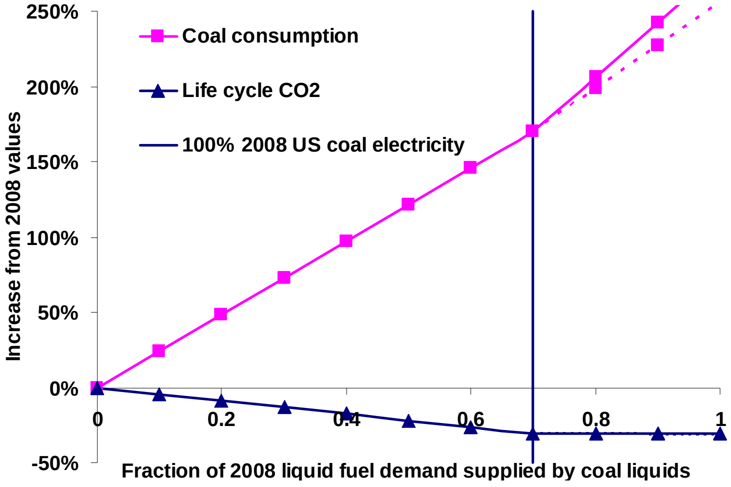


Figure 9.9: Change in coal consumption and CO2 emissions as a function of the US liquid fuel demand met by coal liquids, co-production CTL plants displacing coal power plants. Beyond 70% substitution of coal liquids, all the coal based electricity is displaced. Dotted lines show the variations assuming liquids-only CTL plants are built thereafter.

Figure 9.9 shows, for the same scenario, the increase in coal consumption and decrease in overall CO_2 emissions for different fractions of petroleum demand met by coal liquids. If 70% of the liquid fuel demand is met by coal liquids, all of US electricity coming from coal is displaced. Since these calculations have the underlying assumption that the rest of the energy system remains unchanged, after 70% substitution, the electricity generated by co-production CTL plants acts as capacity addition. However, there is another option of using liquids-only configuration once all the coal power plants are displaced by co-production CTL plants. In such a case, coal increase in coal consumption is less than if co-production plants were used, as shown with dotted lines on the figure. However, the difference in CO_2 reduction is not highly different. From the figure, it is clear that 30% of overall CO_2 emissions can be reduced just from co-production plants with CCS replacing conventional coal power plants, rest of the energy system being unchanged. Though this is a hypothetical scenario, it shows the potential for net overall CO_2 reduction of co-production plants. It must also be noted that these calculations are valid for the energy system as it was in 2008 and if all the CTL plants were built in that year. A more thorough analysis requires dynamic simulation of changes in oil and electricity demands and changes in other sectors of the energy system, which is beyond the scope of this thesis.

Chapter 10: Policy Recommendations and Conclusion

In this chapter, the role of coal-derived liquids is analyzed from the perspective of a broader policy framework. The policy analysis is divided into three aspects, based on the methodology of Farrell and Brandt (2006) – environmental, economic and strategic implications of coal liquids.

The US consumed 19.4 million barrels per day of petroleum products during 2008. Roughly 60% of these were imported. Coal liquids, produced at competitive prices, can contribute as a source of domestic fuels, and decrease dependence on imports. As seen in the previous chapters, the cost of producing coal liquids depends on various factors such as coal type, technology choice, carbon constraints and uncertainty in parameters. Large scale production of coal liquids will also significantly affect resource consumption and CO_2 emissions.

10.1 Environmental implications of coal liquids

The primary environmental impacts of coal liquids occur in the form of emissions and increased resource consumption. It was seen in Chapter 9 that if coal liquids substitute 20% of the 2008 US petroleum demand, US coal consumption increases by 67% to 85%. Increased coal consumption results in increased mining, transportation and their associated effects. In this thesis, only CO_2 emissions associated with coal mining and transportation were considered, in the form of life cycle emissions of coal liquids. Without CCS, the overall life cycle CO_2 emissions will increase by 14 – 21% from the 2008 levels, as found in Chapter 9.Given the high concerns about climate change, this increase is very significant. However, when CCS is implemented, the increases are only marginal (of the order of 1.5%). However, CCS can mitigate only the plant level CO_2 emissions. Emissions from the combustion of coal-derived liquid fuels in automobiles and other sources still remain.

It was also shown in Chapter 9 that CO_2 emissions can actually be reduced if co-production plants with CCS displace conventional coal power plants. Depending on what fraction of petroleum demand is supplied by coal liquids, overall CO_2 emissions can be reduced by as much as 30% (Figure 9.9). But the quantity of CO_2 to be sequestered would be of the order of millions of tonnes per day, or billions of tonnes per year. Theoretically, there is enough storage capacity in the US to sequester that much CO_2. Nevertheless, these are still tremendously high volumes, considering that large scale CCS has not yet been commercially demonstrated at the scale of several million tonnes per year. Thus, without CCS, production and use of coal liquids poses a high environmental risk, particularly in terms of life cycle CO_2 emissions.

Co-production plants produce liquids at a lower cost ($/barrel) than stand-alone plants because of the revenues from by-product electricity sales. In Chapters 7 and 8, it was shown that to make CCS an economically viable option for co-production plants, CO_2 price must be at least $30/tonne. Considering that climate change policies are just getting started in the US, such CO_2 prices are not expected in the near future. That means, in that time frame, it will be cheaper to emit CO_2 than to mitigate using CCS.

Thus, while co-production plants with CCS have the potential to mitigate overall CO_2 emissions, the actual prospects depend critically on commercial implementation of CCS. Regulations have to be devised to encourage the use of CCS for CTL plants.

On the other hand, FT fuels are ultra-clean in terms of criteria air pollutants like NOx and SOx. FT diesel has been proved to be an excellent automobile fuel and can be used even as blends in normal diesel [Norton et al, 1998; Dry 1999]. FT diesel offers a considerable advantage over other alternate fuels in that there is no need for any modifications to existing diesel automobile engine designs. FT gasoline, on the other hand, has a low octane value and requires subsequent treatment to meet the fuel standards. There are methods of converting low octane FT gasoline to motor standard fuel [Marano, 2007]. However, no literature is available on the actual testing of FT gasoline in commercial vehicles. This is a significant matter for consideration because most of the automobile fleet in the U.S. uses gasoline as the fuel.

10.2 Economic implications of CTL technology

It was seen in previous chapters that the capital cost of a 50,000 barrels/day CTL plant vary from about \$80,000 to \$160,000 per daily barrel, depending on the fuel, technology and plant configuration. This translates to a capital investment of \$4 billion - \$8 billion for each plant. Similarly, the cost of coal liquids can be anywhere in the range of \$35 - \$110/barrel, depending on the coal type, configuration and technology choice. The lower end of this range requires the sale of by-product electricity from co-production plants. The economic feasibility of CTL plants depends mainly on where the price of crude oil stands in this range. Unless crude oil prices are sufficiently high, investment in CTL is fraught with significant financial risk. Considering the volatility of oil prices, CTL plants may become uneconomical, should oil prices fall. Though low prices benefit consumers, they cause major financial risk to investors.

One way of mitigating economic risk is by producing diverse products from CTL plants. FT reactors can be operated in different modes, maximizing one set of hydrocarbons over another. If CTL plants produce chemicals besides transportation fuels, that adds a revenue stream to the plant, with the potential of reducing the cost of liquid fuel product.

Government policies with direct or indirect financial assistance can mitigate some of the financial risk involved in CTL plants. Plants in South Africa were built with the help of government support, and such a model can be practiced in the U.S. as well. However, such a decision needs to weigh the environmental risk posed by coal liquids.

10.3 Strategic implications of CTL technology

In 2008, approximately 60% of US oil consumption came from imports, roughly half (about 6 million barrels/day) of which are from countries with uncertain political stability. In scenarios of high crude oil prices and uncertainty in supply, coal liquids offer a cheaper and more stable alternative to crude oil. Thus, CTL technology has the potential to increase the energy security of the U.S, with its large coal reserves, by reducing the dependence on imports. As seen in chapter 9, if all of the imports are substituted by coal liquids, co-production plants can displace almost all of the coal based electricity. By co-production of liquids and power, the net increase in coal consumption would be smaller than for separate plants, though it would still be a large increase over current levels.

One strategic advantage of using coal liquids for transportation is that there would be no need for any change in the existing transportation infrastructure. These fuels can be used directly or blended with normal automotive fuels. This offers a comparative advantage for coal liquids over other alternative fuels, such as H_2.

From a policy perspective, CTL thus offers considerable advantages as well as significant risks. As pointed out by Farrell and Brandt (2006), any decision regarding the implementation of CTL on a large scale has to consider simultaneously all of the implications described above.

10.4 CTL – Different investor and regulator perspectives

CTL technology is of interest to different industries, government and regulatory agencies. In this section lists the likely perspectives of industries such as oil and power utilities, the US Department of Defense (DoD), research organization such as US Department of Energy (DoE) and regulatory agency such as US Environmental Protection Agency (EPA).

Petroleum industry

Since liquids are the primary products from a CTL plant, this technology is well suited for the oil industry to invest in. The petroleum industry has both technical and market expertise to operate CTL plants. A CTL plant is essentially a chemical engineering plant with processes involving reactors, catalysts, heat exchangers, refrigeration plants, and refineries and so on. Gasification and cleanup processes are also essentially chemical processes. Since the crude oil production and refinery industry already handles most of these processes, oil companies are technically well-suited to operate CTL plants. Apart from operational advantages, the oil industry also has the advantage of familiar market conditions.

The high capital investment is a cause of concern if market prices of oil were to drop. Possible future CO_2 regulations will also affect the cost of liquid products. However, the large amounts of high-purity CO_2 from a CTL plant can be used for enhanced oil recovery (EOR), adding a revenue stream that can push the cost liquid products down. EOR also increases the production of conventional crude oil from oil wells.

Power utility industry

Power utility industry is another likely investor in CTL plants, mainly because of the electricity co-production potential. It was seen in Chapter 6 that the by-product electricity from a co-production plant is a significant source of revenue which makes co-production configuration more profitable than a corresponding liquids-only plant, even at low electricity prices.

In terms of operation, a co-production CTL plant is an extension of coal integrated gasification combined cycle power plant (IGCC). However, owing to the near absence of any IGCC plants in the US, today’s power industry has minimal operational experience with regards to gasification facilities. This, coupled with the complicated chemical processes associated with CTL plants make them challenging for the power industry to operate. The liquid fuel market is also a relatively unfamiliar territory for the utility industry. Though co-production plants are more profitable, their capital cost is at least 50% higher than a liquids-only plant, thus increasing the financial risk. Also, unlike liquids, electricity can be sold only when there is demand. Going by the reluctance of the power utility industry with respect to investment in IGCC power plants, whose capital cost is higher than the conventional pulverized coal power plant, it is unlikely that power utility industry will be ready to invest in CTL.

Joint investment of petroleum and utility industries

CTL technology offers a platform for a joint venture between the oil and power industries. While the liquids-only configuration is the more likely choice for oil industry, the co-production configuration, which is more relevant for utility industry, has higher profitability. The likelihood of CTL becoming economically viable over a range of conditions increases if the technical and operational expertise of both the petroleum and utility industries were combined. However, it is also a challenge because of the differences in business cultures in the two industries.

US Department of Defense

CTL can be an attractive investment for the US Department of Defense because of the technology's potential to reduce the dependence on foreign oil for defense purposes. DoD has already shown interest in the development of innovative CTL concepts so that cheap and environmentally friendly transportation fuels [DoD, 2008]. The key challenge for using CTL for defense purposes is the high capital cost of the technology. The consumption of petroleum based fuels for defense purposes was close to 300,000 barrels/day. Based on the cost estimates made in this study, a 50,000 barrels/day plant would require a capital investment of the order of \$4 - \$8 billion. To meet the total requirement, a capital investment on the order of \$40 billion is needed. The defense budget in fiscal 2009 was close to \$530 billion [source: www.defense.gov]. Investment in CTL would result in approximately 7% increase over this. The risk of there being a cut in defense oil supplies must be sufficiently high to make investment in CTL economically viable for defense purposes, particularly in the light of more important war expenditures. According to the kind of research proposals sought by DARPA, the innovative CTL technology should not cost more than \$15,000/bbl/day in capital cost [DoD, 2008]. Clearly, the conventional FT-based CTL plants dealt with in this study are far costlier than what is in the interest of DoD. Thus, even though CTL has strategic advantages for DoD, the economic constraints are unfavorable for this technology.

US Department of Energy (DoE)

CTL offers a strategic advantage of enhancing the country’s energy security by producing domestic liquid fuels. By appropriate measures, it is also possible to reduce the environmental risk of CTL, as explained previously in Section 10.1 and also in Chapter 9. From the different investor perspectives discussed in the preceding paragraphs, it is clear that economic risk is the biggest factor that can prevent CTL technology from becoming commercial. The financial risk can be reduced by providing government support in covering a fraction of the high capital costs of CTL plants. DoE already has loan guarantee programs for investors in clean coal technologies like IGCC power plants. Considered in that light, CTL technology is also a clean coal technology because of the low emissions of criteria air pollutants in liquid fuel production as well as in power production. Also, CCS cost is internalized in a CTL plant, unlike in power plants. Thus, it is possible for DoE to expand loan guarantees to CTL technologies also. The CTL industry in South Africa was initially supported by the government and played an important role in making it profitable. However, any kind of support for CTL must be coupled with CO_2 sequestration, because finding ways to reduce greenhouse gas emissions is also one of the objectives of DoE. At the same time, DoE must invest in research to find novel ways of producing liquid fuels from coal which will be more efficient than the current technology.

US Environmental Protection Agency (EPA)

As discussed in Section 10.1, without CCS, large-scale CTL implementation will lead to massive increase in CO_2 emissions. There must be a sufficiently high CO_2 price to make CCS economically feasible. It was also seen that when co-production plants with CCS displace conventional coal-fired power plants, there is scope for significant net-reduction in overall CO_2 emissions. EPA will play a major role in devising regulations such that large-scale CTL implementation does not compromise with the objective of minimizing greenhouse gas emissions. Keeping this in view, any reasonable regulation should include the following factors:

- CTL plants can be built only when there is a way to sequester CO_2
- CO_2 prices must be sufficiently high to make CCS the more economical option. But a high CO_2 price will result in higher prices of energy over the whole system. On the other hand, making CCS mandatory for CTL plants will affect only the CTL industry and not the whole system.
- Incentives must be given for the building of co-production CTL plants while phasing out inefficient conventional coal-fired power plants
- Since large-scale CTL will increase mining of coal, the existing regulations about mining might need to be revised to ensure protection of environment

10.4 Conclusions

In this thesis, performance, cost and impact assessment models were developed for the evaluation of CTL plants, including the effects of different feedstock, technology choice, carbon constraints and uncertainty in economic parameters. The following general conclusions can be drawn from the analyses performed in this thesis:

- Depending on various factors, the costs of liquid product from both liquids-only and co-generation plants are in the range of \$40 - \$100/barrel, which is comparable to the crude oil prices seen in the past 2-3 years. From the cost breakdown, it can be seen that CTL plants are highly capital intensive, with the capital cost component accounting for about half the total product cost.
- For a case-study liquids-only configuration producing 50,000 barrels/day from Illinois#6 coal, the addition of CCS is a cheaper option when the CO_2 price exceeds \$12/tonne. However, for a co-generation plant with revenues from electricity sales, the CO_2 price has to be more than \$35/tonne to make CCS cost-effective, based on electricity prices in the range of \$0 - \$100/MWh. Without CCS, there will be at least a 40% increase in CO_2 emissions.
- The process using a dry-feed Shell gasification has the lowest capital and product cost of the three systems analyzed (GE, E-Gas and Shell). Coal consumption for a Shell-based CTL process is much lower than the other two options, as are the CO_2 emissions without CCS. The main reason for better performance and economics of a Shell system is the low amount of CO_2 produced in the gasifier, which translates into lower coal requirement for the production of same amount of syngas (CO and H_2), compared to the other two systems. The combined volume fraction of CO and H_2 in the syngas from a Shell gasifier is about 85%, compared to only around 60% in the GE and EGas gasifiers.
- Even though performance-wise bituminous coals are better, in terms of cost of liquid product, sub-bituminous and lignite are more cost-effective, mainly because of lower coal prices.

- Unless crude oil prices are sufficiently high, investment in CTL is fraught with significant financial risk. Considering the volatility of oil prices, CTL plants would become uneconomical, should the oil prices fall.
- Large-scale implementation of CTL will have adverse impacts on resources and environment. Even though CO_2 emissions increase marginally by 1% (compared to 2008 levels) if CCS were used, the coal consumption will still go up by a huge extent. CTL plants also require significant amount of land. If mitigation measures are not taken in other sectors, using CTL on a large-scale leads to environmental risk.
- Co-production plants consume less coal than separate production of liquids and power. When there is no CCS, co-production plants consume 10 – 35% less coal than separate production. With CCS, the savings with co-production are much higher, ranging between 30 – 100%. Thus it is clear that co-production is more efficient than separate production of liquids and power.
- Co-production CTL plants with CCS, supplying 20% of petroleum demand, can meet around 30% of US electricity demand (energy basis) and by displacing conventional coal power plants, have the potential of reducing the US CO_2 emissions by 9% from the 2008 emissions.
- CTL offers considerable advantages as well as significant risks. Environmental, economic as well as strategic implications are intricately linked with each other and therefore all of them must be considered simultaneously in order to devise policies regarding large scale implementation of CTL.
- Though large-scale CTL offers a strategic advantage by producing domestic liquid fuels, for likely investors such as the oil and power industries and the Department of

Defense, financial risk of CTL is the greatest limiting factor in pursuing investments in CTL plants. By combining the operational and market experience of oil and power industries to form a new CTL industry can mitigate the technical as well as the economic risk to a certain extent. Government support such as DoE's loan guarantee program for clean coal technologies would reduce the risk further.

- For regulatory organizations such as EPA, the significant environmental risk that CTL (without carbon constraints) poses in terms of CO_2 emissions is of primary importance in devising environmental regulations for CTL plants. CO_2 prices must be sufficiently high to make CCS the more economical option. But a high CO_2 price will result in higher prices of energy over the whole system. On the other hand, making CCS mandatory for CTL plants will affect only the CTL industry and not the whole system.

In summary it can be said that CTL has significant scope for producing domestic liquid fuels from the abundant coal resources. By implementing CTL in conjunction with CCS and displacing conventional coal-fired power plants, there is potential to achieve net reductions in CO_2 emissions. The commercialization of the technology depends on how the investors and regulatory agencies deal with the economic and environmental risks associated with CTL.

References

Applied Catalysis A, 2004, General, Editorial, 276, 1 – 3.

Aspen Technology, Inc., 2007, Ten Canal Park, Cambridge, MA 02141-2201

Audus H, Choi G, Heath A, Tam S. S, 2001, CO2 abatement in gsa-to-liquids plants, Studies in Surface Science and Catalysis, 519 - 524.

Bechtel, 1990, Slurry reactor design studies. Slurry vs fixed bed reactors for Fischer-Tropsch and methanol: final report, DoE, DE91005752

Boerrigter H and Zwart R.W.R, 2004, High efficiency production of Fischer-Tropsch transportation fuels and substitute natural gas from biomass, Netherlands Organization of Energy and Environment, ECN-CX-03-003.

Bridgwater A. V and Anders M, "Economics of liquid fuels production by coal gasification", Fuel 70, October 1991, pp. 1193 - 1205.

Chen C, 2005, A technical and economic assessment of CO2 capture technology for IGCC power plants, PhD Thesis, Carnegie Mellon University.

CTL newsletter, Coal to liquids coalition, www.FutureCoalFuels.org

DoD, 2008, Broad agency announcement: Coal-to-liquids (CTL), Strategic Technology Office, DARPA-BAA-08-59, Sep 4.

DoE, 1992, Baseline design/economics for advanced Fischer-Tropsch technology, Quarterly Report, DE-AC22-91PC90027.

DoE, 1998, Baseline design/economics for advanced Fischer-Tropsch technology, Final Report, DE-AC22-91PC90027.

DoE, 2006, Report to congress on the itnerdependency of energy and water, December

Dry M. E, 1996, Practical and theoretical aspects of the catalytic Fischer-Tropsch process, Applied Catalysis A: General, 138, 1996, pp. 319 – 344.

Dry M. E.,1999, Fischer-Tropsch reactions and the environment, Applied Catalysis A: General, 189, 185 – 190.

EERE, 2006, US DoE – Energy Efficiency and Renewable Energy Geothermal Tech Program, http://www1.eere.energy.gov/geothermal/printable_versions/geopower_landuse.html

Eldrid R, Kaufman L and Marks P., 2004, The 7FB: the next evolution of the F gas turbine, GE Power Systems, Schenectady, NY.

Energy Information Agency, USA, www.eia.gov

EPRI, 1986, TAG^{TM} – Technical assessment guide, volume 1: Electricity supply, P-4463-SR, Electric Power Research Inst, Inc., Palo Alto, CA, December.

Espinoza R.L, Steynberg A.P, Jager B and Vosloo A.C, 1999, Low temperaure Fischer-Tropsch synthesis from a Sasol perspective, Applied Catalysis A: General, 186, 13 - 26

Farrell A.E and Brandt A.R., 2006, Risks of oil transition, Environmental Research Letters 1, 014004.

Fthenakis V and Kim H.C, 2009, Land use and electricity generation: A life-cycle analysis, Renewable and Sustainable Energy Reviews, 13, 1465 - 1474.

Gray D and Tomlinson G.C, 1990, Assessing the economic impact of indirect liquefaction process improvements: vol 1, development of the integrated indirect liquefaction model and baseline case, DoE DE91004668

Holt N.A.H and Alpert S.B, 2001, Integrated Gasification Combined-Cycle Power Plants, Encyclopedia of Physical Science and Technology, 897 – 924

IECM, 2009, Carnegie Mellon University Center for Energy and Environmental Studies, IECM-cs Integrated Environmental Control Model Carbon Sequestration Edition. http://www.iecm-online.com.

IPCC, 2005, Intergovernmental Panel on Climate Change special report on Carbon dioxide capture and sequestration, summary for policymakers.

Jaramillo P, 2007, A life cycle comparison of coal and natural gas for electricity generation and the production of transportation fuels, PhD Thesis, Carnegie Mellon University.

Joseph H. Field, 2000, Fischer-Tropsch process, in AccessScience@McGraw-Hill, http://www.accessscience.com, DOI 10.1036/1097-8542.258800, last modified: April 10, 2000.

Larson E. D and Tingjin R, 2003, Synthetic fuel production by indirect coal liquefaction, Energy for Sustainable Development, 7, 4, 79 – 102.

Marano J.J, 2007, Options for upgrading and refining Fischer-Tropsch liquids, 2nd Intl Freiberg conf. on IGCC and XtL technologies, Freiberg, Germany, May 8 - 12.

Marano J.J, and Ciferno J.P, 2001, Life cycle greenhouse gas inventory for Fischer-Tropsch fuels, NETL

Matar S, 1982, Synfuels: Hydrocarbons of the future, PennWell Books, Oklahoma.

