Techno Economic Assessment of the Gas to Liquid and Coal to Liquid Processes

by

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Abstract

With the fluctuations in conventional crude oil production and uncertainty in its global price, alternative sources of liquid fuels from natural gas and coal are being considered. In addition, formulation of policies in several jurisdictions on phase-out of coal power plants due to climate change considerations has also created a need for the development of alternative utilization of coal. Gas-to-liquid (GTL) and coal-to-liquid (CTL) processes are two liquefaction technologies that respectively convert natural gas and coal to liquid fuels. There is very limited work on development of scale factors for estimation of capital cost of these plants. In this study, the economic potentials of the GTL and CTL processes are investigated. A case study for western Canada is conducted which has large deposits of coal and natural gas. The capital costs of the key equipment of the plants are estimated through development of cost scale-up factors. The production cost for a 50,000 bbl/day of liquid fuels from the GTL and CTL plant is estimated through development of data-intensive techno-economic models using bottom-up methodology. The developed scale-up factor for the GTL and CTL was found to be 0.7 and 0.65 respectively. For both plants, benefits of economey of scale is achieved at a capacity above 20,000 bbl/day. The production cost of the GTL and CTL process are 44.61 and 57.65 cent/lit respectively. On the other hand, when carbon capture and sequestration (CCS) was considered, the production cost of the CTL plant increases significantly. The potential usage of the GTL is attractive due to its simplicity and the relatively low capital investment. On the other hand, the CTL is complex due to the additional CCS and sulphur removal unit.

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Nomenclature

GTL	Gas to liquid
CTL	Coal to liquid
FT	Fischer-Tropsch
ATR	Auto-thermal reactor
IGCC	Integrated gasification combined cycle
CCS	Carbon capture and sequestration
EOR	Enhanced oil recovery
ECBM	Enhanced coal bed methane
NETL	National energy technology laboratory
DME	Dimethyl ether
GHG	Greenhouse gas
LCA	Life cycle assessment
CPO	Catalytic partial oxidation
CMR	Ceramic membrane reforming
MPa	Mega Pascal
°C	Centigrade degree
NO_X	Nitrogen oxides
LPG	Liquefied petroleum gas
bbl	Barrels
ASF	Anderson-Schulz-Flory
LTFT	Low temperature Fischer-Tropsch
HTFT	High temperature Fischer-Tropsch
ASU	Air separation unit
MTG	Methanol to gasoline
GTG	Gas to gasoline
C_3/C_4	Propane and butane
DCL	Direct coal liquefaction
ICL	Indirect coal liquefaction
MMBtu	Million British thermal units
MJ	Mega Joules
LNG	Liquefied natural gas
CO_2e	Equivalent carbon dioxide

ULSD	Ultra-low sulphur diesel
MCF	Million cubic feet
TCI	Total capital investment
BIG-FT	Biomass integrated Fischer-Tropsch
PSA	Pressure swing adsorption
KW	Kilo watt
C$	Canadian dollars
CBGTL	Coal, biomass and gas to liquid
CBTL	Coal and biomass to liquid
C_b	The base capacity refers to a particular capacity size
C_r	The required capacity
C_b	The cost of base case capacity
C_r	The cost of the required equipment
f	Scale factor
w_n	Mass fraction of n-carbon chain
α	Chain growth probability

Chapter 1.   Introduction

1.1.   Background and motivation

There is an increasing need globally to reduce the reliance on crude oil, especially in light of environmental impacts and economic risks. The fluctuation in crude oil prices in the last decade and uncertainty in the availability of fossil fuels have led to the need to develop alternative sources for transport fuels. Oil prices fluctuated between \$140/barrel and \$40/barrel in 2008, and the average price was a little over \$100/barrel in 2014 [1]. However, recently the oil prices have declined to about half of 2014 level and is expected to be short term. In some countries the availability of crude oil depends on the local political situation. Canada has huge fossil fuel natural resources, among them natural gas and coal are the major ones. Canada's total natural gas production rate in 2014 was 12.4 billion cubic meters, and 34.5 million tonnes of coal were produced in Alberta province alone in that same year [2].