Mills S. A, 1994, Status and future opportunities for conversion of synthesis gas to liquid fuels, Fuel 73, 8, 1243 – 1279.

Morgan G. M. and Henrion M., Uncertainty, Cambridge University Press, 1990.

Neathery J, Gray D, Challman D and Derbyshire F, 1999, The pioneer-plant concept: co-production of electricity and added-value products from coal", Fuel 78, 815 – 823.

NETL 2007a, Baseline technical and economic assessment of a commercial scale Fischer-Tropsch liquids facility", NETL/DoE-2007/1260, April 2007.

NETL 2007b, "Cost and performance baseline for fossil energy plants", NETL/DoE-2007/1281, May

Norton P., Vertin K., Bailey B., Clark N.N., Lyons D.W., Goguen S., Eberhardt J, 1998, Emissions from trucks using Fischer-Tropsch diesel fuel, SAE paper 982526.

Patzlaff J, Liu Y, Graffmann C and Gaube J, 1999, Studies on product distributions of iron and cobalt catalyzed Fischer-Tropsch synthesis, Applied Catalysis A: General, 186, 109 - 119.

Prelipceanu A, Kaballo, H.P and Kerestecioglu, U, 2007, Linde Rectisol® wash process, 2nd Intl Freiberg conf. on IGCC and XtL tech, Freiberg, Germany, May 8 - 12.

Probstein R. F and Hicks R. E, 1985, Synthetic Fuels, Intl Student Edition, McGraw Hill Book Co., Singapore.

Raje A.P and Davis B.H, 1997, Fischer-Tropsch synthesis over iron-based catalysts in a slurry reactor. Reaction rates, selectivities and implications for improving hydrocarbon productivity, Catalysis Today, 36, 335 - 345.

Rubin, E. S.; Rao, A. B.; Chen, C. 2004, Comparative assessments of fossil fuel power plants with CO2 capture and storage, 7th International Conference on Greenhouse Gas Control Technologies (GHGT-7), Vancouver, Canada, September 5-9.

Schulz H and Claeys M, 1999, Kinetic modeling of Fischer-Tropsch product distributions, Applied Catalysis A: General, 186, 91 - 107.

Schulz H, 1999, Short history and present trends of Fischer-Tropsch synthesis, Applied Catalysis A: General, 186, 3 - 12

Shi B and Davis B.H, 2004, Fischer-Tropsch synthesis: accounting for chain-length related phenomena, Applied Catalysis A: General, 277, 61 - 69.

Sie S.T and Krishna R, 1999, Fundamentals and selection of advanced Fischer-Tropsch reactors, Applied Catalysis A: General, 186, 55 – 70.

SSEB, 2006, American energy security – building a bridge to energy independence and to a sustainable energy future, The Southern States Energy Board, Norcross, Georgia.

Stelmachowski M and Nowicki L, 2003, Fuel from the synthesis gas – the role of process engineering, Applied Energy, 74, 85 – 93.

Steynberg A and Dry M, 2004, eds., Fischer-Tropsch Technology, Studies in Surface Science and Catalysis, 152, Elsevier publication, Amsterdam.

Steynberg A.P and Nel H.G, 2004, Clean coal conversion options using Fischer-Tropsch technology, Fuel, 83, 765 – 770.

Steynberg A.P, Espinoza R.L, Jager B and Vosloo A.C, 1999, High temperature Fischer-Tropsch synthesis in commercial practice, Applied Catalysis A: General, 186, 41 – 54.

Tri-state, 2009, Tri-state generation and transmission association Inc., http://www.tristategt.org/Aboutus/baseload-resources.cfm

UOP, 2007, UOP Selexol^{TM} process, UOP LLC, Des Plaines, Illinois, USA.

UOP, 2009, UOP Benfield^{TM} process, UOP LLC, Des Plaines, Illinois, USA.

Vallentin D, 2008, Policy drivers and barriers for coal-to-liquids technologies in the United States, Energy Policy, 36, 3198 - 3211.

van der Laan G.P, Beenackers A.C.M, 2000, Intrinsic kinetics of the gas-solid Fischer-Tropsch and water gas shift reactions over a precipitated iron catalyst, Applied Catalysis A: General, 193, 39 – 53

W. R. Epperly, 2001, Coal liquefaction, in AccessScience@McGraw-Hill, http://www.accessscience.com, DOI 10.1036/1097-8542.143400, last modified: February 20, 2001.

Wender I., 1996, Reactions of synthesis gas, Fuel Processing Technology, 48, 189 – 297.

Wilhelm D.J, Simbeck, D.R, Karp A.D and Dickenson R.L, 2001, Syngas production for gas-to-liquids applications: technologies, issues and outlook, Fuel Processing Technology, 71, 139 – 148

Williams R. H, Larson E. D and Jin H, 2006, Comparing climate-change mitigating potentials of alternative synthetic liquid fuel technologies using biomass and coal, 5th Annual Conference on Carbon Capture and Sequestration – DOE/NETL, 8 – 11 May 2006

Williams R. H, Larson E. D, Liu G and Kreutz T.G, 2009, Fischer-Tropsch fuels from coal and biomass: strategic advantages of once-through (poly-generation) configurations, Energy Procedia, 1,1, 4379 - 4386.

Bibliography

Probstein R. F and Hicks R. E, “Synthetic Fuels”, Intl Student Edition, McGraw Hill Book Co., Singapore, 1985.

Matar S, “Synfuels: Hydrocarbons of the future”, PennWell Books, Oklahome, 1982.

Smith J. M, Van Ness H. C, Abbott M. M, “Introduction to chemical engineering thermodynamics”, 7th ed, McGraw Hill publication, New York, 2005.

Anderson R. B, “The Fischer-Tropsch synthesis”, Academic Press Inc, Florida, 1984.

“Fischer-Tropsch Technology”, Studies in Surface Science and Catalysis, 152, edited by Steynberg A and Dry M., Elsevier publication, Amsterdam, 2004.

Supp E, “How to Produce Methanol from Coal”, Springer Verlag, New York, 1990.

Appendix A1: Application of the Gasifier Model

To analyze the behavior of the gasification process under different input conditions, the following inputs are chosen to be varied over a range of values:

- Temperature
- Heat loss from the gasifier
- Steam/carbon ratio in the input
- Oxygen/carbon ratio in the input

The gasification pressure is fixed at 40 bar for all the cases.

Inputs to the model

As described before, either the temperature at which reactions take place or the heat duty of the reactor has to be specified to run the RGIBBS block. Accordingly, two cases are considered here:

- Fixed temperature, variable heat loss
- Variable temperature, fixed heat loss

In practical applications, both the temperature and the heat loss from the gasifier are variable. However, to maintain a high efficiency, heat losses from the gasifier are minimized. Temperature is controlled by varying other inputs such as the oxygen and steam flow rates. The various input ranges and results from the model are presented in the following sections.

3.2.8.1 Variable heat loss case

This section demonstrates the use of this model for a fixed temperature, variable heat loss case. Table 2 gives the ranges of different inputs:

Table 0.1: Ranges of inputs to the variable heat loss model

Temperature	1000 – 1600 ^{o}C
Pressure	40 bar
Heat loss	Calculated
Oxygen/carbon mole ratio	0.1 – 0.7
Steam/carbon mole ratio	0.2 - 1

Effect of steam and oxygen inputs on product composition and heat loss:

The effects of variations in oxygen and steam feed rates on the product gas composition are shown in Figs 3a – 3c, when the gasification reactions take place at 1250 ^{o}C. Since the main products of gasification are CO, CO_2, H_2, H_2O and CH_4, only their mole fractions have been shown. From the figures, the following observations can be made:

- For any particular H_2O/C ratio, with increase in oxygen, CO content increases initially and then starts decreasing, as CO_2 increases. This means that when there is sufficient oxygen, total combustion of carbon is the preferred reaction compared to partial combustion, this increasing the amount of CO_2 in the products.
- For a fixed H_2O/C ratio, H_2 formation decreases and H_2O content increases with increasing oxygen. It is likely that those reactions where H_2 is a reactant are preferred over those in which H_2 is a product.
- When H_2O content in the feed increases, CO decreases accompanied by a slight increase in CO_2. Since oxygen in the feed is fixed, there must be competing reactions involving oxygen in the steam.

- When H_2O/C ratio is increased, mole fraction of H_2 increases and then decreases slightly and H_2O content increases with increasing steam. Some of the feed steam might come out unreacted.
- Methane formation is negligible

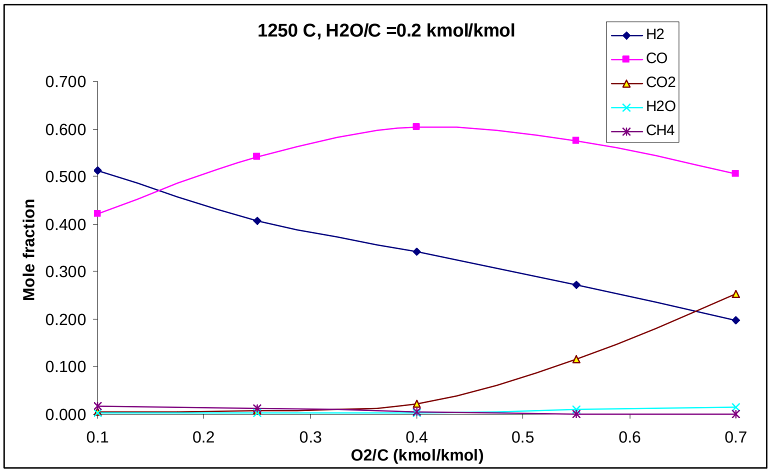


Figure 3a: Change in gas composition with varying oxygen feed rate, for H2O/C = 0.2 kmol/kmol, temperature = 1250 °C

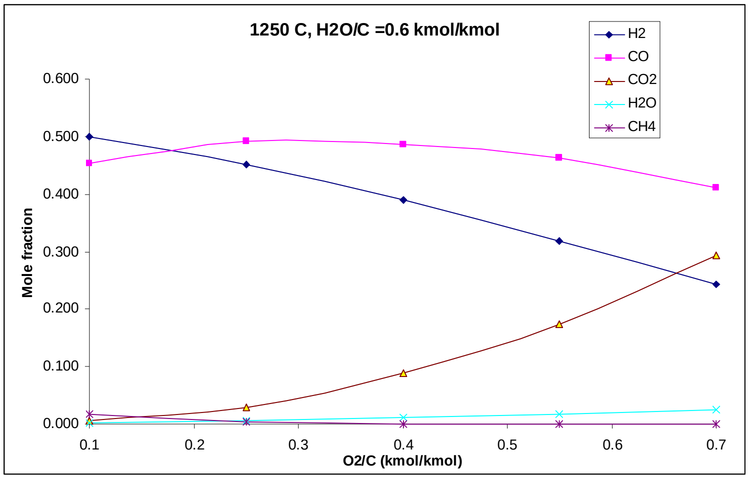


Figure 3b: Change in gas composition with varying oxygen feed rate, for H2O/C = 0.6 kmol/kmol, temperature = 1250 °C

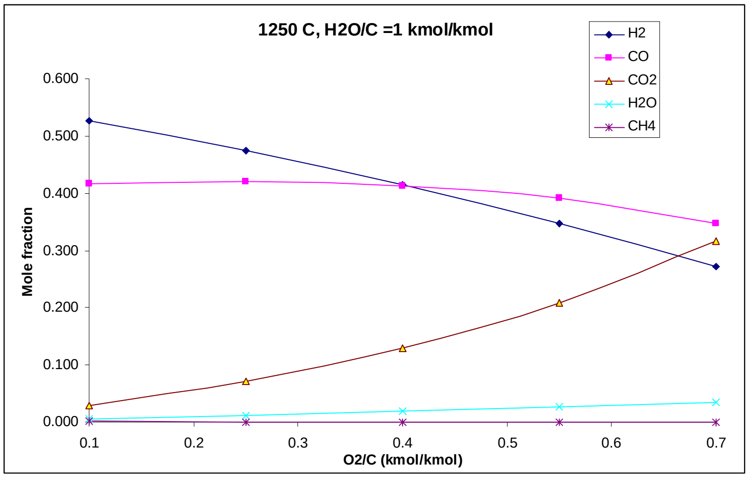


Figure 3c: Change in gas composition with varying oxygen feed rate, for H2O/C = 1 kmol/kmol, temperature = 1250 °C

Variation in heat loss with changing steam and oxygen feeds can be seen in Fig 4. For a given H_2O/C ratio, at low oxygen levels, heat loss from the gasifier is shown as to be negative. This means that for the reactions to take place there needs to be additional heat input to the gasifier. The heat from the combustion reaction of carbon is not sufficient to sustain other gasification reactions. As the oxygen input increases, heat loss goes from negative to positive, where there is excess heat in the gasifier which is not carried away by the syngas. Ideally, the net heat duty (heat loss) of the gasifier must be zero. This shows that for these input conditions, there must be about 0.4 – 0.5 moles of oxygen for every mole of carbon in coal. With increasing steam, heat loss decreases because reactions involving steam (Rxn 3) are endothermic and so more heat is required from the combustion reactions to sustain the series of reactions.

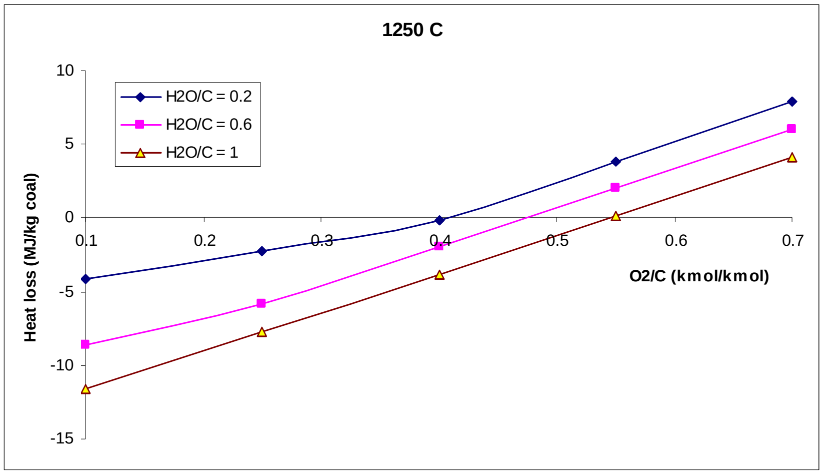


Figure 4: Heat loss from the gasifier with varying oxygen and steam flow rates at 1250 °C

Effect of temperature on product composition and heat loss

Figures 5a – 5c show the effect of changing temperature on the product composition for O_2/C of 0.55 mol/mol and different H_2O/C ratios. The following observations can be made:

- For this oxygen/carbon ratio, for all the H_2O/C ratios, CO and H2O increase with temperature and CO_2 and H_2 decrease. CO and H_2O are the reactants in water gas shift reaction (Rxn 6), whose products are CO_2 and H_2. This behavior of the product composition hints at the predominance of the reverse shift reaction.
- With increasing steam input, CO decreases while CO_2, H_2 and H_2O increase

The variation in heat loss with temperature is shown in Fig 6. As temperature increases, heat loss decreases. This could also be attributed to the reverse shift reaction. Another reason could be the predominance of partial combustion reaction (CO as product) over the total combustion reaction (CO_2 as product) leading to lesser heat release. Increasing steam also decreases heat loss.

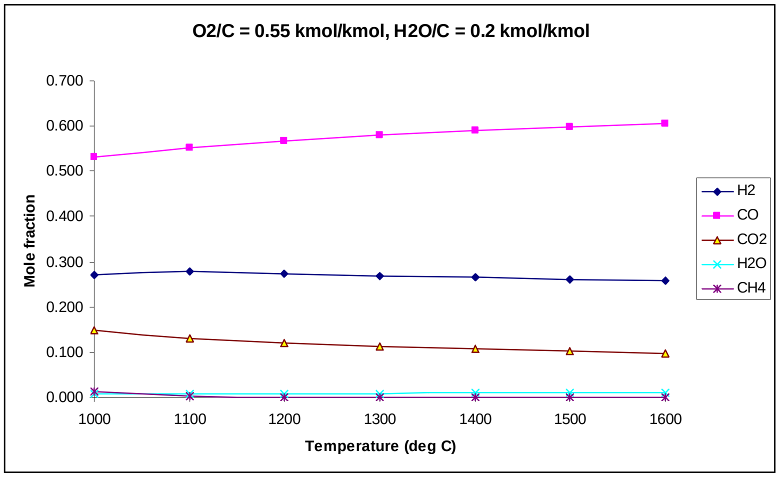


Figure 5a: Change in gas composition with varying temperature for O2/C = 0.55 kmol/kmol and H2O/C = 0.2 kmol/kmol

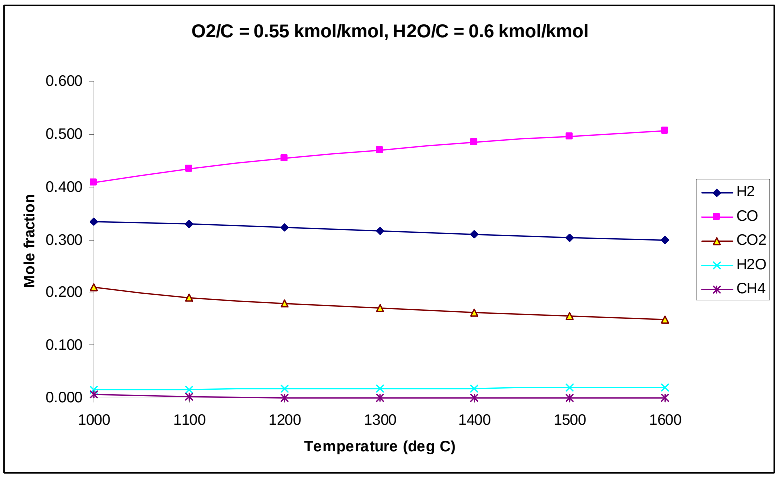


Figure 5b: Change in gas composition with varying temperature for O2/C = 0.55 kmol/kmol and H2O/C = 0.6 kmol/kmol

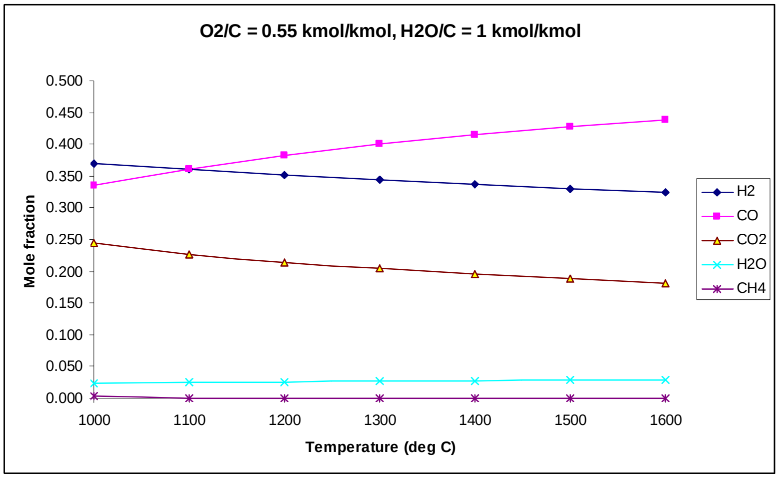


Figure 5c: Change in gas composition with varying temperature for O2/C = 0.55 kmol/kmol and H2O/C = 1 kmol/kmol

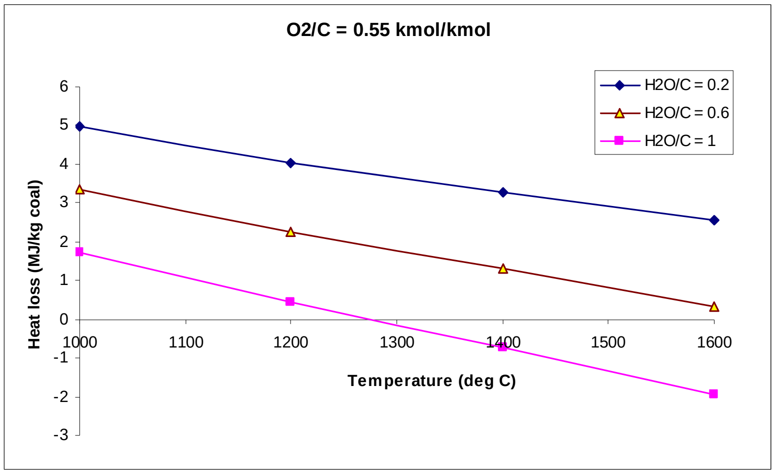


Figure 6: Heat loss from the gasifier with varying temperatures and at different steam inputs and O2/C ratio = 0.55 kmol/kmol

3.2.8.2 Fixed heat loss case

To avoid the problem of negative heat loss, heat loss can be fixed and other variables calculated to reach maintain this constant heat loss. This also reflects the conditions of a real gasifier from which there is a certain amount of heat loss. This section shows the results for a case where heat loss from the gasifier is 1% of the input coal higher heating value.

Table 3: Ranges of inputs to the fixed heat loss model

Temperature	Calculated
Pressure	40 bar
Heat loss	1% coal HHV
Oxygen/carbon mole ratio	0.1 – 0.7
Steam/carbon mole ratio	0.2 - 1

Effect of steam and oxygen inputs on product composition and temperature:

The effects of variations in oxygen and steam feed rates on the product gas composition are shown in Figs 7a – 7c. From the figures, the following observations can be made:

- For any particular H_2O/C ratio, both CO and H_2 increase initially and then decrease, reaching maximum values at an intermediate O_2/C ratio. This is accompanied by CO_2 and H_2O decreasing initially and increasing later after reaching minimum values at intermediate O_2/C ratios. This is, however, not true for the case of H_2O/C ratio of 1 where CO_2 concentration increases first at very low oxygen concentrations.
- Methane formation continuously decreases with increasing O_2. The irregular behavior of CO_2 in Fig 7c might be because of the high methane concentration at very low O_2 levels.
- With increasing H_2O/C ratios, CO concentration reduces whereas all the others increase.

The behavior of syngas temperature with varying O_2 and H_2O feeds is shown in Fig 8. Though temperature increases continuously, the rate of increase is low for lower O_2/C ratios and higher for higher O_2/C ratios. At low O_2/C ratios, exothermic CO formation increases which drives the temperature rise. At higher O_2/C ratios, this reaction is dominated by the more exothermic CO_2 formation, increasing the temperature rise.

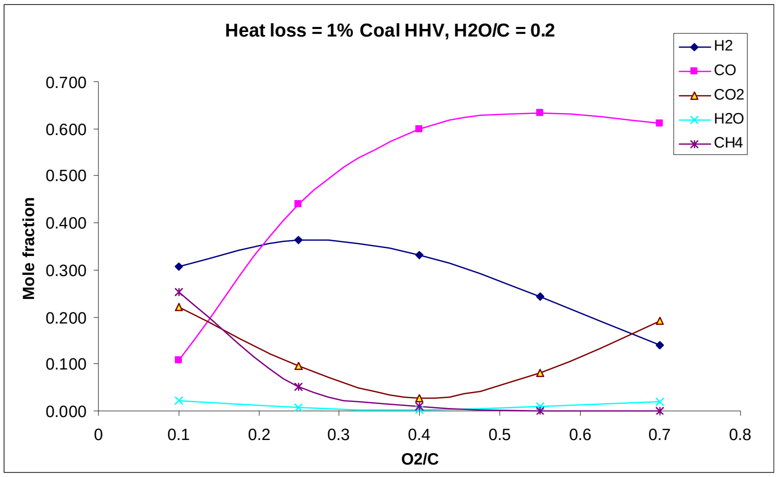


Figure 7a: Change in gas composition for a heat loss equivalent to 1% of input coal heating value, with varying O2/C ratio and at H2O/C = 0.2 kmol/kmol

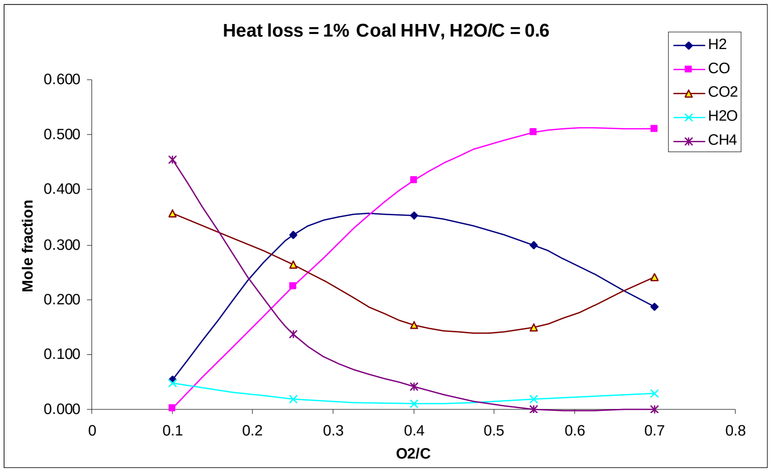


Figure 7b: Change in gas composition for a heat loss equivalent to 1% of input coal heating value, with varying O2/C ratio and at H2O/C = 0.6 kmol/kmol

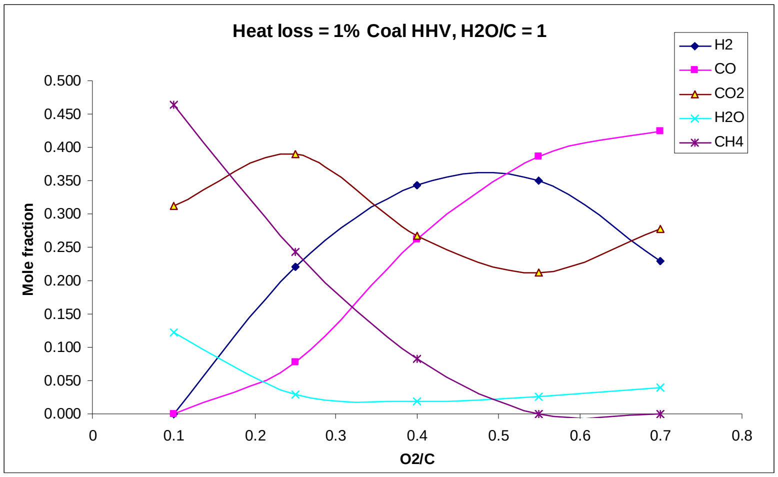


Figure 7c: Change in gas composition for a heat loss equivalent to 1% of input coal heating value, with varying O2/C ratio and at H2O/C = 1 kmol/kmol

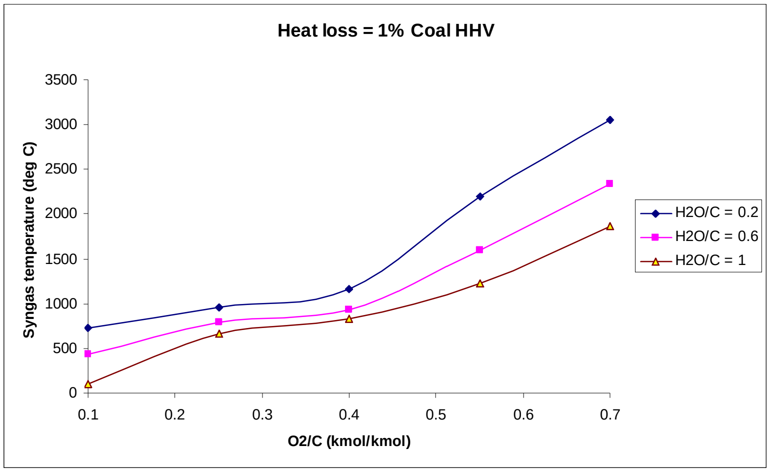


Figure 8: Change in temperature with varying oxygen and steam inputs for the fixed heat loss case

Efficiency of the gasification process

For the reactor described above, gasification efficiency is calculated as the ratio of the higher heating value of syngas to the higher heating value of coal feed. The variation in this efficiency is shown in Fig 9, for different O_2/C and H_2O/C ratios. The graph shows that efficiency reaches a maximum at a O_2/C ratio of around 0.4, for all the ratios of

H_2O/C. It can also be seen that there is no particular trend in how the efficiency changes with change in H_2O/C ratio. The useful products in the syngas are CO and H_2. Since both these components attain a maximum and then decrease with O_2/C ratios, efficiency also varies accordingly. CO_2 and H_2O are combustion products and as such do not have a heat of combustion. Thus they do not contribute towards useful energy in syngas.

The efficiency of the whole process can be improved by recovering heat from the hot syngas leaving the gasifier. This heat source has not been considered here. Adding that would increase the value of efficiency.

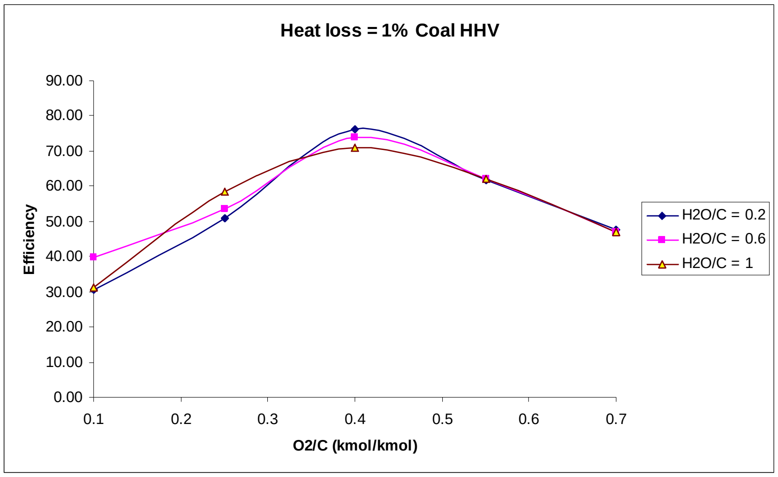


Figure 9: Effect of steam/carbon ratio and oxygen/carbon ratio on gasifier efficiency.

Effect of carbon loss on gasification efficiency

In practical gasifiers, some amount of carbon from coal goes out unreacted, in the form of slag. Table 4 shows the effect of carbon loss (% weight basis) on the product composition and efficiency.

Table 4: Effect of carbon loss on gasification temperature and gas composition

Carbon loss	**0%**	**1%**	**2%**	**3%**
Syngas temp (^oC)	1172	1192	1212	1233
CO	0.437	0.434	0.431	0.427
CO2	0.085	0.086	0.086	0.087
H2	0.310	0.307	0.304	0.301
H2O	0.142	0.147	0.153	0.159
NH3	0.000	0.000	0.000	0.000
H2S	0.007	0.007	0.007	0.007
CH4	0.001	0.001	0.001	0.000
N2	0.009	0.009	0.009	0.009
COS	0.000	0.000	0.000	0.000
AR	0.009	0.009	0.009	0.009
SO2	0.000	0.000	0.000	0.000
Efficiency	**72.49**	**71.52**	**70.55**	**69.58**

It can be seen that the formation of CO and H_2 decreases with increasing carbon loss. This is accompanied by a decrease in gasification efficiency too. Thus it is required to minimize the carbon loss in slag so as to improve efficiency.

Modifying equilibrium concentrations with approach temperatures

Though the gasification reactions approach chemical equilibrium conditions, they are still governed by chemical kinetics. To adjust the difference, Aspen Plus uses a parameter called ‘approach temperature’ for each reaction. Products from practical gasifiers have compositions different then the equilibrium ones. To model the real systems, some reactions have to be modified using approach temperatures so that the actual syngas compositions are obtained. In this section, the effect of approach temperature given to 4 reactions on the product composition is described. The reactions are 6, 8, 10 and 11. For a variation in approach temperature from – 750 ^oC to + 750 ^oC, the results are shown in tables 5 – 8 respectively for each reaction. The O2/C ratio in the feed is 0.44 and the H2O/C ratio is 0.46.

Table 5: Effect of approach temperature on syngas composition

CO + H2O <=> CO2 + H2						
Appr. Temp. (°C)	-750	-375	0	375	750	Effect of increasing appr. temp
CO	0.330	0.396	0.434	0.454	0.466	Increases
H2	0.411	0.348	0.311	0.291	0.280	Decreases
CO2	0.190	0.126	0.087	0.067	0.056	Decreases
H2O	0.041	0.103	0.140	0.160	0.171	Increases
CH4	0.004	0.002	0.002	0.002	0.002	--
NH3	0.000	0.000	0.000	0.000	0.000	--
H2S	0.005	0.007	0.007	0.007	0.007	--
COS	0.003	0.001	0.000	0.000	0.000	--
Syngas temp (°C)	1234	1178	1146	1130	1121	Decreases

Table 6: Effect of approach temperature on syngas composition

CH4 + H2O ⇔ CO + H2						
Appr. Temp. (°C)	-750	-375	0	375	750	Effect of increasing appr. temp
CO	0.391	0.424	0.434	0.435	0.435	Increases
H2	0.158	0.253	0.311	0.315	0.315	Increases
CO2	0.134	0.098	0.087	0.087	0.087	Decreases
H2O	0.208	0.169	0.140	0.138	0.138	Decreases
CH4	8.04E-02	2.89E-02	1.81E-03	3.85E-05	2.85E-06	Decreases
NH3	7.31E-06	2.53E-05	5.30E-05	5.58E-05	5.59E-05	--
H2S	8.03E-03	7.57E-03	7.26E-03	7.24E-03	7.24E-03	--
COS	8.89E-04	5.63E-04	4.52E-04	4.46E-04	4.46E-04	--
Syngas temp (°C)	1544	1297	1146	1136	1136	Decreases

Table 7 Effect of approach temperature on syngas composition

N2 + 3H2 ⇔ 2 NH3						
Appr. Temp. (°C)	-750	-375	0	375	750	Effect of increasing appr. temp
CO	0.437	0.434	0.434	0.434	0.434	--
H2	0.304	0.310	0.311	0.311	0.311	Slightly increases
CO2	0.088	0.087	0.087	0.087	0.087	--
H2O	0.140	0.140	0.140	0.140	0.140	--
CH4	1.54E-03	1.80E-03	1.81E-03	1.81E-03	1.81E-03	--
NH3	6.46E-03	2.86E-04	5.30E-05	1.97E-05	1.05E-05	Decreases
H2S	7.30E-03	7.27E-03	7.26E-03	7.26E-03	7.26E-03	--
COS	4.66E-04	4.52E-04	4.52E-04	4.52E-04	4.52E-04	--
Syngas temp (°C)	1154	1147	1146	1146	1146	--

Table 8: Effect of approach temperature on syngas composition

CO2 + H2S ⇔ COS + H2O						
Appr. Temp. (°C)	-750	-375	0	375	750	Effect of increasing appr. temp
CO	0.435	0.434	0.434	0.434	0.434	--
H2	0.310	0.310	0.311	0.311	0.311	--
CO2	0.087	0.087	0.087	0.087	0.087	--
H2O	0.140	0.140	0.140	0.140	0.140	--
CH4	1.81E-03	1.81E-03	1.81E-03	1.81E-03	1.82E-03	--
NH3	5.29E-05	5.29E-05	5.30E-05	5.30E-05	5.31E-05	--
H2S	7.69E-03	7.53E-03	7.26E-03	6.99E-03	6.74E-03	--
COS	2.55E-05	1.85E-04	4.52E-04	7.31E-04	9.79E-04	--
Syngas temp (°C)	1146	1146	1146	1146	1146	--

The results show that approach temperature of WGS reaction can be modified to adjust the concentrations of CO, H_2, CO_2 and H_2O in the products. The methane hydrolysis reaction also affects the formation of CO and H_2. Ammonia formation reaction can be used to adjust the concentration of ammonia by a slight amount. Providing approach temperature for the COS hydrolysis reaction shows no effect on any of the concentrations.