Liquid fuel, by nature, is one of the cleanest fuels (with a sulfur content of less than 1 ppm compared to the 10 ppm sulfur in crude oil fuels) [3, 4]. Alternative fuels that can be substituted for conventional oil can reduce the dependency on conventional crude oil and help to produce clean fuels. Synthetic liquids fuel like diesel and gas oil, which are produced from natural gas and coal, are therefore attractive. Global fuel demand is expected to increase by 2.1% annually in the next 5 years [5]. Based on current consumption rates, proven conventional oil resources is expected to cover the demand for only four decades, so there is need to find the alternative sources [5-7].

Increased production of synthetic liquid fuels could be a sign of a global shift toward fuels that are not produced from conventional feedstocks. Gas-to-liquid (GTL) and coal-to-liquid (CTL) processes can be explored as alternative technologies for liquid fuel production. A comprehensive

economic assessment of fuels from natural gas and coal and their comparison with those from conventional petroleum-based fuels can provide insights for decision makers in formulating policies and making investment decisions. Understanding the fundamental aspects of CTL and GTL technologies is critical for federal and provincial planning and for policy making. The recent climate change policy announcement in Canada along with the Alberta governments' decisions to phase out coal-fired power plants by 2030 bring opportunities to use excess coal [8].

1.2. Natural gas-to-liquid

Currently, there is interest in natural gas conversion technologies. GTL technology in countries such as Canada and the United States with large natural gas resources would allow the transport sector to reduce its dependence on crude oil and to replace conventional fuels with liquid fuels. In addition, GTL technology can monetize small natural gas reservoirs, so stranded gases can be considered as feedstock for GTL plants. In addition, liquid fuels have a sulfur content of less than 1 ppm, while conventional fuels have 10 ppm [3, 4]. Also GTL products are free from aromatic components [9]. Thus liquid fuels are recognized as clean fuels.

In the GTL process, first syngas (a mixture of hydrogen and carbon monoxide) is produced, and then the syngas is converted to different products such as diesel, gasoline, and wax [5, 10-14]. Syncrude, which is obtained from the Fischer-Tropsch (F-T) reaction, is upgraded to produce marketable products. Sasol Canada [15] leads a GTL project in Canada. At full capacity, the GTL plant is expected to consume 1 billion cubic feet per day of natural gas to produce 96,000 barrels per day of diesel, naphtha, and liquefied petroleum gas. The results of a feasibility study of this project are under review. GTL fuels are, however, already commercialized in Qatar and Malaysia.

In this chapter, literature in the area of liquefaction is briefly reviewed to give the reader some of the history of the GTL and CTL. A comprehensive literature review is covered in chapter 2.

Jaramillo et al. simulated the GTL process and studied capital and manufacturing costs [16]; and this research compared petroleum-based fuel with GTL fuel cost. Lee et al. used Aspen Plus to simulate three processes, including GTL, and to perform an economic assessment [12]. Their results are focused on the effect of feedstock price on a GTL plant's profitability and, in the end, an optimal GTL fuel cost was chosen to account for fluctuations in natural gas price. Rafiee et al. studied the economic impacts of different syngas configurations on the GTL process [17] and they considered the autothermal reactor (ATR) the most economic technology for syngas production. Wood et al. reviewed the different routes to monetize natural gas and GTL was introduced as commercially viable technology [11].

There are studies that focus on the economic aspects of the GTL process as mentioned above [12, 14, 16, 18-25]. However, there are very few studies which focus on development of scale factors of the key equipment for the GTL plants. These studies, moreover, focused on the U.S.; none of these look at the economics of GTL in Canada. This study is an effort to address this gap. Economy of scale is the cost advantages due to reduce in cost per unit of products from a larger scale plant. Scale factor is a coefficient between 0 and 1 and it quantifies the benefits from larger plants comparing to the smaller ones.