Appendix A2: MATLAB Cost Estimation Code

A2.1 Liquids-only Plant Cost Estimation

```
% This is the economics model for a CTL plant. The formulae are taken
from
% IECM documentation. The process section is divided into a number of
% different sections
clear;

% technology designation is based on gasfier and coal type. Units place
-
% 1=GE, 2=EGas, 3=Shell; decimals 1=App med S, 2=Ill6, 3=PRB,
4=NDlignite,
% for ex, 1.1 = GE+App med S

technology = [1.1; 1.2; 1.3; 1.4; 2.1; 2.2; 2.3; 2.4; 3.1; 3.2; 3.3;
3.4];

ratio_gasification = [11.710    8.475   -3.664  0.356   28.102  1.213
0.006   0.007   1.193   53.000  0.163   90.138  38.000  0.586   1.000
0.248   0.212   0.036   0.016   6.135   30.81   100.00
13.556  9.624   -3.901  0.356   29.467  1.242   0.008   0.009   1.219
53.000  0.181   90.087  38.000  0.664   1.000   0.338   0.293   0.045
0.015   3.375   26.14   60.00
19.156  14.133  -4.790  0.380   35.392  1.337   0.001   0.002   1.321
53.000  0.245   90.157  38.000  0.980   1.000   0.070   0.062   0.008
0.014   6.393   19.38   15.00
26.234  17.864  -6.060  0.379   42.667  1.429   0.006   0.009   1.406
53.000  0.291   90.145  38.000  1.238   1.000   0.301   0.273   0.028
0.012   7.177   13.99   15.00
13.135  7.932   -3.583  0.357   30.278  1.202   0.007   0.008   1.181
39.000  0.154   66.107  38.000  0.547   1.000   0.277   0.253   0.024
0.016   3.070   30.81   100.00
14.978  8.560   -3.732  0.351   31.161  1.220   0.009   0.011   1.195
39.000  0.163   66.077  38.000  0.589   1.000   0.372   0.342   0.030
0.016   5.867   26.14   60.00
20.066  11.135  -4.224  0.356   34.876  1.269   0.002   0.002   1.253
39.000  0.204   66.217  38.000  0.770   1.000   0.074   0.068   0.006
0.015   6.057   19.38   15.00
26.019  13.829  -5.263  0.336   41.214  1.336   0.007   0.009   1.315
39.000  0.241   66.245  38.000  0.957   1.000   0.299   0.280   0.018
0.013   3.443   13.99   15.00
10.557  3.770   -1.962  0.287   21.468  1.096   0.006   0.006   1.096
28.170  0.069   46.283  38.000  0.228   1.000   0.223   0.195   0.028
0.014   2.406   30.81   100.00
12.162  3.833   -2.024  0.285   21.890  1.100   0.008   0.008   1.100
28.170  0.069   46.201  38.000  0.230   1.000   0.303   0.265   0.038
0.014   2.403   26.14   60.00
16.899  5.801   -2.199  0.300   24.467  1.137   0.002   0.002   1.137
28.170  0.107   46.885  38.000  0.368   1.000   0.062   0.054   0.008
0.014   4.960   19.38   15.00
```

```
22.883  6.081   -2.508  0.295   26.028  1.150   0.006   0.007   1.150
28.170  0.111   46.877  38.000  0.386   1.000   0.263   0.231   0.032
0.015   5.065   13.99   15.00];

%[MCOAL CO21 STPOW O2MOL LTSGAS SXLGAS XH2S H2SFLO SCO2GS PSXL1 XCO21
CO2DN1 CO2TM1 WCO2 SYNGAS SULFUR CLSULF BSSULF O2CLS]
%[kg/hr kg/hr kW kmol/hr kg/hr kmol/hr      kmol/hr kmol/hr bar
kg/m3 C kW kmol/hr kg/hr kg/hr kg/hr kmol/hr]

ratio_FT = [1.174   10.431  -4.648  0.813   24.900  0.293   34.828
105.281 0.715   0.013   0.047   0.650   0.007   0.000
1.171   9.068   -4.652  0.762   24.900  0.272   34.792  105.677 0.621
0.012   0.035   0.629   0.007   0.000
1.166   6.262   -4.669  0.574   24.900  0.249   34.622  107.537 0.429
0.011   0.009   0.551   0.007   0.000
1.184   2.126   -4.622  0.446   24.900  0.109   34.392  110.080 0.145
0.010   0.010   0.567   0.007   0.000
1.206   14.460  -4.009  1.821   24.900  0.181   35.116  102.186 0.992
0.036   0.163   1.450   0.007   0.000
1.205   13.288  -4.066  1.690   24.900  0.180   35.099  102.361 0.911
0.034   0.151   1.349   0.007   0.000
1.201   11.229  -4.247  1.310   24.900  0.196   35.033  103.077 0.770
0.027   0.109   1.035   0.007   0.000
1.190   6.052   -4.374  0.912   24.900  0.152   34.893  104.581 0.414
0.019   0.029   0.810   0.007   0.000
1.223   14.038  -4.291  1.978   24.900  0.162   35.101  102.338 0.963
0.013   0.084   2.173   0.007   0.000
1.232   14.042  -4.227  2.156   24.900  0.149   35.118  102.159 0.963
0.013   0.088   2.424   0.007   0.000
1.260   14.057  -4.043  2.675   24.900  0.120   35.155  101.764 0.964
0.013   0.102   3.153   0.007   0.000
1.300   14.067  -3.762  3.460   24.900  0.093   35.191  101.381 0.965
0.013   0.124   4.251   0.007   0.000];

% [SYNGAS CO22 STPOW SXLFL2 PSXL2 XCO22 CO2DN2 CO2TM2 WCO2 OUTPUT
HHV_purge PURGE ]
% [kmol/hr kg/hr kW kmol/hr bar     kg/m3 C kW m3/hr  kJ/kg  kg/hr]

for k = 1: size(ratio_gasification,1)
%for k = 2

output = 50000; %bbl/day
syngas = output*ratio_FT(k,1); %kmol/hr of syngas required to produce
'output' bbl/day

%Calculating all the other variables based on 'output' and 'syngas'


m_coal = syngas*ratio_gasification(k,1)*24/1000; % Coal flow rate (TPD)
CO2_emission =
(syngas*ratio_gasification(k,2)+output*ratio_FT(k,2)+output*20*ratio_FT
(k,10)+output*ratio_FT(k,14))*24/1000; % Total CO2 emissions (TPD)
net_output_power = 0; % Net power output (MW)
%GT_output = 0; % Power output from gas turbines (MW)
```

```
ST_output = -(syngas*ratio_gasification(k,3) +
output*ratio_FT(k,3))/1000; %Power output from steam turbines (MW)
oxygen = syngas*ratio_gasification(k,4); %Oxygen flow rate to gasifier
(kmol/hr)
LT_syngas = syngas*ratio_gasification(k,5); % Syngas input into low
temp cooling (kg/hr)
selexol_syngas = syngas*ratio_gasification(k,6); %Syngas input into
Selexol process (kmol/hr)
sulfur_claus = syngas*ratio_gasification(k,17); %Sulfur output from
Claus process (kg/hr)
sulfur_BS = syngas*ratio_gasification(k,18); % Sulfur output from
Beavon Stretford process (kg/hr)
%HP_steam = 0; %Flow rate of high pressure steam (kg/hr)
x_H2S = ratio_gasification(k,7); %Mole fraction of H2S in the inlet
syngas to Selexol
H2S_flow = syngas*ratio_gasification(k,8); %Flow rate of H2S into the
Selexol process (kmol/hr)
selexol_CO2_syngas_1 = syngas*ratio_gasification(k,9); % Syngas inlet
into CO2 removal system (kmol/hr)
selexol_CO2_syngas_2 = output*ratio_FT(k,4); % Syngas inlet into CO2
removal system (kmol/hr)
p_Selexol_1 = ratio_gasification(k,10); %Pressure in the CO2 absorption
column (bar)
p_Selexol_2 = ratio_FT(k,5); %Pressure in the CO2 absorption column
(bar)
x_CO2_1 = ratio_gasification(k,11); %Mole fraction of CO2 in the inlet
syngas
x_CO2_2 = ratio_FT(k,6); %Mole fraction of CO2 in the inlet syngas
CO2_density_1 = ratio_gasification(k,12); %Density of CO2 in the first
selexol process (kg/m3)
CO2_density_2 = ratio_FT(k,7); %Density of CO2 in the second selexol
process(kg/m3)
CO2_temp_1 = ratio_gasification(k,13)+273; %Temperature of CO2 (K)
CO2_temp_2 = ratio_FT(k,8)+273; %Temperature of CO2 (K)
CO2_compr_work = syngas*ratio_gasification(k,14)+output*ratio_FT(k,9);
% CO2 compression work (kW)
purge_MW = 9000*output*ratio_FT(k,12)/3600/1000; %9,000 kJ/kg is the
average HHV of purge gases
H2_MW = 142919*output*ratio_FT(k,11)/3600/1000;
p_HP = 98; % High pressure steam (bar)
HHV_coal = ratio_gasification(k,21); %MJ/kg

solvent_price = 3.3; % $/kg of Selexol solvent
CL_catalyst_price = 603.95; % $/ton of Claus catalyst
coal_price = ratio_gasification(k,22); % $/ton of coal
labour_price = 35; % $/day
carbon_tax = 25; % $/ton of CO2 emitted to atmosphere
CO2_transport = 5; % $/ton of CO2 trasported. Has a range of 1.3 - 10.4
$/ton
CO2_storage = 5; % $/ton of CO2 stored. Has a range of 0.65 - 10.4
$/ton
CO2_monitor = 0.25; % $/ton of CO2 monitored at the site. Range 0.13 -
0.39;
sulfur_credit = 0; % $/ton of sulfur
%CCS_geo_seq = 4; % $/ton of CO2 for sequestration and monitoring, ref
IPCC report
elec_price = 0; % $/kWh
```

```
CF = 0.85; % Plant capacity factor

CPI = 525.4/395; % Chem Engg Plant Index correction for 2007 to 2000 $

%%%%%%%%% CAPITAL COST CALCULATIONS BEGIN %%%%%%%%%%%%
%--------------
% Coal handling section
    max_CH = 25000/1.1; % max TPD of coal in one train

    if m_coal < max_CH
        n_OT_CH = 1; % no. of operating trains of coal handling
    else
        n_OT_CH = ceil(m_coal/max_CH);
    end
    n_EX_CH = 0; % no. of spare trains
    n_T_CH = n_OT_CH + n_EX_CH;

    DC_CH = n_T_CH*9.92*(m_coal*1.1/n_OT_CH)/1000*CPI; % Direct cost of
coal handling in 2006 $
%----------------
% Oxidant feed section
    max_OF = 7730; % kmol/hr of oxygen in one train

    if oxygen < max_OF
        n_OT_OF = 1; % no. of operating trains
    else
        n_OT_OF = ceil(oxygen/max_OF);
    end
    n_EX_OF = 0; % no. of spare trains
    n_T_OF = n_OT_OF + n_EX_OF;

    DC_OF =
n_T_OF*31.15*(65^0.067)*((oxygen/n_OT_OF)^0.852)/(0.05^0.073)/1000*CPI;
% Direct cost of oxidant feed
%----------------
% Gasification section
    max_G = 2903; % TPD of coal in one train, for GE radiant and EGas
%    max_G = 2722; % TPD of coal in one train, for Shell radiant

    if m_coal < max_G
        n_OT_G = 1; % no. of operating trains
    else
        n_OT_G = ceil(m_coal/max_G);
    end
    n_EX_G = 1; % no. of spare trains
    n_T_G = n_OT_G + n_EX_G;

%    DC_G = n_T_G*15.88*((m_coal*1.1/n_OT_G)^0.943)/1000*CPI; % Direct
cost,
%    for quench gasifiers
    if k <= 4
        DC_G = n_T_G*43.00*((m_coal/n_OT_G)^0.943)/1000; % Direct cost,
2006$M, for GE radiant
    else if 4<k<=8
```

```
            DC_G = n_T_G*40.77*((m_coal/n_OT_G)^0.943)/1000; % Direct
cost, 2006$M, for EGas radiant
        else
            DC_G = n_T_G*55.23*((m_coal/n_OT_G)^0.943)/1000; % Direct
cost, 2006$M, for Shell radiant
        end
    end

%-----------------
% Low temperature gas cooling section

    max_LT = 590900; % kg/hr of syngas in one train

    if LT_syngas < max_LT
        n_OT_LT = 1; % no. of operating trains
    else
        n_OT_LT = ceil(LT_syngas/max_OF);
    end
    n_EX_LT = 1; % no. of spare trains
    n_T_LT = n_OT_LT + n_EX_LT;

    DC_LT = n_T_LT*0.0343*(LT_syngas/n_OT_LT)/1000*CPI; % Direct cost
%-----------------
% Selexol H2S removal section
    max_SXL = 30590; % kmol/hr of syngas in one train

    if selexol_syngas < max_SXL
        n_OT_SXL = 1; % no. of operating trains
    else
        n_OT_SXL = ceil(selexol_syngas/max_SXL);
    end
    n_EX_SXL = 1; % no. of spare trains
    n_T_SXL = n_OT_SXL + n_EX_SXL;

    DC_SXL =
n_T_SXL*0.659*((selexol_syngas/n_OT_SXL)^0.981)/(0.01^0.059)/1000*CPI;
% Direct cost
    initial_solvent = n_T_SXL*(-25200 +
34.7*(H2S_flow/n_OT_SXL)/x_H2S^1.04)/2.2; % kg of initial solvent
loading
    initial_solvent_cost = initial_solvent*solvent_price;
    makeup_solvent = CF*(-350 +
3.476*selexol_syngas/n_OT_SXL)*n_OT_SXL/2.2; % kg/yr of Selexol solvent

%-----------------
% Claus plant section
    max_CL = 8227; % kg/hr of Sulfur in one train

   if sulfur_claus < max_CL
        n_OT_CL = 1; % no. of operating trains
    else
        n_OT_CL = ceil(sulfur_claus/max_CL);
    end
    n_EX_CL = 1; % no. of spare trains
    n_T_CL = n_OT_CL + n_EX_CL;
```

```
    DC_CL = n_T_CL*11.79*((sulfur_claus/n_OT_CL)^0.668)/1000*CPI; %
Direct cost
    initial_CL_catalyst = n_T_CL*0.0111*sulfur_claus/n_OT_CL; % kg of
initial Claus catalyst loading
    initial_catalyst_cost = initial_CL_catalyst*CL_catalyst_price;
    makeup_catalyst = n_OT_CL*0.00211*CF*sulfur_claus/n_OT_CL; %kg/yr
of Claus catalyst
%------------------
% Beavon Stretford plant section
    max_BS = 545; % kg/hr of Sulfur in one train

    if sulfur_BS < max_BS
        n_OT_BS = 1; % no. of operating trains
    else
        n_OT_BS = ceil(sulfur_BS/max_BS);
    end
    n_EX_BS = 1; % no. of spare trains
    n_T_BS = n_OT_BS + n_EX_BS;

    DC_BS = (63.76 +
n_T_CL*121.56*((sulfur_BS/n_OT_BS)^0.645))/1000*CPI; % Direct cost
    initial_BS_chemical = 188.76*sulfur_BS*CPI; % cost of initial
chemical loading in $
    makeup_BS_chemical = 374*CF*sulfur_BS*CPI; % $/yr
%------------------
% Fischer Tropsch reactor system
    DC_FT = 0.0086*output;

    initial_FT_catalyst = 120*output; % cost of initial catalyst
loading, $
    makeup_FT_catalyst = 674*output*CF; %annual cost of make up
catalyst $/year
%------------------
% Gas turbine section
    %DC_GT = 168*GT_output/1000*CPI;
    DC_GT = 0;
%------------------
%Heat recovery steam generator section
    %DC_HRSG =
794968*((p_HP/1500)^1.526)*((HP_steam/600000)^0.242)/1000*CPI;
    DC_HRSG = 0;
%------------------
%Steam turbine section
    DC_ST = 158.7*ST_output/1000*CPI;
%------------------
%CO2 removal section
    rho_selexol = 1030; % Density of Selexol solvent (kg/m3)
    M_selexol = 280; % Molecular weight of Selexol solvent (kg/kmol)
    alpha = 0.99; % Efficiency of CO2 removal system

    selexol_mol_1 = 17.44*alpha^1.013/(1-
alpha)^0.06261*x_CO2_1^0.1163*selexol_CO2_syngas_1^0.987116/p_Selexol_1
^0.85745/3600;
```

```
    selexol_mol_2 = 17.44*alpha^1.013/(1-
alpha)^0.06261*x_CO2_2^0.1163*selexol_CO2_syngas_2^0.987116/p_Selexol_2
^0.85745/3600;
    %kmol/s
    selexol_mass_1 = selexol_mol_1*M_selexol; %kg/s
    selexol_vol_1 = selexol_mass_1/rho_selexol; %m3/s

    selexol_mass_2 = selexol_mol_2*M_selexol; %kg/s
    selexol_vol_2 = selexol_mass_2/rho_selexol; %m3/s

    CO2_mass_1 = syngas*ratio_gasification(2)/3600;
    CO2_volume_1 = CO2_mass_1/CO2_density_1*298/CO2_temp_1;
    solvent_out_vol_1 = selexol_vol_1 + CO2_volume_1; % After CO2
capture, inlet to power recovery turbine (m3/s)
    solvent_out_mass_1 = selexol_mass_1 + CO2_mass_1;% kg/s

    CO2_mass_2 = output*ratio_FT(2)/3600;
    CO2_volume_2 = CO2_mass_2/CO2_density_2*298/CO2_temp_2;
    solvent_out_vol_2 = selexol_vol_2 + CO2_volume_2; % After CO2
capture, inlet to power recovery turbine (m3/s)
    solvent_out_mass_2 = selexol_mass_2 + CO2_mass_2;% kg/s

    p_exit_turb1_1 = 0.1212*p_Selexol_1^1.415; % Exit pres of first
power recov turbine (bar)
    p_exit_turb2_1 = 4.2; % Exit pres of second power recov turbine
(bar)

    p_exit_turb1_2 = 0.1212*p_Selexol_2^1.415; % Exit pres of first
power recov turbine (bar)
    p_exit_turb2_2 = 4.2; % Exit pres of second power recov turbine
(bar)

    power_turb1_1 = (p_Selexol_1 -
p_exit_turb1_1)*100*solvent_out_vol_1*0.77; % Power from first turbine
(kW)
    power_turb2_1 = (p_exit_turb1_1 -
p_exit_turb2_1)*100*solvent_out_vol_1*0.77; % kW

    power_turb1_2 = (p_Selexol_2 -
p_exit_turb1_2)*100*solvent_out_vol_2*0.77; % Power from first turbine
(kW)
    power_turb2_2 = (p_exit_turb1_2 -
p_exit_turb2_2)*100*solvent_out_vol_2*0.77; % kW

    recycle_compr_power_1 = 1780; %kW
    recycle_compr_power_2 = 1780; %kW

    %Cost calculations
    DC_abs_column_1 = (-1375.356 + 16.536*p_Selexol_1 +
0.1404*(selexol_mol_1*3600+selexol_CO2_syngas_1))*CPI/1000;
    DC_abs_column_2 = (-1375.356 + 16.536*p_Selexol_2 +
0.1404*(selexol_mol_2*3600+selexol_CO2_syngas_2))*CPI/1000;
    DC_abs_column = DC_abs_column_1 + DC_abs_column_2;
```

```
    DC_turb_1 = (2*219.086 + 0.1085*(power_turb1_1+power_turb2_1) +
0.0201*(p_exit_turb1_1^2+p_exit_turb2_1^2))*CPI/1000;
    DC_turb_2 = (2*219.086 + 0.1085*(power_turb1_2+power_turb2_2) +
0.0201*(p_exit_turb1_2^2+p_exit_turb2_2^2))*CPI/1000;
    DC_turb = DC_turb_1 + DC_turb_2;

    n_OT_slumptank_1 = ceil(solvent_out_mass_1/800);
    n_OT_slumptank_2 = ceil(solvent_out_mass_2/800);
    n_EX_slumptank_1 = 1; % no. of spare trains
    n_EX_slumptank_2 = 1; % no. of spare trains
    n_T_slumptank_1 = n_OT_slumptank_1 + n_EX_slumptank_1;
    n_T_slumptank_2 = n_OT_slumptank_2 + n_EX_slumptank_2;

    DC_slumptank_1 =
2.0049*n_T_slumptank_1*(solvent_out_mass_1/n_OT_slumptank_1)^0.7446*CPI
/1000;
    DC_slumptank_2 =
2.0049*n_T_slumptank_2*(solvent_out_mass_2/n_OT_slumptank_2)^0.7446*CPI
/1000;
    DC_slumptank = DC_slumptank_1 + DC_slumptank_2;

    DC_recycle_compr_1 = 5.598*recycle_compr_power_1^0.7784*CPI/1000;
    DC_recycle_compr_2 = 5.598*recycle_compr_power_2^0.7784*CPI/1000;
    DC_recycle_compr = DC_recycle_compr_1 + DC_recycle_compr_2;

    %Cost of just venting CO2
    DC_CO2_VENT = DC_abs_column + DC_turb + DC_slumptank +
DC_recycle_compr;

    %Compression costs
    DC_CO2_compr = 15.8*CO2_compr_work^0.64*CPI/1000;
    DC_CO2_CCS = DC_CO2_VENT + DC_CO2_compr;

% It is assumed that the plant will install only the compressor.
% Transportation and storage are not considered in the capital cost but
% will be taken into account in the operating costs using IPCC
estimates.
%    %Transportation costs, assuming midwest region
%   L = 100; % distance transported ((km)
%    D_NPS = 22; % standard dia of pipeline (in)
%    C_material = exp(3.112)*L^0.901*D_NPS^1.590;
%    C_labour = exp(4.487)*L^0.820*D_NPS^0.940;
%    C_ROW = exp(3.950)*L^1.049*D_NPS^0.403;
%    C_misc = exp(4.390)*L^0.783*D_NPS^0.791;
%    DC_pipeline = (C_material + C_labour + C_ROW +
C_misc)*(515/442)/1e6; %$M
%    DC_CO2_CCS = DC_abs_column + DC_turb + DC_slumptank +
DC_recycle_compr + DC_CO2_compr + DC_pipeline;
%    OM_pipeline = 3250*(515/442)*L; %$/yr
%--------------------
% DIRECT COST MATRIX %
DC(1,1) = DC_CH;
DC(2,1) = DC_OF;
DC(3,1) = DC_G;
DC(4,1) = DC_LT;
DC(5,1) = DC_SXL;
```

```
DC(6,1) = DC_CL;
DC(7,1) = DC_BS;
DC(8,1) = DC_FT;
DC(9,1) = DC_GT;
DC(10,1) = DC_HRSG;
DC(11,1) = DC_ST;

for a = 1:11
    DC_CCS(a,1) = DC(a,1);
    DC_NO_CCS(a,1) = DC(a,1);
end
DC_CCS(12,1) = DC_CO2_CCS;
DC_NO_CCS(12,1) = DC_CO2_VENT;
PFC_NO_CCS = sum(DC_NO_CCS);
PFC_CCS = sum(DC_CCS);
DC = [DC_CCS DC_NO_CCS];
%---------------------
% INDIRECT CAPITAL COST %
IC_GFC = 0.15; % General facilities capital 15% of direct cost
IC_EHO = 0.10; % Engg & home office capital, 10% of direct cost
IC_PROC = 0.25; % Process contingency 5% of direct cost
IC_PROJ = 0.15; % Project contingency 15% of direct cost
IC_RLTY = 0.10; % Royalty charges 5% of direct cost

IC_VEC = [IC_GFC, IC_EHO, IC_PROC, IC_PROJ, IC_RLTY];

GFC = IC_GFC*DC;
EHO = IC_EHO*DC;
PROC = IC_PROC*DC;
PROJ = IC_PROJ*DC;
RLTY = IC_RLTY*DC;
%---------------------
% TOTAL CAPITAL COST %
TPC_VEC = DC + GFC + EHO + PROC + PROJ + RLTY;
TPC_CCS = sum(TPC_VEC(1:12,1));
TPC_NO_CCS = sum(TPC_VEC(1:12,2));
%---------------------
% INITIAL CATALYST AND CHEMICAL LOADING COSTS %
initial_cost =
(initial_solvent_cost+initial_catalyst_cost+initial_BS_chemical+initial
_FT_catalyst)/1e6; % $M
%initial_cost = (initial_solvent_cost+initial_FT_catalyst)/1e6; % $M
%---------------------
% OPERATION AND MAINTENANCE COSTS %
    coal_cost = m_coal*365*CF*coal_price; % $/yr
    sulfur_total = (sulfur_claus + sulfur_BS)*24/1000; %tons/day
    sulfur_revenue = sulfur_total*sulfur_credit*CF*365/1e6; % $M/yr

    VOM = (makeup_solvent*solvent_price +
makeup_catalyst*CL_catalyst_price + makeup_BS_chemical +
makeup_FT_catalyst + coal_cost)/1e6; % M$/yr

    VOM_matrix(1,1) = makeup_solvent*solvent_price/1e6;
    VOM_matrix(2,1) = makeup_catalyst*CL_catalyst_price/1e6;
    VOM_matrix(3,1) = makeup_BS_chemical/1e6;
    VOM_matrix(4,1) = makeup_FT_catalyst/1e6;
```

```
    VOM_matrix(5,1) = coal_cost/1e6;
%    VOM_matrix(5,1) = OM_pipeline/1e6;
    VOM_matrix(6,1) = -sulfur_revenue/1e6;

    VOM_matrix;

    FOM_labour = labour_price*100*2*40*52*CPI/1e6;
    FOM_maint_CCS = 0.02*TPC_CCS;
    FOM_maint_NO_CCS = 0.02*TPC_NO_CCS;
    FOM_maint_labour_CCS = 0.4*FOM_maint_CCS;
    FOM_maint_labour_NO_CCS = 0.4*FOM_maint_NO_CCS;
    FOM_admin_CCS = 0.3*(FOM_labour + FOM_maint_labour_CCS);
    FOM_admin_NO_CCS = 0.3*(FOM_labour + FOM_maint_labour_NO_CCS);
    FOM_CCS = FOM_labour + FOM_maint_CCS + FOM_admin_CCS; % $M
    FOM_NO_CCS = FOM_labour + FOM_maint_NO_CCS + FOM_admin_NO_CCS; % $M
%--------------------
% OTHER CAPITAL COSTS %
    inventory_cost_CCS = 0.005*TPC_CCS;
    inventory_cost_NO_CCS = 0.005*TPC_NO_CCS;
    pre_production_CCS = FOM_CCS/12; % 1 month of FOM $M
    pre_production_NO_CCS = FOM_NO_CCS/12; % 1 month of FOM $M
    post_production = VOM/12; % 1 month of VOM $M
%--------------------

CRF = 0.15; % capital recovery factor
annual_CO2 = (CO2_emission)*365*CF/1e6; % MT/y
CCS_geo_seq_cost = (CO2_transport+CO2_storage+CO2_monitor)*annual_CO2;
% $M/yr
%elec_revenue = net_output_power*1000*24*365*CF*elec_price./1e6; %$M/yr
elec_revenue = 0; %$M/yr
TCR_CCS = 1.25*(TPC_CCS + initial_cost + inventory_cost_CCS +
pre_production_CCS + post_production); % total capital reqmt $M
TRR_CCS = TCR_CCS*CRF + VOM + FOM_CCS + CCS_geo_seq_cost - elec_revenue
- sulfur_revenue;
specific_cap_cost_CCS = TCR_CCS*1e6/output; % Capital cost per daily
barrel ($/DB)
output_cost_CCS = TRR_CCS*1e6/(output*CF*365) % $/bbl of output

TCR_NO_CCS = 1.25*(TPC_NO_CCS + initial_cost + inventory_cost_NO_CCS +
pre_production_NO_CCS + post_production); % total capital reqmt $M
specific_cap_cost_NO_CCS = TCR_NO_CCS*1e6/output; % Capital cost per
daily barrel ($/DB)
%TRR_NO_CCS = TCR_NO_CCS*CRF + VOM + FOM_NO_CCS + annual_CO2*carbon_tax
- elec_revenue;
%output_cost_NO_CCS = TRR_NO_CCS*1e6/(output*CF*365) % $/bbl of output
TRR_NO_CCS_ctax = TCR_NO_CCS*CRF + VOM + FOM_NO_CCS +
annual_CO2*carbon_tax - elec_revenue - sulfur_revenue;
TRR_NO_CCS_no_ctax = TCR_NO_CCS*CRF + VOM + FOM_NO_CCS - elec_revenue -
sulfur_revenue;
output_cost_NO_CCS_ctax = TRR_NO_CCS_ctax*1e6/(output*CF*365) % $/bbl
of output
output_cost_NO_CCS_no_ctax = TRR_NO_CCS_no_ctax*1e6/(output*CF*365) %
$/bbl of output

% RESULT MATRIX
```

```
result_CCS(1,k) = technology(k);
result_CCS(2,k) = output;
result_CCS(3,k) = m_coal;
result_CCS(4,k) = output*20*ratio_FT(k,10)*24/1000;
result_CCS(5,k) = net_output_power;
result_CCS(6,k) = TCR_CCS;
result_CCS(7,k) = specific_cap_cost_CCS;
result_CCS(8,k) = output_cost_CCS;
result_CCS(9,k) = output_cost_CCS;
result_CCS(10,k) =
100*(net_output_power+output*0.0648)/(m_coal*0.0116*HHV_coal);
%efficiency_CCS = (net_output_power+output*0.058)/(m_coal*0.0116*24)

result_NO_CCS(1,k) = technology(k);
result_NO_CCS(2,k) = output;
result_NO_CCS(3,k) = m_coal;
result_NO_CCS(4,k) = CO2_emission;
result_NO_CCS(5,k) = net_output_power + CO2_compr_work/1000;
result_NO_CCS(6,k) = TCR_NO_CCS;
result_NO_CCS(7,k) = specific_cap_cost_NO_CCS;
result_NO_CCS(8,k) = output_cost_NO_CCS_no_ctax;
result_NO_CCS(9,k) = output_cost_NO_CCS_ctax;
result_NO_CCS(10,k) = 100*(net_output_power +
output*0.0648)/(m_coal*0.0116*HHV_coal);
%efficiency_NO_CCS = (net_output_power+ CO2_compr_work/1000 +
output*0.058)/(m_coal*0.0116*24)

result_matrix = [result_NO_CCS result_CCS];
water(k,1) = technology(k);
water(k,2) = ST_output*2.90*1.18*24 - output*0.164; %m3/day; 85% Water
consumption is for cooling tower. Scaling factor = 2.90m3/MWh. FT water
production = 1bbl/bbl

contribution(1,1) = TCR_CCS*CRF*1e6/(output*365*CF); %capital cost
contribution(2,1) = VOM*1e6/(output*365*CF); % consumables
contribution(3,1) = FOM_CCS*1e6/(output*365*CF); % maintenance
contribution(4,1) = CCS_geo_seq_cost*1e6/(output*365*CF); %CCS
operating cost
contribution(5,1) = -sulfur_revenue*1e6/(output*365*CF); %sulfur
revenue
contribution(6,1) = -elec_revenue*1e6/(output*365*CF); % elec revenue
contribution(7,1) = output_cost_CCS; %total

contribution(1,2) = TCR_NO_CCS*CRF*1e6/(output*365*CF);
contribution(2,2) = VOM*1e6/(output*365*CF);
contribution(3,2) = FOM_NO_CCS*1e6/(output*365*CF);
contribution(4,2) = 0;
contribution(5,2) = -sulfur_revenue*1e6/(output*365*CF);
contribution(6,2) = -elec_revenue*1e6/(output*365*CF);
contribution(7,2) = output_cost_NO_CCS_no_ctax;

% Sensitivity analysis of output price as a function of capital cost
and
% O&M costs
%s = [-1 -0.75 -0.5 -0.25 0 0.25 0.5 0.75 1];
%for s = -1:0.25:1
```

```
 %   TRR_CCS_TCRsens = (1+s).*TCR_CCS*CRF + VOM + FOM_CCS +
CCS_geo_seq_cost - elec_revenue - sulfur_revenue; %sensitivity to
capital cost
 %   TRR_CCS_VOMsens = TCR_CCS*CRF + (1+s).*VOM + FOM_CCS +
CCS_geo_seq_cost - elec_revenue - sulfur_revenue; %sensitivity to VOM
 %   TRR_CCS_FOMsens = TCR_CCS*CRF + VOM + (1+s).*FOM_CCS +
CCS_geo_seq_cost - elec_revenue - sulfur_revenue; %sensitivity to
capital cost
 %   TRR_CCS_CCSsens = TCR_CCS*CRF + VOM + FOM_CCS +
(1+s).*CCS_geo_seq_cost - elec_revenue - sulfur_revenue; %sensitivity
to capital cost
 %   output_cost_CCS_TCRsens = TRR_CCS_TCRsens*1e6/(output*CF*365); %
$/bbl of output
 %   output_cost_CCS_VOMsens = TRR_CCS_VOMsens*1e6/(output*CF*365); %
$/bbl of output
 %   output_cost_CCS_FOMsens = TRR_CCS_FOMsens*1e6/(output*CF*365); %
$/bbl of output
 %   output_cost_CCS_CCSsens = TRR_CCS_CCSsens*1e6/(output*CF*365); %
$/bbl of output
 %   pct_chg_TCR = (output_cost_CCS_TCRsens/output_cost_CCS - 1)*100;
%percentage change in output from base case
 %   pct_chg_VOM = (output_cost_CCS_VOMsens/output_cost_CCS - 1)*100;
%percentage change in output from base case
 %   pct_chg_FOM = (output_cost_CCS_FOMsens/output_cost_CCS - 1)*100;
%percentage change in output from base case
 %   pct_chg_CCS = (output_cost_CCS_CCSsens/output_cost_CCS - 1)*100;
%percentage change in output from base case
 %   sensitivity = [s; output_cost_CCS_TCRsens; pct_chg_TCR;
output_cost_CCS_VOMsens; pct_chg_VOM; output_cost_CCS_FOMsens;
pct_chg_FOM; output_cost_CCS_CCSsens; pct_chg_CCS];
%end

end
```

A2.2 Co-production Plant Cost Estimation

```
% This is the economics model for a CTL plant. The formulae are taken
from
% IECM documentation. The process section is divided into a number of
% different sections
% In this model, 1 ton = 1000 kg
clear;

% technology designation is based on gasfier and coal type. Units place
-
% 1=GE, 2=EGas, 3=Shell; decimals 1=App med S, 2=Ill6, 3=PRB,
4=NDlignite,
% for ex, 1.1 = GE+App med S

technology = [1.1; 1.2; 1.3; 1.4; 2.1; 2.2; 2.3; 2.4; 3.1; 3.2; 3.3;
3.4];
```

```
ratio_gasification = [11.710    8.475   -3.664  0.356   28.102  1.213
0.006   0.007   1.193   53.000  0.163   90.138  38.000  0.586   1.000
0.248   0.212   0.036   0.016   6.135   30.81   100.00
13.556  9.624   -3.901  0.356   29.467  1.242   0.008   0.009   1.219
53.000  0.181   90.087  38.000  0.664   1.000   0.338   0.293   0.045
0.015   3.375   26.14   60.00
19.156  14.133  -4.790  0.380   35.392  1.337   0.001   0.002   1.321
53.000  0.245   90.157  38.000  0.980   1.000   0.070   0.062   0.008
0.014   6.393   19.38   15.00
26.234  17.864  -6.060  0.379   42.667  1.429   0.006   0.009   1.406
53.000  0.291   90.145  38.000  1.238   1.000   0.301   0.273   0.028
0.012   7.177   13.99   15.00
13.135  7.932   -3.583  0.357   30.278  1.202   0.007   0.008   1.181
39.000  0.154   66.107  38.000  0.547   1.000   0.277   0.253   0.024
0.016   3.070   30.81   100.00
14.978  8.560   -3.732  0.351   31.161  1.220   0.009   0.011   1.195
39.000  0.163   66.077  38.000  0.589   1.000   0.372   0.342   0.030
0.016   5.867   26.14   60.00
20.066  11.135  -4.224  0.356   34.876  1.269   0.002   0.002   1.253
39.000  0.204   66.217  38.000  0.770   1.000   0.074   0.068   0.006
0.015   6.057   19.38   15.00
26.019  13.829  -5.263  0.336   41.214  1.336   0.007   0.009   1.315
39.000  0.241   66.245  38.000  0.957   1.000   0.299   0.280   0.018
0.013   3.443   13.99   15.00
10.557  3.770   -1.962  0.287   21.468  1.096   0.006   0.006   1.096
28.170  0.069   46.283  38.000  0.228   1.000   0.223   0.195   0.028
0.014   2.406   30.81   100.00
12.162  3.833   -2.024  0.285   21.890  1.100   0.008   0.008   1.100
28.170  0.069   46.201  38.000  0.230   1.000   0.303   0.265   0.038
0.014   2.403   26.14   60.00
16.899  5.801   -2.199  0.300   24.467  1.137   0.002   0.002   1.137
28.170  0.107   46.885  38.000  0.368   1.000   0.062   0.054   0.008
0.014   4.960   19.38   15.00
22.883  6.081   -2.508  0.295   26.028  1.150   0.006   0.007   1.150
28.170  0.111   46.877  38.000  0.386   1.000   0.263   0.231   0.032
0.015   5.065   13.99   15.00];

%[MCOAL CO21 STPOW O2MOL LTSGAS SXLGAS XH2S H2SFLO SCO2GS PSXL1 XCO21
CO2DN1 CO2TM1 WCO2 SYNGAS SULFUR CLSULF BSSULF O2CLS WAUX HHV_coal
Price]
%[kg/hr kg/hr kW kmol/hr kg/hr kmol/hr      kmol/hr kmol/hr bar
kg/m3 C kW kmol/hr kg/hr kg/hr kg/hr kmol/hr kW MH/kg $/tonne]

ratio_FT = [1.463   10.229  -4.719  0.515   24.900  0.453   34.583
107.973 0.701   0.007   0.846   1.466   0.563
1.449   8.875   -4.719  0.467   24.900  0.434   34.505  108.824 0.608
0.007   0.791   1.466   0.526
1.427   6.093   -4.695  0.369   24.900  0.377   34.283  111.308 0.417
0.007   0.683   0.910   0.453
1.401   1.977   -4.646  0.227   24.900  0.199   33.611  118.986 0.135
0.007   0.522   0.654   0.340
1.629   14.140  -4.565  0.766   24.900  0.422   34.830  105.260 0.970
0.007   1.741   0.276   1.297
1.603   12.959  -4.574  0.710   24.900  0.417   34.792  105.683 0.889
0.007   1.625   1.461   1.209
```

```
1.557   10.926  -4.578  0.605   24.900  0.412   34.697  106.714 0.749
0.007   1.399   1.344   1.042
1.484   5.788   -4.559  0.391   24.900  0.338   34.349  110.566 0.396
0.007   0.994   1.137   0.734
1.564   13.817  -4.696  0.712   24.900  0.443   34.777  105.845 0.948
0.007   0.991   0.276   0.593
1.575   13.821  -4.690  0.723   24.900  0.436   34.784  105.768 0.948
0.007   0.989   1.405   0.580
1.610   13.843  -4.673  0.758   24.900  0.417   34.804  105.549 0.949
0.007   0.987   1.413   0.544
1.661   13.856  -4.648  0.809   24.900  0.391   34.831  105.250 0.950
0.007   0.985   1.435   0.491];

% [SYNGAS CO22 STPOW SXLFL2 PSXL2 XCO22 CO2DN2 CO2TM2 WCO2 OUTPUT
UNCGAS WAUX N2DIL]
% [kmol/hr kg/hr kW kmol/hr bar     kg/m3 C kW m3/hr kmol/hr kW
kmol/hr]

ratio_PB = [20.984  -16.465 -9.380  -25.845 1.000   0.042   0.862
4.670   134.394 1.103   50.000  7.757
20.894  -16.410 -9.340  -25.750 1.000   0.041   0.844   4.650   133.682
1.102   50.000  7.592
20.767  -16.332 -9.284  -25.616 1.000   0.040   0.819   4.622   132.614
1.100   50.000  7.373
20.293  -16.042 -9.072  -25.114 1.000   0.036   0.725   4.516   128.715
1.093   50.029  6.526
21.950  -17.311 -9.812  -27.123 1.000   0.038   0.822   4.900   140.466
1.099   49.984  7.402
21.894  -17.285 -9.787  -27.073 1.000   0.037   0.800   4.881   139.826
1.098   50.000  7.196
21.684  -17.155 -9.693  -26.848 1.000   0.035   0.747   4.849   138.928
1.098   50.002  6.726
21.497  -17.048 -9.610  -26.658 1.000   0.033   0.692   4.804   137.449
1.097   50.000  6.228
21.339  -16.680 -9.539  -26.219 1.000   0.045   0.936   4.748   137.266
1.108   49.994  8.427
21.339  -16.679 -9.539  -26.218 1.000   0.045   0.936   4.747   137.268
1.109   49.953  8.427
21.331  -16.673 -9.536  -26.209 1.000   0.045   0.935   4.746   137.251
1.109   50.000  8.419
21.328  -16.671 -9.534  -26.205 1.000   0.045   0.936   4.746   137.230
1.109   50.014  8.428];

%[HPSTM GTPOW STPOW TOTPOW SYNGAS XCO2 CO2EXH FGMOLE FGMASS FGDENS
FGTEMP CO23]
%[kg/hr kW kW kW kmol/hr     kg/hr kmol/hr kg/hr kg/m3 C kg/hr]

for k = 1: size(ratio_gasification,1)
%for k = 8

output = 50000; %bbl/day
syngas = output*ratio_FT(k,1); %kmol/hr of syngas required to produce
'output' bbl/day
uncgas = output*ratio_FT(k,11); %Unconverted syngas to power block

%Calculating all the other variables based on 'output' and 'syngas'
```

```
m_coal = syngas*ratio_gasification(k,1)*24/1000; % Coal flow rate (TPD)
CO2_emission =
(syngas*ratio_gasification(k,2)+output*ratio_FT(k,2)+uncgas*ratio_PB(k,
12))*24/1000; % Total CO2 emissions (TPD)
GT_output = -uncgas*ratio_PB(k,2)/1000; % Power output from gas
turbines (MW)
ST_output = -(syngas*ratio_gasification(k,3) + output*ratio_FT(k,3) +
uncgas*ratio_FT(k,3))/1000; %Power output from steam turbines (MW)
auxillary_power = 1.15*(syngas*ratio_gasification(k,20) +
output*ratio_FT(k,12)+output*0.384125)/1000; %Total auxillary power
(MW), not counting the MEA power
net_output_power = GT_output + ST_output - auxillary_power; % Net power
output (MW)
oxygen = syngas*ratio_gasification(k,4); %Oxygen flow rate to gasifier
(kmol/hr)
LT_syngas = syngas*ratio_gasification(k,5); % Syngas input into low
temp cooling (kg/hr)
selexol_syngas = syngas*ratio_gasification(k,6); %Syngas input into
Selexol process (kmol/hr)
sulfur_claus = syngas*ratio_gasification(k,17); %Sulfur output from
Claus process (kg/hr)
sulfur_BS = syngas*ratio_gasification(k,18); % Sulfur output from
Beavon Stretford process (kg/hr)
HP_steam = uncgas*ratio_FT(k,1); %Flow rate of high pressure steam
(kg/hr)
x_H2S = ratio_gasification(k,7); %Mole fraction of H2S in the inlet
syngas to Selexol
H2S_flow = syngas*ratio_gasification(k,8); %Flow rate of H2S into the
Selexol process (kmol/hr)
selexol_CO2_syngas_1 = syngas*ratio_gasification(k,9); % Syngas inlet
into CO2 removal system (kmol/hr)
selexol_CO2_syngas_2 = output*ratio_FT(k,4); % Syngas inlet into CO2
removal system (kmol/hr)
p_Selexol_1 = ratio_gasification(k,10); %Pressure in the CO2 absorption
column (bar)
p_Selexol_2 = ratio_FT(k,5); %Pressure in the CO2 absorption column
(bar)
x_CO2_1 = ratio_gasification(k,11); %Mole fraction of CO2 in the inlet
syngas
x_CO2_2 = ratio_FT(k,6); %Mole fraction of CO2 in the inlet syngas
x_CO2_3 = ratio_PB(k,6); %Mole fraction of CO2 in the fluegases before
MEA CO2 removal
CO2_density_1 = ratio_gasification(k,12); %Density of CO2 in the first
selexol process (kg/m3)
CO2_density_2 = ratio_FT(k,7); %Density of CO2 in the second selexol
process(kg/m3)
CO2_temp_1 = ratio_gasification(k,13)+273; %Temperature of CO2 (K)
CO2_temp_2 = ratio_FT(k,8)+273; %Temperature of CO2 (K)
CO2_compr_work = syngas*ratio_gasification(k,14)+output*ratio_FT(k,9);
% CO2 compression work (kW)
CO2_exhaust = uncgas*ratio_PB(k,7)*24/1000; % CO2 emissions which are
not captured (TPD)
FG_mole_flow = uncgas*ratio_PB(k,8); % Mole flow rate of flue gases
entering MEA (kmole/hr)
FG_density = uncgas*ratio_PB(k,10); % Density of flue gases entering
MEA (kg/m3)
```

```
FG_temp = uncgas*ratio_PB(k,11)+273; % Temperature of flue gas at which
density is measured
FG_mass_flow = uncgas*ratio_PB(k,9); % Mass flow rate of flue gas
(kg/hr)

p_HP = 98; % High pressure steam (bar)

CPI = 525.4/395; % Chem Engg Plant Index correction for 2007 to 2000 $

solvent_price = 3.3; % $/kg of Selexol solvent
MEA_price = 1250*CPI; % $/tonne
CL_catalyst_price = 603.95; % $/ton of Claus catalyst
coal_price = ratio_gasification(k,22); % $/ton of coal, 10 for sub-
bituminous, 35 for bituminous
labour_price = 35; % $/day
carbon_tax = 25; % $/ton of CO2 emitted to atmosphere
CO2_transport = 5; % $/ton of CO2 trasported. Has a range of 1.3 - 10.4
$/ton
CO2_storage = 5; % $/ton of CO2 stored. Has a range of 0.65 - 10.4
$/ton
CO2_monitor = 0.25; % $/ton of CO2 monitored at the site. Range 0.13 -
0.39;
sulfur_credit = 106; % $/ton of sulfur
elec_price = [0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.10]; %
$/kWh
%elec_price = 0; % this is for convenience of sensitivity analysis,
remove otherwise
CF = 0.85; % Plant capacity factor

HHV_coal = ratio_gasification(k,21); % Higher heating value MJ/kg of
coal

%%%%%%%%% CAPITAL COST CALCULATIONS BEGIN %%%%%%%%%%%%
%--------------
% Coal handling section
    max_CH = 25000; % max TPD of coal in one train

    if m_coal < max_CH
        n_OT_CH = 1; % no. of operating trains of coal handling
    else
        n_OT_CH = ceil(m_coal/max_CH);
    end
    n_EX_CH = 0; % no. of spare trains
    n_T_CH = n_OT_CH + n_EX_CH;

    DC_CH = n_T_CH*9.92*(m_coal*1.1/n_OT_CH)/1000*CPI; % Direct cost of
coal handling in 2006 $
%----------------
% Oxidant feed section
    max_OF = 7730; % kmol/hr of oxygen in one train

    if oxygen < max_OF
        n_OT_OF = 1; % no. of operating trains
    else
        n_OT_OF = ceil(oxygen/max_OF);
```

```
    end
    n_EX_OF = 0; % no. of spare trains
    n_T_OF = n_OT_OF + n_EX_OF;

    DC_OF =
n_T_OF*31.15*(65^0.067)*((oxygen/n_OT_OF)^0.852)/(0.05^0.073)/1000*CPI;
% Direct cost of oxidant feed
%----------------
% Gasification section
%    max_G = 2903; % TPD of coal in one train, for GE radiant and EGas
    max_G = 2722; % TPD of coal in one train, for Shell radiant

    if m_coal < max_G
        n_OT_G = 1; % no. of operating trains
    else
        n_OT_G = ceil(m_coal/max_G);
    end
    n_EX_G = 1; % no. of spare trains
    n_T_G = n_OT_G + n_EX_G;

%    DC_G = n_T_G*15.88*((m_coal*1.1/n_OT_G)^0.943)/1000*CPI; % Direct
cost,
%    for quench gasifiers
    if k <= 4
        DC_G = n_T_G*43.00*((m_coal/n_OT_G)^0.943)/1000; % Direct cost,
2006$M, for GE radiant
    else if 4<k<=8
            DC_G = n_T_G*40.77*((m_coal/n_OT_G)^0.943)/1000; % Direct
cost, 2006$M, for EGas radiant
        else
            DC_G = n_T_G*55.23*((m_coal/n_OT_G)^0.943)/1000; % Direct
cost, 2006$M, for Shell radiant
        end
    end

%-----------------
% Low temperature gas cooling section

    max_LT = 590900; % kg/hr of syngas in one train

    if LT_syngas < max_LT
        n_OT_LT = 1; % no. of operating trains
    else
        n_OT_LT = ceil(oxygen/max_OF);
    end
    n_EX_LT = 1; % no. of spare trains
    n_T_LT = n_OT_LT + n_EX_LT;

    DC_LT = n_T_LT*0.0343*(LT_syngas/n_OT_LT)/1000*CPI; % Direct cost
%-----------------
% Selexol H2S removal section
    max_SXL = 30590; % kmol/hr of syngas in one train

    if selexol_syngas < max_SXL
        n_OT_SXL = 1; % no. of operating trains
```

```
    else
        n_OT_SXL = ceil(selexol_syngas/max_SXL);
    end
    n_EX_SXL = 1; % no. of spare trains
    n_T_SXL = n_OT_SXL + n_EX_SXL;

    DC_SXL =
n_T_SXL*0.659*((selexol_syngas/n_OT_SXL)^0.981)/(0.01^0.059)/1000*CPI;
% Direct cost
    initial_solvent = n_T_SXL*(-25200 +
34.7*(H2S_flow/n_OT_SXL)/x_H2S^1.04)/2.2; % kg of initial solvent
loading
    initial_solvent_cost = initial_solvent*solvent_price;
    makeup_solvent = CF*(-350 +
3.476*selexol_syngas/n_OT_SXL)*n_OT_SXL/2.2; % kg/yr of Selexol solvent

%------------------
% Claus plant section
    max_CL = 8227; % kg/hr of Sulfur in one train

    if sulfur_claus < max_CL
        n_OT_CL = 1; % no. of operating trains
    else
        n_OT_CL = ceil(sulfur_claus/max_CL);
    end
    n_EX_CL = 1; % no. of spare trains
    n_T_CL = n_OT_CL + n_EX_CL;

    DC_CL = n_T_CL*11.79*((sulfur_claus/n_OT_CL)^0.668)/1000*CPI; %
Direct cost
    initial_CL_catalyst = n_T_CL*0.0111*sulfur_claus/n_OT_CL; % kg of
initial Claus catalyst loading
    initial_catalyst_cost = initial_CL_catalyst*CL_catalyst_price;
    makeup_catalyst = n_OT_CL*0.00211*CF*sulfur_claus/n_OT_CL; %kg/yr
of Claus catalyst
%------------------
% Beavon Stretford plant section
    max_BS = 545; % kg/hr of Sulfur in one train

    if sulfur_BS < max_BS
        n_OT_BS = 1; % no. of operating trains
    else
        n_OT_BS = ceil(sulfur_BS/max_BS);
    end
    n_EX_BS = 1; % no. of spare trains
    n_T_BS = n_OT_BS + n_EX_BS;

    DC_BS = (63.76 +
n_T_CL*121.56*((sulfur_BS/n_OT_BS)^0.645))/1000*CPI; % Direct cost
    initial_BS_chemical = 188.76*sulfur_BS*CPI; % cost of initial
chemical loading in $
    makeup_BS_chemical = 374*CF*sulfur_BS*CPI; % $/yr
%------------------
% Fischer Tropsch reactor system
    DC_FT = 0.0092*output;
```

```
    initial_FT_catalyst = 120*output; % cost of initial catalyst
loading, $
    makeup_FT_catalyst = 674*output; %annual cost of make up catalyst
$/year
%-----------------
% Gas turbine section
%    DC_GT = 168*GT_output/1000*CPI; older model for 7FA
    DC_GT = 194.393*GT_output/1000; % $M 2006, for 7FB from NETL
report, base = 232MW
%-----------------
%Heat recovery steam generator section
    DC_HRSG =
794968*((p_HP/1500)^1.526)*((HP_steam/600000)^0.242)/1000*CPI;
%-----------------
%Steam turbine section
    DC_ST = 158.7*ST_output/1000*CPI;
%-----------------
%CO2 removal section - Selexol
    rho_selexol = 1030; % Density of Selexol solvent (kg/m3)
    M_selexol = 280; % Molecular weight of Selexol solvent (kg/kmol)
    alpha = 0.99; % Efficiency of CO2 removal system

    selexol_mol_1 = 17.44*alpha^1.013/(1-
alpha)^0.06261*x_CO2_1^0.1163*selexol_CO2_syngas_1^0.987116/p_Selexol_1
^0.85745/3600;
    selexol_mol_2 = 17.44*alpha^1.013/(1-
alpha)^0.06261*x_CO2_2^0.1163*selexol_CO2_syngas_2^0.987116/p_Selexol_2
^0.85745/3600;
    %kmol/s
    selexol_mass_1 = selexol_mol_1*M_selexol; %kg/s
    selexol_vol_1 = selexol_mass_1/rho_selexol; %m3/s

    selexol_mass_2 = selexol_mol_2*M_selexol; %kg/s
    selexol_vol_2 = selexol_mass_2/rho_selexol; %m3/s

    CO2_mass_1 = syngas*ratio_gasification(2)/3600;
    CO2_volume_1 = CO2_mass_1/CO2_density_1*298/CO2_temp_1;
    solvent_out_vol_1 = selexol_vol_1 + CO2_volume_1; % After CO2
capture, inlet to power recovery turbine (m3/s)
    solvent_out_mass_1 = selexol_mass_1 + CO2_mass_1;% kg/s

    CO2_mass_2 = output*ratio_FT(2)/3600;