1.3. Coal-to-liquid

Canada has large coal resources. That said, the federal government plans to phase out coal power plants, and this leaves the potential for CTL plants to use the coal that will no longer be burned in power plants. Moreover, liquid fuels are assumed to be clean fuels compared to conventional fuels, as mentioned in section 1.2. Two major coal-to-liquid conversion pathways are considered:

indirect coal liquefaction and direct coal liquefaction. In the indirect process, a hydrogen (i.e., steam) is combined with carbon (the coal); following the chemical reactions, hydrocarbon chains of various lengths form. The Fischer-Tropsch (F-T) synthesis is the key component of CTL processing [26, 27]. Syncrude, which is obtained from the F-T reaction, is upgraded to produce marketable products. In direct coal liquefaction, however, the gasification process is eliminated. After coal slurry preparation, liquefaction occurs and liquid products are upgraded [26]. Secunda CTL is a synthetic fuel plant in South Africa that uses direct coal liquefaction to produce liquid fuels from coal. Secunda, with almost 160,000 barrels per day production capacity, is the largest coal liquefaction plant in the world [28]. The Shenhua Group Corporation constructed the world's first commercial direct coal liquefaction plant in Inner Mongolia in 2003. The capacity of the plant's phase one is 22,000 barrels per day liquid fuels [28].

As with the GTL process, there are some studies that focus on the economic aspects of the CTL process, but few that assess the scaling factors of the key equipment. All of these studies, moreover, focused on the U.S. There are no economic analyses of CTL based in Canada.

A brief literature review on CTL is presented and it is further described in detail in chapter 2. Mantripragada et al. simulated two configurations of the CTL process and calculated the capital and operating costs of each [3]. Costs of the all the process equipment were obtained from the Integrated Gasification Combined Cycle (IGCC) plant. Two low bituminous coal types were selected and the cost of the feedstock coal was assumed to be \$15/tonne [3]. Since coal emits twice the CO_2 of fossil fuels per unit of energy produced, the conversion of syngas to liquid fuels produces significant amounts of CO_2 emissions [29, 30]. The plant can compensate for these high emissions through carbon capture and sequestration (CCS). Sequestered CO_2 is used in enhanced oil recovery (EOR) or enhanced coal bed methane (ECBM) recovery [31]. Mantripragada et al.

also calculated the final product cost of the CTL with and without CCS unit [30]. Another concern related to this process is the type of coal used. Mantripragada et al. compared three types of coal, bituminous, sub-bituminous, and lignite and showed that a bituminous coal liquefaction plant has a lower capital cost than a plant processing other grades of coal [32]. Bae et al. considered economic data for direct, indirect, and hybrid coal liquefaction plants operating at a production capacity of 50,000 barrels per day [26]. The authors calculated the internal rate of return, net present value, and payback period for all three pathways, compared the results, and performed a sensitivity analysis. The results indicated that indirect coal liquefaction has the highest capital cost and payback period of the three processes [26] and direct coal liquefaction has the highest internal rate of return. Since coal gasification is the most costly part of the liquefaction plant, Vosloo compared the operating parameters of the different gasifiers, including fixed bed, fluidized bed, and entrained bed [33]. He demonstrated that gasifier type is determined by the coal properties [33]. The National Energy Technology Laboratory (NETL) has done comprehensive technical and economic assessments on indirect coal liquefaction plants based on assumed capacities of 50,000 barrels per day and bituminous coal as feedstock are assumed [20]. NETL reported the capital cost and operating cost of the CTL plant. However, there are few studies on the economic model of CTL plants and very rare studies which focus on development of scale factors of the key equipment for the CTL plants [3, 9, 26, 33-36]. These studies, moreover, focused on the U.S.; none of these look at the economics of CTL in Canada. This study is an effort to address this gap. Economy of scale determines the cost benefits from bigger capacities and scale factors described these advantages in forms of numbers.

1.4. Objectives and motivations

The overall objective of the thesis is to conduct techno-economic assessment of gas-to-liquid and coal-to-liquid processes. The specific objectives of this thesis are as follows:

- To develop a techno-economic model that can estimate the total cost of basic GTL and indirect and direct CTL plants in Canada specifically;

- To develop scaling factors for all key equipment in the both GTL and CTL plants as well as for the entire plants based on the Canadian jurisdiction;

- To develop the capital cost of these plants at varying scale;

- To develop the production cost of liquid fuels based on CTL and GTL;

- To assess a CTL plant with a CCS unit, given the massive amount of greenhouse gas emissions from the coal liquefaction process;

- To perform a sensitivity analysis to investigate the effects of changes in critical input parameters to the techno-economic model.

1.5. Thesis organization

This thesis is organized in a paper-based format as described below. Chapters 2, 3, and 4 are expected to be published as a paper, hence some background information is repeated.