    CO2_volume_2 = CO2_mass_2/CO2_density_2*298/CO2_temp_2;
    solvent_out_vol_2 = selexol_vol_2 + CO2_volume_2; % After CO2
capture, inlet to power recovery turbine (m3/s)
    solvent_out_mass_2 = selexol_mass_2 + CO2_mass_2;% kg/s

    p_exit_turb1_1 = 0.1212*p_Selexol_1^1.415; % Exit pres of first
power recov turbine (bar)
    p_exit_turb2_1 = 4.2; % Exit pres of second power recov turbine
(bar)

    p_exit_turb1_2 = 0.1212*p_Selexol_2^1.415; % Exit pres of first
power recov turbine (bar)
```

```
    p_exit_turb2_2 = 4.2; % Exit pres of second power recov turbine
(bar)

    power_turb1_1 = (p_Selexol_1 -
p_exit_turb1_1)*100*solvent_out_vol_1*0.77; % Power from first turbine
(kW)
    power_turb2_1 = (p_exit_turb1_1 -
p_exit_turb2_1)*100*solvent_out_vol_1*0.77; % kW

    power_turb1_2 = (p_Selexol_2 -
p_exit_turb1_2)*100*solvent_out_vol_2*0.77; % Power from first turbine
(kW)
    power_turb2_2 = (p_exit_turb1_2 -
p_exit_turb2_2)*100*solvent_out_vol_2*0.77; % kW

    recycle_compr_power_1 = 1780; %kW
    recycle_compr_power_2 = 1780; %kW

    %Cost calculations
    DC_abs_column_1 = (-1375.356 + 16.536*p_Selexol_1 +
0.1404*(selexol_mol_1*3600+selexol_CO2_syngas_1))*CPI/1000;
    DC_abs_column_2 = (-1375.356 + 16.536*p_Selexol_2 +
0.1404*(selexol_mol_2*3600+selexol_CO2_syngas_2))*CPI/1000;
    DC_abs_column = DC_abs_column_1 + DC_abs_column_2;

    DC_turb_1 = (2*219.086 + 0.1085*(power_turb1_1+power_turb2_1) +
0.0201*(p_exit_turb1_1^2+p_exit_turb2_1^2))*CPI/1000;
    DC_turb_2 = (2*219.086 + 0.1085*(power_turb1_2+power_turb2_2) +
0.0201*(p_exit_turb1_2^2+p_exit_turb2_2^2))*CPI/1000;
    DC_turb = DC_turb_1 + DC_turb_2;

    n_OT_slumptank_1 = ceil(solvent_out_mass_1/800);
    n_OT_slumptank_2 = ceil(solvent_out_mass_2/800);
    n_EX_slumptank_1 = 1; % no. of spare trains
    n_EX_slumptank_2 = 1; % no. of spare trains
    n_T_slumptank_1 = n_OT_slumptank_1 + n_EX_slumptank_1;
    n_T_slumptank_2 = n_OT_slumptank_2 + n_EX_slumptank_2;

    DC_slumptank_1 =
2.0049*n_T_slumptank_1*(solvent_out_mass_1/n_OT_slumptank_1)^0.7446*CPI
/1000;
    DC_slumptank_2 =
2.0049*n_T_slumptank_2*(solvent_out_mass_2/n_OT_slumptank_2)^0.7446*CPI
/1000;
    DC_slumptank = DC_slumptank_1 + DC_slumptank_2;

    DC_recycle_compr_1 = 5.598*recycle_compr_power_1^0.7784*CPI/1000;
    DC_recycle_compr_2 = 5.598*recycle_compr_power_2^0.7784*CPI/1000;
    DC_recycle_compr = DC_recycle_compr_1 + DC_recycle_compr_2;

    %Cost of just venting CO2
    DC_CO2_VENT = DC_abs_column + DC_turb + DC_slumptank +
DC_recycle_compr;

    %Compression costs
```

```
    DC_CO2_compr = 15.8*CO2_compr_work^0.64*CPI/1000;


%--------------------------------------
% CO2 removal section - Amine-based
    phi_lean = 0.2; % Lean solvent loading
    eff_CO2_MEA = 90; % Efficiency of CO2 removal in the MEA process
    C_MEA = 30; % Concentration of MEA sorbent in the solvent
    T_FG_in = 50; % Temperature of flue gases entering MEA process (deg
C)
    FG_vol_flow = FG_mass_flow/FG_density*298/FG_temp;
    % Reference values of a few parameters
    T_FG_ref = 318; % K
    FG_vol_flow_ref = 0.9e6; % Nm3/hr
    sorbent_vol_flow_ref = 3030.3; % m3/hr
    sorbent_makeup_ref = 1060; % kg/hr
    CO2_mass_flow_ref = 7150; % TPD
    sorbent_reclaimer_ref = 353.5; % kg/hr
    MEA_steam_ref = 83.3; % tonne/hr
    MEA_vol_ref = 757.6; %m3/hr
    MEA_loss_nominal = 1.5; % kg/tonneCO2
    MEA_loss_HSS = 0.5*MEA_loss_nominal;
    NAOH_reclaimer = 0.13; % kg/tonneCO2
    MEA_reclaimed = NAOH_reclaimer/40;
    CO2_compr_work_ref = 38.5; %MW
    CO2_compr_mass_ref = 7200; % TPD

    % Process parameter calculations
    L_G_ratio = exp(-
1.4352+0.1239*x_CO2_3*100+3.4863*phi_lean+0.0174*eff_CO2_MEA-
0.0397*C_MEA+0.0027*T_FG_in);
    sorbent_mole_flow = L_G_ratio*FG_mole_flow; % MEA sorbent flow rate
kmol/hr

    Q_L_ratio = exp(-2.4452-0.0037*x_CO2_3*100-
6.2743*phi_lean+0.0254*C_MEA);
    heat_req_MEA = Q_L_ratio*sorbent_mole_flow; % Regenerative heat
required in MEA process MJ/hr;
    m_steam = heat_req_MEA/2000; %tonne/hr
    MW_lean = 16.907 + 2.333*phi_lean + 0.204*C_MEA; % Average
molecular wt of lean solvent kg/kmol
    sorbent_vol_flow = sorbent_mole_flow*MW_lean/1000; %m3/hr

    CO2_compr_work_MEA = (-51.632 +
19.207*log(2000+14.7))*uncgas*ratio_PB(12)/1e6; % Work required for CO2
compression, MW

    sorbent_makeup = (MEA_loss_nominal+MEA_loss_HSS-
MEA_reclaimed)*uncgas*ratio_PB(12)/1000; % kg/hr

    % Cost calculations

    max_CO2_MEA = 5000; % TPD. Maximum train size of MEA unit. Each
train has 1 per train of the
```

```
    %following pieces of equipment. 2 pumps per train and 4 reboilers
per
    %train
    if uncgas*ratio_PB(12)*24/1000 < max_CO2_MEA
        n_OT_MEA = 1; % no. of operating trains
    else
        n_OT_MEA = ceil(uncgas*ratio_PB(12)*24/1000/max_CO2_MEA);
    end

    n_EX_MEA = 1;
    n_T_MEA = n_OT_MEA+n_EX_MEA;

    DC_absorber_MEA =
13.667*n_T_MEA*((T_FG_in+273)*FG_vol_flow/T_FG_ref/FG_vol_flow_ref/n_OT
_MEA)^0.6*CPI; %$M
    DC_sorb_regen =
8.3*n_T_MEA*(sorbent_vol_flow/sorbent_vol_flow_ref/n_OT_MEA)^0.6*CPI; %
$M
    DC_HX =
1.1*n_T_MEA*(sorbent_vol_flow/sorbent_vol_flow_ref/n_OT_MEA)^0.6*CPI; %
$M
    DC_sorb_proc =
3.5*(sorbent_makeup/sorbent_makeup_ref*n_T_MEA/n_OT_MEA)^0.6*CPI; % $M
    DC_pumps =
1.133*2*n_T_MEA*(sorbent_vol_flow/sorbent_vol_flow_ref/n_OT_MEA/2)^0.6*
CPI; %$M
    n_CO2_compr_MEA =
ceil(uncgas*ratio_PB(12)*24/1000/CO2_compr_mass_ref);
    DC_CO2_compr_MEA =
n_CO2_compr_MEA*16.85*(CO2_compr_work_MEA/CO2_compr_work_ref*n_T_MEA/n_
CO2_compr_MEA)^0.7*CPI;
    DC_FG_blower =
0.967*n_T_MEA*(T_FG_in*FG_vol_flow/T_FG_ref/FG_vol_flow_ref/n_OT_MEA)^0
.6*CPI;
    DC_sorb_reclaimer =
0.967*n_T_MEA*(sorbent_makeup/sorbent_reclaimer_ref/n_OT_MEA)^0.6*CPI;
%$M
    DC_reboiler =
n_T_MEA*4*1.117*(m_steam/83.3*sorbent_vol_flow/757.6/n_OT_MEA^2/4)^0.6*
CPI;

    DC_CCS_MEA =
DC_absorber_MEA+DC_sorb_regen+DC_HX+DC_sorb_proc+DC_pumps+DC_CO2_compr_
MEA+DC_FG_blower+DC_sorb_reclaimer+DC_reboiler;

%--------Total CCS cost-----------%
    DC_CO2_CCS = DC_CO2_VENT + DC_CO2_compr+DC_CCS_MEA;
    %DC_CO2_CCS = DC_CO2_VENT + DC_CO2_compr;
% It is assumed that the plant will install only the compressor.
% Transportation and storage are not considered in the capital cost but
% will be taken into account in the operating costs using IPCC
estimates.

%--------------------
% DIRECT COST MATRIX %
DC(1,1) = DC_CH;
```

```
DC(2,1) = DC_OF;
DC(3,1) = DC_G;
DC(4,1) = DC_LT;
DC(5,1) = DC_SXL;
DC(6,1) = DC_CL;
DC(7,1) = DC_BS;
DC(8,1) = DC_FT;
DC(9,1) = DC_GT;
DC(10,1) = DC_HRSG;
DC(11,1) = DC_ST;

for a = 1:11
    DC_CCS(a,1) = DC(a,1);
    DC_NO_CCS(a,1) = DC(a,1);
end
DC_CCS(12,1) = DC_CO2_CCS;
DC_NO_CCS(12,1) = DC_CO2_VENT;
PFC_NO_CCS = sum(DC_NO_CCS);
PFC_CCS = sum(DC_CCS);
DC = [DC_CCS DC_NO_CCS];
%--------------------
% INDIRECT CAPITAL COST %
IC_GFC = 0.15; % General facilities capital 15% of direct cost
IC_EHO = 0.10; % Engg & home office capital, 10% of direct cost
IC_PROC = 0.25; % Process contingency 5% of direct cost
IC_PROJ = 0.15; % Project contingency 15% of direct cost
IC_RLTY = 0.10; % Royalty charges 5% of direct cost

IC_VEC = [IC_GFC, IC_EHO, IC_PROC, IC_PROJ, IC_RLTY];

GFC = IC_GFC*DC;
EHO = IC_EHO*DC;
PROC = IC_PROC*DC;
PROJ = IC_PROJ*DC;
RLTY = IC_RLTY*DC;
%--------------------
% TOTAL CAPITAL COST %
TPC_VEC = DC + GFC + EHO + PROC + PROJ + RLTY;
TPC_CCS = sum(TPC_VEC(1:12,1));
TPC_NO_CCS = sum(TPC_VEC(1:12,2));
%--------------------
% INITIAL CATALYST AND CHEMICAL LOADING COSTS %
initial_cost =
(initial_solvent_cost+initial_catalyst_cost+initial_BS_chemical+initial
_FT_catalyst)/1e6; % $M
%--------------------
% OPERATION AND MAINTENANCE COSTS %
    coal_cost = m_coal*365*CF*coal_price; % $/yr
    sulfur_total = (sulfur_claus + sulfur_BS)*24/1000; %tons/day
    sulfur_revenue = sulfur_total*sulfur_credit*CF*365/1e6; %$M/yr
    MEA_cost = MEA_price*sorbent_makeup*24/1000*CF*365/1e6; % $M/yr
    VOM = (makeup_solvent*solvent_price +
makeup_catalyst*CL_catalyst_price + makeup_BS_chemical +
makeup_FT_catalyst + coal_cost)/1e6; % M$/yr
    VOM_matrix(1,1) = makeup_solvent*solvent_price/1e6;
    VOM_matrix(2,1) = makeup_catalyst*CL_catalyst_price/1e6;
```

```
    VOM_matrix(3,1) = makeup_BS_chemical/1e6;
    VOM_matrix(4,1) = coal_cost/1e6;
%    VOM_matrix(5,1) = OM_pipeline/1e6;
    VOM_matrix(5,1) = -sulfur_revenue/1e6;
    VOM_matrix;

    FOM_labour = labour_price*100*2*40*52*CPI/1e6;
    FOM_maint_CCS = 0.02*TPC_CCS;
    FOM_maint_NO_CCS = 0.02*TPC_NO_CCS;
    FOM_maint_labour_CCS = 0.4*FOM_maint_CCS;
    FOM_maint_labour_NO_CCS = 0.4*FOM_maint_NO_CCS;
    FOM_admin_CCS = 0.3*(FOM_labour + FOM_maint_labour_CCS);
    FOM_admin_NO_CCS = 0.3*(FOM_labour + FOM_maint_labour_NO_CCS);
    FOM_CCS = FOM_labour + FOM_maint_CCS + FOM_admin_CCS; % $M
    FOM_NO_CCS = FOM_labour + FOM_maint_NO_CCS + FOM_admin_NO_CCS; % $M
%--------------------
% OTHER CAPITAL COSTS %
    inventory_cost_CCS = 0.005*TPC_CCS;
    inventory_cost_NO_CCS = 0.005*TPC_NO_CCS;
    pre_production_CCS = FOM_CCS/12; % 1 month of FOM $M
    pre_production_NO_CCS = FOM_NO_CCS/12; % 1 month of FOM $M
    post_production = VOM/12; % 1 month of VOM $M
%--------------------

CRF = 0.15; % capital recovery factor
annual_CO2 = (CO2_emission+CO2_exhaust)*365*CF/1e6; % MT/y
annual_CO2_CCS = CO2_exhaust*CF*365/1e6; %MT/y
%annual_CO2_CCS = (CO2_exhaust+aspen_out(i,8)*24/1000)*CF*365/1e6;
%MT/y
CCS_geo_seq_cost = (CO2_transport+CO2_storage+CO2_monitor)*annual_CO2;
% $M/yr

elec_revenue_NO_CCS =
(net_output_power+CO2_compr_work/1000)*1000*24*365*CF*elec_price./1e6;
%$M/yr
elec_revenue_CCS = (net_output_power-
CO2_compr_work_MEA)*1000*24*365*CF*elec_price./1e6; %$M/yr
%elec_revenue_CCS = (net_output_power)*1000*24*365*CF*elec_price./1e6;
%$M/yr
TCR_CCS = 1.25*(TPC_CCS + initial_cost + inventory_cost_CCS +
pre_production_CCS + post_production); % total capital reqmt $M
TRR_CCS_ctax = TCR_CCS*CRF + VOM + MEA_cost + FOM_CCS +
CCS_geo_seq_cost + annual_CO2_CCS*carbon_tax- elec_revenue_CCS -
sulfur_revenue;
%TRR_CCS_ctax = TCR_CCS*CRF + VOM + FOM_CCS + CCS_geo_seq_cost +
annual_CO2_CCS*carbon_tax- elec_revenue_CCS - sulfur_revenue;
TRR_CCS_no_ctax = TCR_CCS*CRF + VOM + MEA_cost + FOM_CCS +
CCS_geo_seq_cost - elec_revenue_CCS - sulfur_revenue;
%TRR_CCS_no_ctax = TCR_CCS*CRF + VOM + FOM_CCS + CCS_geo_seq_cost -
elec_revenue_CCS - sulfur_revenue;
specific_cap_cost_CCS = TCR_CCS*1e6/output; % Capital cost per daily
barrel ($/DB)
output_cost_CCS_ctax = TRR_CCS_ctax*1e6/(output*CF*365); % $/bbl of
output
output_cost_CCS_no_ctax = TRR_CCS_no_ctax*1e6/(output*CF*365); % $/bbl
of output
```

```
TCR_NO_CCS = 1.25*(TPC_NO_CCS + initial_cost + inventory_cost_NO_CCS +
pre_production_NO_CCS + post_production); % total capital reqmt $M
specific_cap_cost_NO_CCS = TCR_NO_CCS*1e6/output; % Capital cost per
daily barrel ($/DB)
TRR_NO_CCS_ctax = TCR_NO_CCS*CRF + VOM + FOM_NO_CCS +
annual_CO2*carbon_tax - elec_revenue_NO_CCS - sulfur_revenue;
TRR_NO_CCS_no_ctax = TCR_NO_CCS*CRF + VOM + FOM_NO_CCS -
elec_revenue_NO_CCS - sulfur_revenue;
output_cost_NO_CCS_ctax = TRR_NO_CCS_ctax*1e6/(output*CF*365); % $/bbl
of output
output_cost_NO_CCS_no_ctax = TRR_NO_CCS_no_ctax*1e6/(output*CF*365); %
$/bbl of output

elec_effect = [elec_price*1000; output_cost_NO_CCS_no_ctax;
output_cost_NO_CCS_ctax; output_cost_CCS_no_ctax;
output_cost_CCS_ctax];
% RESULT MATRIX
result_CCS(1,k) = technology(k);
result_CCS(2,k) = output;
result_CCS(3,k) = m_coal;
result_CCS(4,k) = CO2_exhaust;
%result_CCS(3,i) = CO2_exhaust+aspen_out(i,8)*24/1000;
result_CCS(5,k) = net_output_power-CO2_compr_work_MEA;
%result_CCS(4,i) = net_output_power;
%result_CCS(i,5) = TCR_CCS;
result_CCS(6,k) = specific_cap_cost_CCS;
result_CCS(7,k) = elec_effect(4,9); %output cost @ $80/MWh, CCS, no
Ctax
result_CCS(8,k) = elec_effect(5,9); %output cost @ $80/MWh, CCS, Ctax
result_CCS(9,k) = 100*(output*0.058 +
result_CCS(5,k))/(m_coal*0.0116*HHV_coal); %Net plant efficiency (HHV)
%result_CCS(i,7) = output_cost_CCS;
%result_CCS(i,8) = (net_output_power+output*0.058)/(m_coal*0.0116*24);
%efficiency_CCS = (net_output_power+output*0.058)/(m_coal*0.0116*24)

result_NO_CCS(1,k) = technology(k);
result_NO_CCS(2,k) = output;
result_NO_CCS(3,k) = m_coal;
result_NO_CCS(4,k) = CO2_emission+CO2_exhaust;
result_NO_CCS(5,k) = net_output_power + CO2_compr_work/1000;
%result_NO_CCS(i,5) = TCR_NO_CCS;
result_NO_CCS(6,k) = specific_cap_cost_NO_CCS;
result_NO_CCS(7,k) = elec_effect(2,9); %output cost @ $80/MWh, no CCS,
no Ctax
result_NO_CCS(8,k) = elec_effect(3,9); %output cost @ $80/MWh, no CCS,
no Ctax
result_NO_CCS(9,k) = 100*(output*0.058 +
result_NO_CCS(5,k))/(m_coal*0.0116*HHV_coal); %Net plant efficiency
(HHV)

comparison = [result_NO_CCS, result_CCS];
water(k,1) = technology(k);
water(k,2) = ST_output*2.90*1.18*24 - output*0.164; %m3/day; 85% Water
consumption is for cooling tower. Scaling factor = 2.90m3/MWh. FT water
production = 1bbl/bbl
```

```
output_comparison = [output_cost_NO_CCS_no_ctax',
output_cost_NO_CCS_ctax', output_cost_CCS_no_ctax',
output_cost_CCS_ctax'];

end
%result_NO_CCS(i,7) = output_cost_NO_CCS_ctax;
%result_NO_CCS(i,8) = output_cost_NO_CCS_no_ctax;
%result_NO_CCS(i,9) = (net_output_power + CO2_compr_work/1000 +
output*0.058)/(m_coal*0.0116*24);
%efficiency_NO_CCS = (net_output_power+ CO2_compr_work/1000 +
output*0.058)/(m_coal*0.0116*24)

%contribution(1,1) = TCR_CCS*CRF*1e6/(output*365*CF);
%contribution(2,1) = sum(VOM_matrix(1:4,1))*1e6/(output*365*CF);
%contribution(3,1) = FOM_CCS*1e6/(output*365*CF);
%contribution(4,1) = CCS_geo_seq_cost*1e6/(output*365*CF);
%contribution(5,1) = -sulfur_revenue*1e6/(output*365*CF);
%contribution(6,1) = -elec_revenue*1e6/(output*365*CF);
%contribution(7,1) = output_cost_CCS;

%contribution(1,2) = TCR_NO_CCS*CRF*1e6/(output*365*CF);
%contribution(2,2) = sum(VOM_matrix(1:4,1))*1e6/(output*365*CF);
%contribution(3,2) = FOM_NO_CCS*1e6/(output*365*CF);
%contribution(4,2) = 0;
%contribution(5,2) = -sulfur_revenue*1e6/(output*365*CF);
%contribution(6,2) = -elec_revenue*1e6/(output*365*CF);
%contribution(7,2) = output_cost_NO_CCS_no_ctax;


% Sensitivity analysis of output price as a function of capital cost
and
% O&M costs
%s = [-1 -0.75 -0.5 -0.25 0 0.25 0.5 0.75 1];
%for s = -1:0.25:1
%    TRR_CCS_TCRsens = (1+s).*TCR_CCS*CRF + VOM + FOM_CCS -
elec_revenue; %sensitivity to capital cost
%    TRR_CCS_VOMsens = TCR_CCS*CRF + (1+s).*VOM + FOM_CCS -
elec_revenue; %sensitivity to VOM
%    TRR_CCS_FOMsens = TCR_CCS*CRF + VOM + (1+s).*FOM_CCS -
elec_revenue; %sensitivity to capital cost
%    output_cost_CCS_TCRsens = TRR_CCS_TCRsens*1e6/(output*CF*365); %
$/bbl of output
%    output_cost_CCS_VOMsens = TRR_CCS_VOMsens*1e6/(output*CF*365); %
$/bbl of output
%    output_cost_CCS_FOMsens = TRR_CCS_FOMsens*1e6/(output*CF*365); %
$/bbl of output
%    pct_chg_TCR = (output_cost_CCS_TCRsens/output_cost_CCS - 1)*100;
%percentage change in output from base case
%    pct_chg_VOM = (output_cost_CCS_VOMsens/output_cost_CCS - 1)*100;
%percentage change in output from base case
%    pct_chg_FOM = (output_cost_CCS_FOMsens/output_cost_CCS - 1)*100;
%percentage change in output from base case
%
```

```
%    sensitivity = [s; pct_chg_TCR; pct_chg_VOM; pct_chg_FOM];
%end
```