Chapter 2 is a review of the different ways of producing liquid fuels from natural gas and coal and technology readiness level. This chapter covers the conversion of natural gas to dimethyl ether (DME) and methanol, the Fischer-Tropsch synthesis, pyrolysis, and indirect and direct coal liquefaction. The life cycle greenhouse gas (GHG) impacts of producing liquid fuel from non-conventional resources are also reviewed.

Chapter 3 discussed the methodology and input data and assumption for developing the economic model for GTL and CTL plants. Moreover, the method of scale factor calculation for the plant equipment is described briefly.

Chapter 4 discusses the development of natural gas to liquid production costs in western Canada. A GTL plant typically has three processes: syngas production, liquefaction, and upgrading. In this study, each process undergoes a cost analysis in the context of the anticipated GTL plant in Canada. Each process or unit operation was analysed in terms of investment cost, operations cost, and scale analysis.

In Chapter 5 the results of the model developed to estimate operation and capital costs of typical indirect and direct coal liquefaction plants are shared. The GTL plant, scaling factor, and economy of scale analysis for all equipment are developed. The addition of a CCS unit to a GTL plant is included, given that GHG emissions from coal are a significant concern.

Chapter 6 includes the main observations from the sensitivity analysis of the techno-economic model. In fact, the impact of input data variation on the production cost of the GTL and CTL are studied in this chapter.

Chapter 7 includes the key conclusions and observations from the research. In the end, recommendations for the future work is discussed.

Chapter 2. Literature Review[1]

2.1. Background

Crude oil has massive drawbacks rising from its limit supply, high fluctuation in the price, environmental impacts and also, economic and political issues. Due to the problems associated with crude oil, countries depending highly on petroleum are searching a suitable substitute for transportation fuels. Therefore, alternative sources of liquid fuel from natural gas and coal with respect to GHG emission reduction are being considered. Moreover, formulation of policies in several jurisdictions on phase-out of coal power plants due to climate change considerations has also created a need for the development of alternative utilization of coal. Liquefaction processes such as Coal to liquid (CTL) and gas to liquid (GTL) are pathways that can be a replacement for the fuel production from conventional crude oils. The benefits of producing these synthetic liquid fuels revolved around the huge deposit of coal and natural gas in some region of the world such as Canada, United States, etc and also, its low sulphur content comparing to crude oil fuels [2-4]. One of the major concerns associated with a new process is the GHG emissions, which is necessary to be addressed. The emissions and energy consumed by the GTL and CTL can be measured through the life cycle assessment (LCA). LCA is a widely used standardized methodology to quantitative the environmental effects of products through the entire life cycle. For liquefaction processes, the

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[1] A version of this chapter has been submitted as Mohajerani, S., Kumar, A., Oni A. A techno-economic assessment of gas-to-liquid and coal-to-liquid plants through development of scale factors, *Energy*, 2016.

total emission burdens of synthetic fuels from natural gas and coal. The comparison of the LCA results from GTL and CTL and conventional petroleum-based fuels can provide a clear view for high-level energy authorities. In addition, understanding the fundamental aspects of coal-to-liquid and gas-to-liquid technologies is critical for the energy mix plans and for the policy implementation.

There is not a recent review paper on the life cycle assessment of the GTL and CTL processes which studied the amount of energy, efficiencies, and emissions of both. Therefore, there is a need to investigate the LCA of the liquefaction processes via energy consumption and energy efficiency of the plant and quantify the GHG emission for the entire process. There is lack of comprehensive date in the field of environment and carbon footprint from natural gas/coal extraction to liquid fuels in public domain.

The aim of this study is to collect current data on existing liquefaction technologies, GHG emissions, and LCA results of GTL and CTL plants. In this chapter, every step of producing liquid fuel from natural gas and coal are introduced and quantitative data which are provided in the literature are discussed briefly. Finally, a range of emission burdens associated with each operating sections from raw materials to end products is tabulated. This chapter gives a general idea about the GHG emission of typical liquefaction plants in terms of environmental impacts.

The overall objective of the present work is to conduct a review of the GTL and CTL technologies including the research so far on their life cycle assessments (LCA). The specific objectives of this chapter are:

- Conduct a review of the different GTL and CTL technologies with respect to their conversion mechanisms, technological characteristics and technology readiness level (TRL).