A2.3 Uncertainty Analysis for Liquids-Only Configuration

```
% This is the economics model for a CTL plant. The formulae are taken
from
% IECM documentation. The process section is divided into a number of
% different sections
clear;
%aspen_out = [948151.77 573310.041 610906.373 -74128.373 -509471.41
23400.1352 24421.9068 2031635.71 80348.7841 21913.5031 1486.63203
0.00860280 691.225296 78738.8109 19684.397 41.67 25 0.16711526
0.71230821 70.8885074 25.2950718 38 250 333.336443 81696.6574];
technology = [1.1; 1.2; 1.3; 1.4; 2.1; 2.2; 2.3; 2.4; 3.1; 3.2; 3.3;
3.4];

ratio_gasification = [11.710    8.475   -3.664  0.356   28.102  1.213
0.006   0.007   1.193   53.000  0.163   90.138  38.000  0.586   1.000
0.248   0.212   0.036   0.016   6.135   30.81   100.00
13.556  9.624   -3.901  0.356   29.467  1.242   0.008   0.009   1.219
53.000  0.181   90.087  38.000  0.664   1.000   0.338   0.293   0.045
0.015   3.375   26.14   60.00
19.156  14.133  -4.790  0.380   35.392  1.337   0.001   0.002   1.321
53.000  0.245   90.157  38.000  0.980   1.000   0.070   0.062   0.008
0.014   6.393   19.38   15.00
26.234  17.864  -6.060  0.379   42.667  1.429   0.006   0.009   1.406
53.000  0.291   90.145  38.000  1.238   1.000   0.301   0.273   0.028
0.012   7.177   13.99   15.00
13.135  7.932   -3.583  0.357   30.278  1.202   0.007   0.008   1.181
39.000  0.154   66.107  38.000  0.547   1.000   0.277   0.253   0.024
0.016   3.070   30.81   100.00
14.978  8.560   -3.732  0.351   31.161  1.220   0.009   0.011   1.195
39.000  0.163   66.077  38.000  0.589   1.000   0.372   0.342   0.030
0.016   5.867   26.14   60.00
20.066  11.135  -4.224  0.356   34.876  1.269   0.002   0.002   1.253
39.000  0.204   66.217  38.000  0.770   1.000   0.074   0.068   0.006
0.015   6.057   19.38   15.00
26.019  13.829  -5.263  0.336   41.214  1.336   0.007   0.009   1.315
39.000  0.241   66.245  38.000  0.957   1.000   0.299   0.280   0.018
0.013   3.443   13.99   15.00
10.557  3.770   -1.962  0.287   21.468  1.096   0.006   0.006   1.096
28.170  0.069   46.283  38.000  0.228   1.000   0.223   0.195   0.028
0.014   2.406   30.81   100.00
12.162  3.833   -2.024  0.285   21.890  1.100   0.008   0.008   1.100
28.170  0.069   46.201  38.000  0.230   1.000   0.303   0.265   0.038
0.014   2.403   26.14   60.00
16.899  5.801   -2.199  0.300   24.467  1.137   0.002   0.002   1.137
28.170  0.107   46.885  38.000  0.368   1.000   0.062   0.054   0.008
0.014   4.960   19.38   15.00
22.883  6.081   -2.508  0.295   26.028  1.150   0.006   0.007   1.150
28.170  0.111   46.877  38.000  0.386   1.000   0.263   0.231   0.032
0.015   5.065   13.99   15.00];
```

```
%[MCOAL CO21 STPOW O2MOL LTSGAS SXLGAS XH2S H2SFLO SCO2GS PSXL1 XCO21
CO2DN1 CO2TM1 WCO2 SYNGAS SULFUR CLSULF BSSULF O2CLS]
%[kg/hr kg/hr kW kmol/hr kg/hr kmol/hr      kmol/hr kmol/hr bar
kg/m3 C kW kmol/hr kg/hr kg/hr kg/hr kmol/hr]

ratio_FT = [1.174   10.431  -4.648  0.813   24.900  0.293   34.828
105.281 0.715   0.013   0.047   0.650   0.007   0.000
1.171   9.068   -4.652  0.762   24.900  0.272   34.792  105.677 0.621
0.012   0.035   0.629   0.007   0.000
1.166   6.262   -4.669  0.574   24.900  0.249   34.622  107.537 0.429
0.011   0.009   0.551   0.007   0.000
1.184   2.126   -4.622  0.446   24.900  0.109   34.392  110.080 0.145
0.010   0.010   0.567   0.007   0.000
1.206   14.460  -4.009  1.821   24.900  0.181   35.116  102.186 0.992
0.036   0.163   1.450   0.007   0.000
1.205   13.288  -4.066  1.690   24.900  0.180   35.099  102.361 0.911
0.034   0.151   1.349   0.007   0.000
1.201   11.229  -4.247  1.310   24.900  0.196   35.033  103.077 0.770
0.027   0.109   1.035   0.007   0.000
1.190   6.052   -4.374  0.912   24.900  0.152   34.893  104.581 0.414
0.019   0.029   0.810   0.007   0.000
1.223   14.038  -4.291  1.978   24.900  0.162   35.101  102.338 0.963
0.013   0.084   2.173   0.007   0.000
1.232   14.042  -4.227  2.156   24.900  0.149   35.118  102.159 0.963
0.013   0.088   2.424   0.007   0.000
1.260   14.057  -4.043  2.675   24.900  0.120   35.155  101.764 0.964
0.013   0.102   3.153   0.007   0.000
1.300   14.067  -3.762  3.460   24.900  0.093   35.191  101.381 0.965
0.013   0.124   4.251   0.007   0.000];

% [SYNGAS CO22 STPOW SXLFL2 PSXL2 XCO22 CO2DN2 CO2TM2 WCO2 OUTPUT
HHV_purge PURGE ]
% [kmol/hr kg/hr kW kmol/hr bar     kg/m3 C kW m3/hr  kJ/kg  kg/hr]

%for k = 1: size(ratio_gasification,1)
for k = 12

output = 50000; %bbl/day
syngas = output*ratio_FT(k,1); %kmol/hr of syngas required to produce
'output' bbl/day

%Calculating all the other variables based on 'output' and 'syngas'


m_coal = syngas*ratio_gasification(k,1)*24/1000; % Coal flow rate (TPD)
CO2_emission =
(syngas*ratio_gasification(k,2)+output*ratio_FT(k,2)+output*20*ratio_FT
(k,10)+output*ratio_FT(k,14))*24/1000; % Total CO2 emissions (TPD)
net_output_power = 0; % Net power output (MW)
%GT_output = 0; % Power output from gas turbines (MW)
ST_output = -(syngas*ratio_gasification(k,3) +
output*ratio_FT(k,3))/1000; %Power output from steam turbines (MW)
oxygen = syngas*ratio_gasification(k,4); %Oxygen flow rate to gasifier
(kmol/hr)
```

```
LT_syngas = syngas*ratio_gasification(k,5); % Syngas input into low
temp cooling (kg/hr)
selexol_syngas = syngas*ratio_gasification(k,6); %Syngas input into
Selexol process (kmol/hr)
sulfur_claus = syngas*ratio_gasification(k,17); %Sulfur output from
Claus process (kg/hr)
sulfur_BS = syngas*ratio_gasification(k,18); % Sulfur output from
Beavon Stretford process (kg/hr)
%HP_steam = 0; %Flow rate of high pressure steam (kg/hr)
x_H2S = ratio_gasification(k,7); %Mole fraction of H2S in the inlet
syngas to Selexol
H2S_flow = syngas*ratio_gasification(k,8); %Flow rate of H2S into the
Selexol process (kmol/hr)
selexol_CO2_syngas_1 = syngas*ratio_gasification(k,9); % Syngas inlet
into CO2 removal system (kmol/hr)
selexol_CO2_syngas_2 = output*ratio_FT(k,4); % Syngas inlet into CO2
removal system (kmol/hr)
p_Selexol_1 = ratio_gasification(k,10); %Pressure in the CO2 absorption
column (bar)
p_Selexol_2 = ratio_FT(k,5); %Pressure in the CO2 absorption column
(bar)
x_CO2_1 = ratio_gasification(k,11); %Mole fraction of CO2 in the inlet
syngas
x_CO2_2 = ratio_FT(k,6); %Mole fraction of CO2 in the inlet syngas
CO2_density_1 = ratio_gasification(k,12); %Density of CO2 in the first
selexol process (kg/m3)
CO2_density_2 = ratio_FT(k,7); %Density of CO2 in the second selexol
process(kg/m3)
CO2_temp_1 = ratio_gasification(k,13)+273; %Temperature of CO2 (K)
CO2_temp_2 = ratio_FT(k,8)+273; %Temperature of CO2 (K)
CO2_compr_work = syngas*ratio_gasification(k,14)+output*ratio_FT(k,9);
% CO2 compression work (kW)
purge_MW = 9000*output*ratio_FT(k,12)/3600/1000; %9,000 kJ/kg is the
average HHV of purge gases
H2_MW = 142919*output*ratio_FT(k,11)/3600/1000;
p_HP = 98; % High pressure steam (bar)
HHV_coal = ratio_gasification(k,21); %MJ/kg

solvent_price = 3.3; % $/kg of Selexol solvent
CL_catalyst_price = 603.95; % $/ton of Claus catalyst
coal_price = ratio_gasification(k,22); % $/ton of coal
labour_price = 35; % $/day
carbon_tax = 25; % $/ton of CO2 emitted to atmosphere
CO2_transport = 5; % $/ton of CO2 trasported. Has a range of 1.3 - 10.4
$/ton
CO2_storage = 5; % $/ton of CO2 stored. Has a range of 0.65 - 10.4
$/ton
CO2_monitor = 0.25; % $/ton of CO2 monitored at the site. Range 0.13 -
0.39;
sulfur_credit = 0; % $/ton of sulfur
%CCS_geo_seq = 4; % $/ton of CO2 for sequestration and monitoring, ref
IPCC report
elec_price = 0; % $/kWh
CF = 0.85; % Plant capacity factor

CPI = 525.4/395; % Chem Engg Plant Index correction for 2007 to 2000 $
```

```
% INDIRECT CAPITAL COST, if not doing Monte-Carlo %
IC_GFC = 0.15; % General facilities capital 15% of direct cost
IC_EHO = 0.10; % Engg & home office capital, 10% of direct cost
IC_PROC = 0.15; % Process contingency 15% of direct cost
IC_PROJ = 0.15; % Project contingency 15% of direct cost
IC_RLTY = 0.05; % Royalty charges 5% of direct cost

% Generation of data for Monte-Carlo uncertainty analysis

p = rand(20000,8); %random probability generation for Monte Carlo
simulation

a_CF = 0.75; % Minimum value of CF
m_CF = 0.85; % Most likely value of CF
b_CF = 0.95; % Maximum value of CF

a_cpr = 10; % Minimum value of coal price historically, uniform
distribution for bituminous. 10 for sub-bit and lignite
b_cpr = 20; % Maximum value of coal price for bituminous. for sub-bit
and lignite 20

a_dc = 0.75; % Direct cost varied between +/- 25%, triangular
distribution
m_dc = 1;
b_dc = 1.25;

a_gfc = 0.1; % Minimum value of general facilities capital for indirect
cap costs
m_gfc = 0.15; % Most likely value general facilities capital for
indirect cap costs
b_gfc = 0.2; % Maximum value of general facilities capital for indirect
cap costs

a_eho = 0.07; % Minimum value of engg and home office for indirect cap
costs
m_eho = 0.10; % Most likely value of engg and home office for indirect
cap costs
b_eho = 0.12; % Maximum value of engg and home office for indirect cap
costs

a_proc = 0.1; % Minimum value of process contingency for indirect cap
costs
m_proc = 0.25; % Most likely value of process contingency for indirect
cap costs
b_proc = 0.4; % Maximum value of process contingency for indirect cap
costs

a_proj = 0.1; % Minimum value of project contingency for indirect cap
costs
m_proj = 0.15; % Most likely value of project contingency for indirect
cap costs
b_proj = 0.2; % Maximum value of project contingency for indirect cap
costs
```

```
a_rlty = 0.1; % Minimum value of royalty charges for indirect cap costs
m_rlty = 0.15; % Most likely value of rolyalty charges for indirect cap
costs
b_rlty = 0.2; % Maximum value of royalty charges for indirect cap costs

a_ic = 0.4; % Sum of all the above indirect costs
m_ic = 0.75;
b_ic = 1;

a_CO2_trpt = 1.3; % Mimimum cost of transport
b_CO2_trpt = 10.4; % Maximum cost of transport

a_CO2_strg = 0.65; % Minimum cost of storage
b_CO2_strg = 10.4; % Maximum cost of storage

a_CO2_mon = 0.13; % Minimum cost of monitoring
b_CO2_mon = 0.39; % Maximum cost of monitoring

a_crf = 0.10; % Minimum of CRF, disc rate 3% 30 years
m_crf = 0.15;
b_crf = 0.2; % Maximum  of CRF, disc rate 20% 20-50 years

for i = 1:size(p,1)

    %Direct cost distribution (triangular)
    if p(i,1) <= (m_dc-a_dc)/(b_dc-a_dc)
        dc(i) = a_dc + sqrt(p(i,1)*(b_dc-a_dc)*(m_dc-a_dc));
    else
        dc(i) = b_dc - sqrt((1-p(i,1))*(b_dc-a_dc)*(b_dc-m_dc));
    end

    %dc(i) = 1; % for deterministic calculations

    % Indirect cost distribution (triangular)
    if p(i,2) <= (m_ic-a_ic)/(b_ic-a_ic)
        IC_TOTAL(i) = a_ic + sqrt(p(i,2)*(b_ic-a_ic)*(m_ic-a_ic));
    else
        IC_TOTAL(i) = b_ic - sqrt((1-p(i,2))*(b_ic-a_ic)*(b_ic-m_ic));
    end
    %IC_TOTAL(i) = m_ic; % for deterministic calculation

    % Coal price distribution (uniform)
    coal_price(i) = a_cpr + (b_cpr - a_cpr)*p(i,3);
    %coal_price(i) = 60; % for deterministic calculations

    % Capacity factor distribution (triangular)
    if p(i,4) <= (m_CF-a_CF)/(b_CF-a_CF)
        CF(i) = a_CF + sqrt(p(i,4)*(b_CF-a_CF)*(m_CF-a_CF));
    else
        CF(i) = b_CF - sqrt((1-p(i,4))*(b_CF-a_CF)*(b_CF-m_CF));
    end
    %CF(i) = 0.85; % for deterministic calculations

    % CCS operating cost distributions (uniform)
```

```
    CO2_transport(i) = a_CO2_trpt + (b_CO2_trpt - a_CO2_trpt)*p(i,5);
%    CO2_transport(i) = 5; % for deterministic calculations
    CO2_storage(i) = a_CO2_strg + (b_CO2_strg - a_CO2_strg)*p(i,6);
%    CO2_storage(i) = 5; % for determinictic calculations
    CO2_monitor(i) = a_CO2_mon + (b_CO2_mon - a_CO2_mon)*p(i,7);
%    CO2_monitor(i) = 0.25; % for deterministic calculations

    % Capital recovery factor distribution (triangular)
    if p(i,8) <= (m_crf-a_crf)/(b_crf-a_crf)
        CRF(i) = a_crf + sqrt(p(i,8)*(b_crf-a_crf)*(m_crf-a_crf));
    else
        CRF(i) = b_crf - sqrt((1-p(i,8))*(b_crf-a_crf)*(b_crf-m_crf));
    end
    %CRF(i) = 0.15; % for deterministic calculations

end


CPI = 525.4/395; % Chem Engg Plant Index correction for 2007 to 2000 $

%%%%%%%%% CAPITAL COST CALCULATIONS BEGIN %%%%%%%%%%%
%--------------
for i = 1:size(p,1)
% Coal handling section
    max_CH = 25000; % max TPD of coal in one train

    if m_coal < max_CH
        n_OT_CH = 1; % no. of operating trains of coal handling
    else
        n_OT_CH = ceil(m_coal/max_CH);
    end
    n_EX_CH = 0; % no. of spare trains
    n_T_CH = n_OT_CH + n_EX_CH;

    DC_CH = n_T_CH*9.92*(m_coal*1.1/n_OT_CH)/1000*CPI; % Direct cost of
coal handling in 2006 $
    IC_CH = IC_TOTAL(i)*DC_CH;
    PFC_CH = DC_CH + IC_CH;
%----------------
% Oxidant feed section
    max_OF = 7730; % kmol/hr of oxygen in one train

    if oxygen < max_OF
        n_OT_OF = 1; % no. of operating trains
    else
        n_OT_OF = ceil(oxygen/max_OF);
    end
    n_EX_OF = 0; % no. of spare trains
    n_T_OF = n_OT_OF + n_EX_OF;

    DC_OF =
n_T_OF*31.15*(65^0.067)*((oxygen/n_OT_OF)^0.852)/(0.05^0.073)/1000*CPI;
% Direct cost of oxidant feed
    IC_OF = IC_TOTAL(i)*DC_OF;
    PFC_OF = DC_OF + IC_OF;
```

```
%----------------
% Gasification section
    max_G = 2903; % TPD of coal in one train, for GE radiant and EGas
%    max_G = 2722; % TPD of coal in one train, for Shell radiant

    if m_coal < max_G
        n_OT_G = 1; % no. of operating trains
    else
        n_OT_G = ceil(m_coal/max_G);
    end
    n_EX_G = 1; % no. of spare trains
    n_T_G = n_OT_G + n_EX_G;

%    DC_G = n_T_G*15.88*((m_coal*1.1/n_OT_G)^0.943)/1000*CPI; % Direct
cost,
%    for quench gasifiers
    if k <= 4
        DC_G = n_T_G*43.00*((m_coal/n_OT_G)^0.943)/1000; % Direct cost,
2006$M, for GE radiant
    else if 4<k<=8
            DC_G = n_T_G*40.77*((m_coal/n_OT_G)^0.943)/1000; % Direct
cost, 2006$M, for EGas radiant
        else
            DC_G = n_T_G*55.23*((m_coal/n_OT_G)^0.943)/1000; % Direct
cost, 2006$M, for Shell radiant
        end
    end


    IC_G = IC_TOTAL(i)*DC_G;
    PFC_G = DC_G + IC_G;
%-----------------
% Low temperature gas cooling section

    max_LT = 590900; % kg/hr of syngas in one train

    if LT_syngas < max_LT
        n_OT_LT = 1; % no. of operating trains
    else
        n_OT_LT = ceil(oxygen/max_OF);
    end
    n_EX_LT = 1; % no. of spare trains
    n_T_LT = n_OT_LT + n_EX_LT;

    DC_LT = n_T_LT*0.0343*(LT_syngas/n_OT_LT)/1000*CPI; % Direct cost
    IC_LT = IC_TOTAL(i)*DC_LT;
    PFC_LT = DC_LT + IC_LT;
%-----------------
% Selexol H2S removal section
    max_SXL = 30590; % kmol/hr of syngas in one train

    if selexol_syngas < max_SXL
        n_OT_SXL = 1; % no. of operating trains
    else
        n_OT_SXL = ceil(selexol_syngas/max_SXL);
```

```
    end
    n_EX_SXL = 1; % no. of spare trains
    n_T_SXL = n_OT_SXL + n_EX_SXL;

    DC_SXL =
n_T_SXL*0.659*((selexol_syngas/n_OT_SXL)^0.981)/(0.01^0.059)/1000*CPI;
% Direct cost
    IC_SXL = IC_TOTAL(i)*DC_SXL;
    PFC_SXL = DC_SXL + IC_SXL;
    initial_solvent = n_T_SXL*(-25200 +
34.7*(H2S_flow/n_OT_SXL)/x_H2S^1.04)/2.2; % kg of initial solvent
loading
    initial_solvent_cost = initial_solvent*solvent_price;
    makeup_solvent = CF(i)*(-350 +
3.476*selexol_syngas/n_OT_SXL)*n_OT_SXL/2.2; % kg/yr of Selexol solvent

%-----------------
% Claus plant section
    max_CL = 8227; % kg/hr of Sulfur in one train

    if sulfur_claus < max_CL
        n_OT_CL = 1; % no. of operating trains
    else
        n_OT_CL = ceil(sulfur_claus/max_CL);
    end
    n_EX_CL = 1; % no. of spare trains
    n_T_CL = n_OT_CL + n_EX_CL;

    DC_CL = n_T_CL*11.79*((sulfur_claus/n_OT_CL)^0.668)/1000*CPI; %
Direct cost
    IC_CL = IC_TOTAL(i)*DC_CL;
    PFC_CL = DC_CL + IC_CL;
    initial_CL_catalyst = n_T_CL*0.0111*sulfur_claus/n_OT_CL; % kg of
initial Claus catalyst loading
    initial_catalyst_cost = initial_CL_catalyst*CL_catalyst_price;
    makeup_catalyst = n_OT_CL*0.00211*CF(i)*sulfur_claus/n_OT_CL;
%kg/yr of Claus catalyst
%-----------------
% Beavon Stretford plant section
    max_BS = 545; % kg/hr of Sulfur in one train

    if sulfur_BS < max_BS
        n_OT_BS = 1; % no. of operating trains
    else
        n_OT_BS = ceil(sulfur_BS/max_BS);
    end
    n_EX_BS = 1; % no. of spare trains
    n_T_BS = n_OT_BS + n_EX_BS;

    DC_BS = (63.76 +
n_T_CL*121.56*((sulfur_BS/n_OT_BS)^0.645))/1000*CPI; % Direct cost
    IC_BS = IC_TOTAL(i)*DC_BS;
    PFC_BS = DC_BS + IC_BS;
    initial_BS_chemical = 188.76*sulfur_BS*CPI; % cost of initial
chemical loading in $
    makeup_BS_chemical = 374*CF(i)*sulfur_BS*CPI; % $/yr
```

```
%-----------------
% Fischer Tropsch reactor system
    DC_FT = 0.0086*output;

    initial_FT_catalyst = 120*output; % cost of initial catalyst
loading, $
    makeup_FT_catalyst = 674*output; %annual cost of make up catalyst
$/year

    IC_FT = IC_TOTAL(i)*DC_FT;
    PFC_FT = DC_FT + IC_FT;
%-----------------
% Gas turbine section
%    DC_GT = 168*GT_output/1000*CPI;
%    IC_GT = IC_TOTAL(i)*DC_GT;
%    PFC_GT = DC_GT + IC_GT;
    DC_GT = 0;
    IC_GT = 0;
    PFC_GT = DC_GT + IC_GT;
%-----------------
%Heat recovery steam generator section
%    DC_HRSG =
794968*((p_HP/1500)^1.526)*((HP_steam/600000)^0.242)/1000*CPI;
%    IC_HRSG = IC_TOTAL(i)*DC_HRSG;
    DC_HRSG = 0;
    IC_HRSG = 0;
    PFC_HRSG = DC_HRSG + IC_HRSG;
%-----------------
%Steam turbine section
    DC_ST = 158.7*ST_output/1000*CPI;
    IC_ST = IC_TOTAL(i)*DC_ST;
    PFC_ST = DC_ST + IC_ST;
%-----------------
%CO2 removal section
    rho_selexol = 1030; % Density of Selexol solvent (kg/m3)
    M_selexol = 280; % Molecular weight of Selexol solvent (kg/kmol)
    alpha = 0.99; % Efficiency of CO2 removal system

    selexol_mol_1 = 17.44*alpha^1.013/(1-
alpha)^0.06261*x_CO2_1^0.1163*selexol_CO2_syngas_1^0.987116/p_Selexol_1
^0.85745/3600;
    selexol_mol_2 = 17.44*alpha^1.013/(1-
alpha)^0.06261*x_CO2_2^0.1163*selexol_CO2_syngas_2^0.987116/p_Selexol_2
^0.85745/3600;
    %kmol/s
    selexol_mass_1 = selexol_mol_1*M_selexol; %kg/s
    selexol_vol_1 = selexol_mass_1/rho_selexol; %m3/s

    selexol_mass_2 = selexol_mol_2*M_selexol; %kg/s
    selexol_vol_2 = selexol_mass_2/rho_selexol; %m3/s

    CO2_mass_1 = syngas*ratio_gasification(2)/3600;
    CO2_volume_1 = CO2_mass_1/CO2_density_1*298/CO2_temp_1;
    solvent_out_vol_1 = selexol_vol_1 + CO2_volume_1; % After CO2
capture, inlet to power recovery turbine (m3/s)
    solvent_out_mass_1 = selexol_mass_1 + CO2_mass_1;% kg/s
```

```
    CO2_mass_2 = output*ratio_FT(2)/3600;
    CO2_volume_2 = CO2_mass_2/CO2_density_2*298/CO2_temp_2;
    solvent_out_vol_2 = selexol_vol_2 + CO2_volume_2; % After CO2
capture, inlet to power recovery turbine (m3/s)
    solvent_out_mass_2 = selexol_mass_2 + CO2_mass_2;% kg/s

    p_exit_turb1_1 = 0.1212*p_Selexol_1^1.415; % Exit pres of first
power recov turbine (bar)
    p_exit_turb2_1 = 4.2; % Exit pres of second power recov turbine
(bar)

    p_exit_turb1_2 = 0.1212*p_Selexol_2^1.415; % Exit pres of first
power recov turbine (bar)
    p_exit_turb2_2 = 4.2; % Exit pres of second power recov turbine
(bar)

    power_turb1_1 = (p_Selexol_1 -
p_exit_turb1_1)*100*solvent_out_vol_1*0.77; % Power from first turbine
(kW)
    power_turb2_1 = (p_exit_turb1_1 -
p_exit_turb2_1)*100*solvent_out_vol_1*0.77; % kW

    power_turb1_2 = (p_Selexol_2 -
p_exit_turb1_2)*100*solvent_out_vol_2*0.77; % Power from first turbine
(kW)
    power_turb2_2 = (p_exit_turb1_2 -
p_exit_turb2_2)*100*solvent_out_vol_2*0.77; % kW

    recycle_compr_power_1 = 1780; %kW
    recycle_compr_power_2 = 1780; %kW

    %Cost calculations
    DC_abs_column_1 = (-1375.356 + 16.536*p_Selexol_1 +
0.1404*(selexol_mol_1*3600+selexol_CO2_syngas_1))*CPI/1000;
    DC_abs_column_2 = (-1375.356 + 16.536*p_Selexol_2 +
0.1404*(selexol_mol_2*3600+selexol_CO2_syngas_2))*CPI/1000;
    DC_abs_column = DC_abs_column_1 + DC_abs_column_2;

    DC_turb_1 = (2*219.086 + 0.1085*(power_turb1_1+power_turb2_1) +
0.0201*(p_exit_turb1_1^2+p_exit_turb2_1^2))*CPI/1000;
    DC_turb_2 = (2*219.086 + 0.1085*(power_turb1_2+power_turb2_2) +
0.0201*(p_exit_turb1_2^2+p_exit_turb2_2^2))*CPI/1000;
    DC_turb = DC_turb_1 + DC_turb_2;

    n_OT_slumptank_1 = ceil(solvent_out_mass_1/800);
    n_OT_slumptank_2 = ceil(solvent_out_mass_2/800);
    n_EX_slumptank_1 = 1; % no. of spare trains
    n_EX_slumptank_2 = 1; % no. of spare trains
    n_T_slumptank_1 = n_OT_slumptank_1 + n_EX_slumptank_1;
    n_T_slumptank_2 = n_OT_slumptank_2 + n_EX_slumptank_2;

    DC_slumptank_1 =
2.0049*n_T_slumptank_1*(solvent_out_mass_1/n_OT_slumptank_1)^0.7446*CPI
/1000;
```

```
    DC_slumptank_2 =
2.0049*n_T_slumptank_2*(solvent_out_mass_2/n_OT_slumptank_2)^0.7446*CPI
/1000;
    DC_slumptank = DC_slumptank_1 + DC_slumptank_2;

    DC_recycle_compr_1 = 5.598*recycle_compr_power_1^0.7784*CPI/1000;
    DC_recycle_compr_2 = 5.598*recycle_compr_power_2^0.7784*CPI/1000;
    DC_recycle_compr = DC_recycle_compr_1 + DC_recycle_compr_2;

    %Cost of just venting CO2
    DC_CO2_VENT = DC_abs_column + DC_turb + DC_slumptank +
DC_recycle_compr;
    IC_CO2_VENT = IC_TOTAL(i)*DC_CO2_VENT;
    PFC_CO2_VENT = DC_CO2_VENT + IC_CO2_VENT;

    %Compression costs
    DC_CO2_compr = 15.8*CO2_compr_work^0.64*CPI/1000;
    DC_CO2_CCS = DC_CO2_VENT + DC_CO2_compr;
    IC_CO2_CCS = IC_TOTAL(i)*DC_CO2_CCS;
    PFC_CO2_CCS = DC_CO2_CCS + IC_CO2_CCS;

%---------------------
% TOTAL PLANT COSTS

TPC_NO_CCS =
PFC_CH+PFC_OF+PFC_G+PFC_LT+PFC_SXL+PFC_CL+PFC_BS+PFC_FT+PFC_GT+PFC_HRSG
+PFC_ST+PFC_CO2_VENT;
TPC_CCS =
PFC_CH+PFC_OF+PFC_G+PFC_LT+PFC_SXL+PFC_CL+PFC_BS+PFC_FT+PFC_GT+PFC_HRSG
+PFC_ST+PFC_CO2_CCS;

%---------------------
% INITIAL CATALYST AND CHEMICAL LOADING COSTS %
initial_cost =
(initial_solvent_cost+initial_catalyst_cost+initial_BS_chemical+initial
_FT_catalyst)/1e6; % $M

%---------------------
% OPERATION AND MAINTENANCE COSTS %
    FOM_labour = labour_price*100*2*40*52*CPI/1e6;
    FOM_maint_CCS = 0.02*TPC_CCS;
    FOM_maint_NO_CCS = 0.02*TPC_NO_CCS;
    FOM_maint_labour_CCS = 0.4*FOM_maint_CCS;
    FOM_maint_labour_NO_CCS = 0.4*FOM_maint_NO_CCS;
    FOM_admin_CCS = 0.3*(FOM_labour + FOM_maint_labour_CCS);
    FOM_admin_NO_CCS = 0.3*(FOM_labour + FOM_maint_labour_NO_CCS);
    FOM_CCS = FOM_labour + FOM_maint_CCS + FOM_admin_CCS; % $M
    FOM_NO_CCS = FOM_labour + FOM_maint_NO_CCS + FOM_admin_NO_CCS; % $M


    coal_cost = 365*CF(i)*coal_price(i)*m_coal; % $/yr
    sulfur_total = (sulfur_claus + sulfur_BS)*24/1000; %tons/day
    sulfur_revenue = sulfur_total*sulfur_credit*CF(i)*365/1e6; % $M/yr
```

```
    VOM = (makeup_solvent*solvent_price +
makeup_catalyst*CL_catalyst_price + makeup_BS_chemical +
makeup_FT_catalyst + coal_cost)./1e6; % M$/yr

%---------------------
% OTHER CAPITAL COSTS %
    inventory_cost_CCS = 0.005*TPC_CCS;
    inventory_cost_NO_CCS = 0.005*TPC_NO_CCS;
    pre_production_CCS = FOM_CCS/12; % 1 month of FOM $M
    pre_production_NO_CCS = FOM_NO_CCS/12; % 1 month of FOM $M
    post_production = VOM/12; % 1 month of VOM $M
%---------------------

annual_CO2 = (CO2_emission)*365*CF(i)/1e6; % MT/y
CCS_geo_seq_cost =
(CO2_transport(i)+CO2_storage(i)+CO2_monitor(i))*annual_CO2; % $M/yr
elec_revenue = net_output_power*1000*24*365*CF(i)*elec_price./1e6;
%$M/yr

TCR_CCS(i) = 1.25*dc(i)*(TPC_CCS + initial_cost + inventory_cost_CCS +
pre_production_CCS + post_production); % total capital reqmt $M
specific_cap_cost_CCS = TCR_CCS(i)*1e6/output; % Capital cost per daily
barrel ($/DB)
TRR_CCS = TCR_CCS(i)*CRF(i) + VOM + FOM_CCS + CCS_geo_seq_cost -
sulfur_revenue - elec_revenue;
output_cost_CCS(i) = TRR_CCS*1e6/(output*CF(i)*365); % $/bbl of output

TCR_NO_CCS(i) = 1.25*dc(i)*(TPC_NO_CCS + initial_cost +
inventory_cost_NO_CCS + pre_production_NO_CCS + post_production); %
total capital reqmt $M
specific_cap_cost_NO_CCS = TCR_NO_CCS(i)*1e6/output; % Capital cost per
daily barrel ($/DB)
TRR_NO_CCS = TCR_NO_CCS(i)*CRF(i) + VOM + FOM_NO_CCS +
(annual_CO2*carbon_tax) - sulfur_revenue - elec_revenue;
output_cost_NO_CCS(i) = TRR_NO_CCS/(output*CF(i)*365)*1e6; % $/bbl of
output

end
stats = [mean(CF) median(CF) prctile(CF,5) prctile(CF,95);
    mean(coal_price) median(coal_price) prctile(coal_price,5)
prctile(coal_price,95);
    mean(TCR_NO_CCS) median(TCR_NO_CCS) prctile(TCR_NO_CCS,5)
prctile(TCR_NO_CCS,95);
    mean(output_cost_NO_CCS) median(output_cost_NO_CCS)
prctile(output_cost_NO_CCS,5) prctile(output_cost_NO_CCS,95);
    mean(TCR_CCS) median(TCR_CCS) prctile(TCR_CCS,5)
prctile(TCR_CCS,95);
    mean(output_cost_CCS) median(output_cost_CCS)
prctile(output_cost_CCS,5) prctile(output_cost_CCS,95)];

end
```

Appendix A3: FT diesel and gasoline – properties and emissions

A3.1 Fischer-Tropsch diesel – properties and performance

Data of tests [28] conducted using FT diesel on trucks shows that it can become a very clean and effective alternative to conventional diesel. Figures A3.1 to A3.5 show the performance of engines using FT diesel, either on a pure basis or as a blend in US 2-D type diesel, which is the commercial diesel available in USA. Also shown in the figures are the California Auto Regulation Board (CARB) standards for diesel fuels. Table A3.3 shows a comparison of FT fuels with CARB standards and the commercial grade US 2-D diesel.

Table A3.1: Desired properties of diesel fuel

Property	**Remarks**
Flash point (minimum temperature at which fuel ignites)	Should be high for safety reasons
Viscosity	Low viscosity leads to poor lubrication and high viscosity causes poor atomization of liquid
Cetane number (indication of combustion performance)	Should be high
API gravity (indicates density and energy content)	Should be high so as to contain more energy
Sulfur and nitrogen	Should be very low
Aromatics	Should be very low

Table A3.2: Comparison of FT diesel with commercial fuel US 2-D and standards [1]

Property	US 2-D	FT diesel	CARB specification
IBP (oC)	184	189	203
Density (kg/L)	0.855	0.777	0.831
Viscosity (cSt)	2.4	2.4	2.4
Cetane no.	40	>70	49
Aromatics (wt %)	32.8	0.5	6.7
Sulfur (mass %)	0.028	0.001	0.022

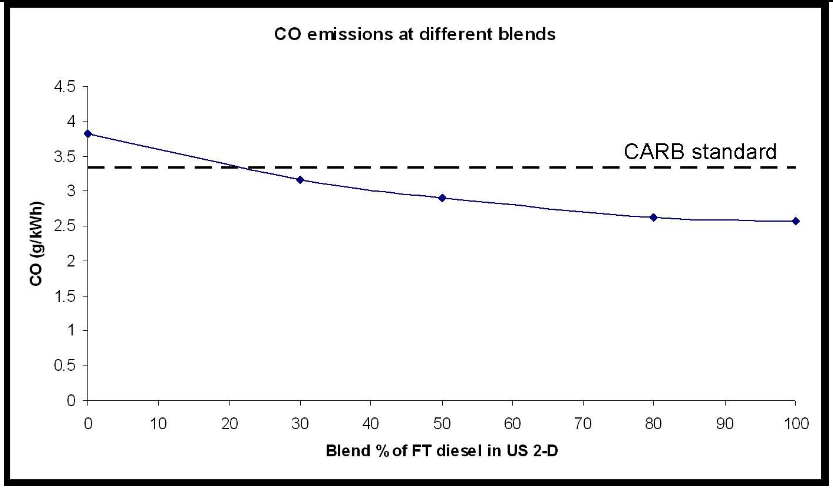


Figure A3.1: Carbon monoxide emissions from diesel blended with FT diesel

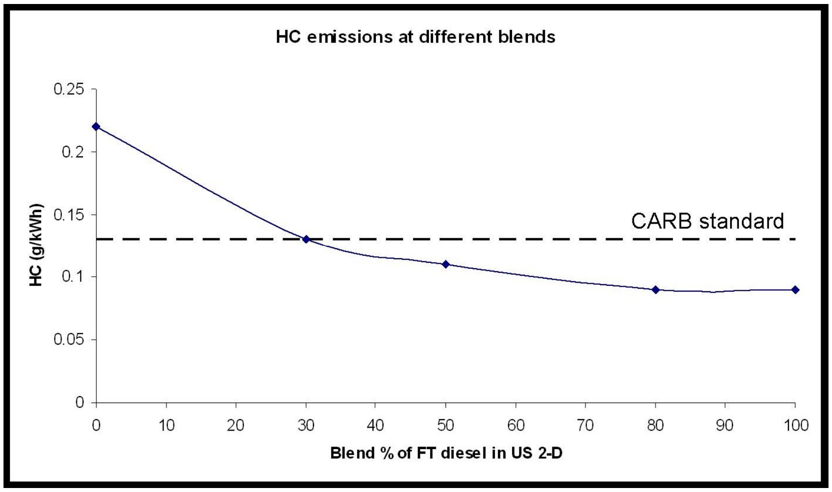


Figure A3.2: Hydrocarbon emissions from diesel blended with FT diesel

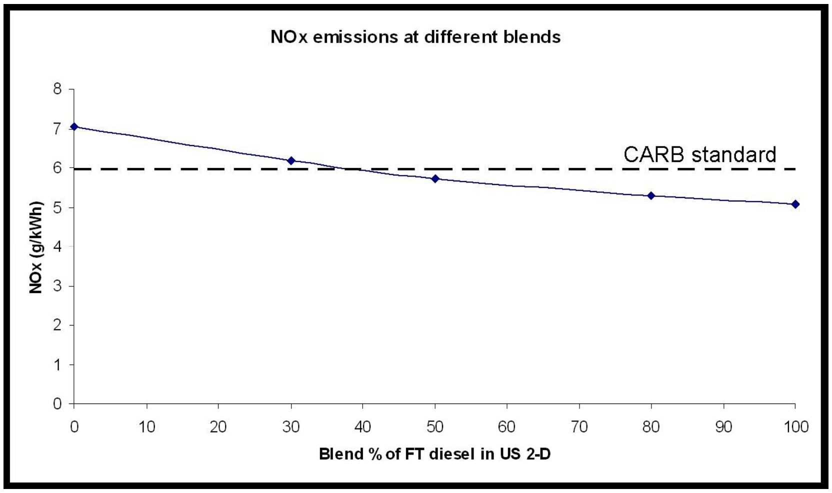


Figure A3.3: Nitrogen oxides emissions from diesel blended with FT diesel

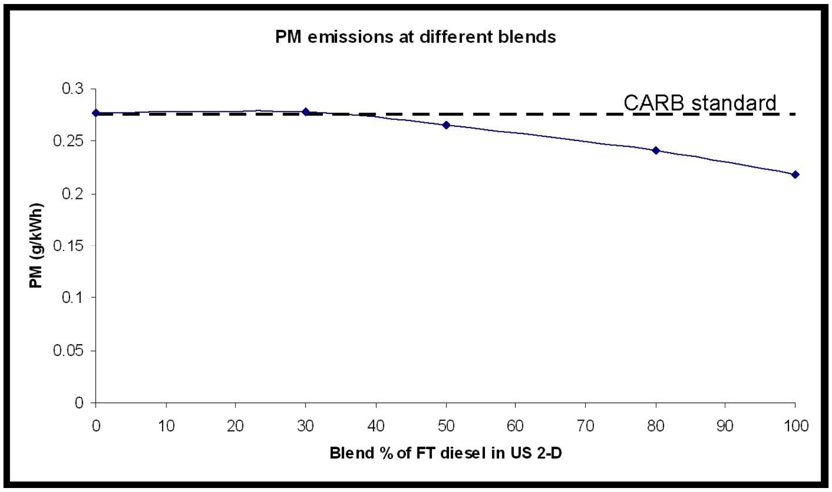


Figure A3.4: Particulate matter emissions from diesel blended with FT diesel

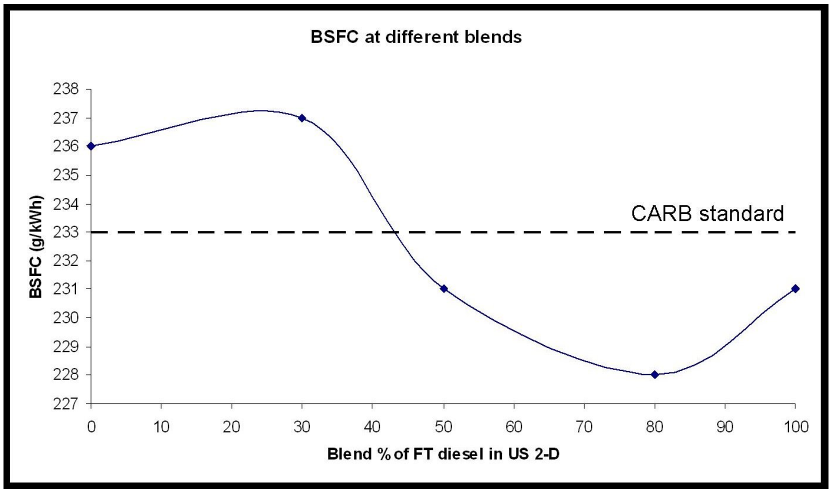


Figure A3.5: Brake specific fuel consumption of an engine using diesel blended with FT diesel

The following conclusions can be drawn from Table A3.2:

- Initial boiling point (IBP) of FT diesel is higher and closer to CARB specification than US 2-D
- FT diesel has better properties than US 2-D and even the CARB standards in terms of cetane number, aromatics and sulfur contents.

- Density of FT diesel is low which makes its heating value slightly lower than the other fuels in consideration.
- It has also been observed in some tests [28] that the lubricity of neat FT diesel was unacceptable. Lower lubricity causes wearing of engine parts, particularly the fuel injection system operating at very high pressures. To prevent this, a lubricity additive like Paradyne 655 has been added.

The trends of emissions and engine performance in terms of brake specific fuel consumption (BSFC) can be interpreted based on the above observations about FT diesel properties. The following conclusions can be drawn from the figures:

- All the emissions including CO, unburnt hydrocarbons (HC), nitrogen oxides (NOx) and particulate matters (PM) decrease as the percentage of FT diesel increases in the engine feed. Because of very high cetane number of FT diesel, its combustion characteristics are greatly enhanced over the lower cetane number fuels. As a result, carbon monoxide and hydrocarbon emissions, which are a result of incomplete combustion, reduce as more FT fuel is blended into engine feed. The same can be said of particulate matter. NOx emissions are much lower in pure FT diesel because the fuel itself is practically nitrogen-free.
- BSFC is a function of the heating value of fuel also. Because of its lower density, BSFC of 100% FT diesel is higher than 80% blend. Still, the performance is much better than pure US 2-D fuel or even CARB standard.

From the above discussion, it can be concluded that FT diesel can form a potential alternative fuel to conventional diesel and can be used without any modifications in the engine technology as such. Engines using FT diesel offer better performance and lower emissions. Also, diesel can be easily produced directly from the FT process without requiring further treatments to improve its properties to make it suitable for use in IC engines.

A3.2. Fischer-Tropsch gasoline – properties and issues

As shown in Table A3.3, the most important property of a good engine gasoline is its octane number. Higher the octane number, higher is the performance of the engine. A good fuel also needs to be low in sulfur, nitrogen and aromatics. Like FT diesel, FT gasoline also is a very clean fuel in terms of criteria air pollutants. However, the gasoline fraction produced in the FT reactor has a very low octane number [14]. The main reasons for FT gasoline being of low octane quality and further steps required to enhance the quality have been examined in this section.

Table A3.3: Desirable properties of gasoline fuel

Property	**Remarks**
Octane number (indication of combustion and anti-knock performance)	Should be high
Aromatics	Should be very low
Olefins (unsaturated hydrocarbons)	Should be low. High olefins lead to low oxidation stability and hence to spontaneous combustion
Oxygenates	Can be present in a moderate amounts to improve octane quality
Sulfur and nitrogen	Should be very low
Lead (earlier added to prevent knocking)	Should not be present

Most of the hydrocarbons produced in an FT process are straight chained. Though straight chains are good in terms of the cetane number, they possess low octane numbers. The straight-chained nature of FT gasoline is the primary reason for its octane number being low. Olefins (unsaturated hydrocarbons) have higher octane numbers than paraffins (saturated hydrocarbons). Because of the nature of FT reaction, the products contain predominantly olefins. FT gasoline has an olefinic content of about 70% [14]. Since the octane number is low in spite of such high olefinic content, it can be inferred that the effect of straight chains is more pronounced in reducing the octane number than the effect of olefins.

As can be seen from table A3.3, for a fuel-grade gasoline, olefin content has to be very low since high olefins cause low oxidation stability of the fuel. The high olefinic nature of FT gasoline is an undesirable property if it has to be used as an engine fuel.

Before looking at the options to improve the properties of FT gasoline, it is important to note another key aspect of octane number. As the chain length of hydrocarbons increases, the difference between the octane numbers of olefins and paraffins also increases. In other words, when the olefinic content of FT gasoline is modified, it is better to modify lighter olefins while keeping heavier olefins to improve the octane quality.

The following changes have to be made in FT gasoline to make it suitable for use in an automobile:

- To improve the octane quality, straight chains have to be converted into branched chains.
- To meet the low olefin requirement, olefins have to be converted into paraffins.

These structural changes in the hydrocarbons are possible by the use of the following reaction mechanisms:

- Isomerization – the process of converting straight chains to branched chains, but not changing the number of carbon and hydrogen atoms (in other words, the weight) of the hydrocarbons

- Hydrogenation – the process of adding hydrogen to olefins to convert them into paraffins
- Oligomerization – the process of adding carbon atoms to increase the length of the chain. This process helps in converting lighter olefins into heavier olefins, which can improve the octane number better than lighter olefins.

These processes are technically feasible and hence theoretically FT gasoline can be modified to meet the commercial fuel standards. However, it is not very clear from the published literature if at all this has been ever undertaken. Data on the tests conducted using FT gasoline in real world engines is also not available. As a result, it is not obvious whether the modified FT gasoline can be used as an effective fuel in automobile engines. What can be inferred is that the immediate gasoline product obtained from FT reaction is not suitable to be used as an engine fuel and a large number of subsequent steps are required to modify it into a commercial fuel. Because of this, the price of FT gasoline is likely to be more than that of FT diesel.