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- Conduct a review of LCA studies of GTL and CTL processes.

- Identify the gaps in knowledge and challenges in commercializing these technologies based on the review.

- Identify the promising technologies.

2.2. Gas to liquid process

The GTL process comprises of three steps: synthetic gas (syngas) production, synthetic liquid, and product upgrading. In the first step, natural gas is consumed and synthesis gas is produced through a reforming process. In the second step, the synthesis gas is converted to the liquid phase with longer chain hydrocarbons. At the end, the liquid hydrocarbons are fed to the upgrader units to produce commercialized grade of liquid products. In every GTL process, syngas production is an intermediate step which means that syngas operated as a transitional material in the liquefaction process. This type of technology in which syngas plays a role as an intermediate is known as the indirect liquefaction process. All three steps of indirect gas liquefaction are explained below.

2.2.1. Syngas production

There are three main methods for converting natural gas to synthesis gas through a combination of carbon monoxide and hydrogen:

- Steam reforming

Steam reforming is the most widely used process for syngas production. The reforming reaction takes place at the temperature ranges 850 - 1000℃ and 3000 kPa pressure depending on the types of catalyst [24] [11]. The catalyst can be either ceramic-supported nickel or nickel-alumina; however, operating temperature is lower for the nickel-alumina than the ceramic ones [37].

Typically, the steam reforming reaction is conducted in a tubular-packed reactor and it is highly exothermic. Therefore, the extra released energy can be recovered through heat exchangers from an outlet stream [11].

$$CH_4 + H_2O \rightarrow CO + 3H_2 \tag{1}$$

- Partial oxidation reforming

Oxygen is a reactant for the oxy-reforming (partial oxidation) process and its role is to adjust the synthetic ratio. Therefore, concentrated and pure oxygen is produced through the air separation unit (ASU) and is fed to the autothermal reforming reactor (ATR). The Natural gas is reacted in the ATR in the presence of oxygen and steam [38][12]. Heat from the reaction maintains the reactor's temperature at a constant level [11].

$$CH_4 + \frac{1}{2}O_2 \rightarrow CO + 2H_2 \tag{2}$$

- CO$_2$ reforming

During carbon dioxide reforming, the reaction conversion rises along with the rise in temperature. Carbon dioxide reforming involves the following reaction:

$$CH_4 + CO_2 \rightarrow 2CO + 2H_2 \tag{3}$$

ATR-based processes cannot provide a suitable H$_2$/CO ratio because of the relatively high level of sulfur that exists naturally in hydrocarbon resources. Basically, a lower S/C ratio improves the syngas composition [37]. Hence, with new technologies researchers are trying to develop gasification techniques such as the next generation of ATR which includes ATR in combination with gas-heated reforming, catalytic partial oxidation (CPO), and ceramic membrane reforming (CMR) [17]. These new methods enhance the gas production for GTL and have the potential to

improve the production pathway by decreasing the amount of oxygen needed, the operational temperature, and the capital cost of GTL process [10, 37, 38]. Syngas is an intermediate for the indirect GTL process. However, new technologies decrease the steps involved in production and help develop direct methods [5, 10, 11, 14, 39].

In the following section, both types and reasons for eliminating the intermediate process are introduced.

2.2.2. *Gas to DME conversion*

DME (dimethyl ether) is a liquid product that comes from natural gas. There are two methods for DME production: direct (one step) and indirect (two steps). In the first step of the indirect method, natural gas is converted to MeOH and then reacted to produce DME through a catalytic synthesis into an adiabatic fixed bed reactor. Figure 2-1 shows the DME process flow diagram. Chemical reactions are shown in equations 4, 5 and 6 [40]. The DME production phase includes the following reaction that occurs at 230℃ and 3000 kPa:

$$CO + 2H_2 \rightarrow CH_2OH \tag{4}$$

The produced methanol is dehydrated and converted to DME. If the reactions continue in a fluidized-bed unit (653°C and 3.3 MPa), DME can be converted to gasoline [7, 41].

$$2CH_3OH \rightarrow CH_3OCH_3 + H_2O \tag{5}$$

$$CO + H_2O \rightarrow CO_2 + H_2 \tag{6}$$
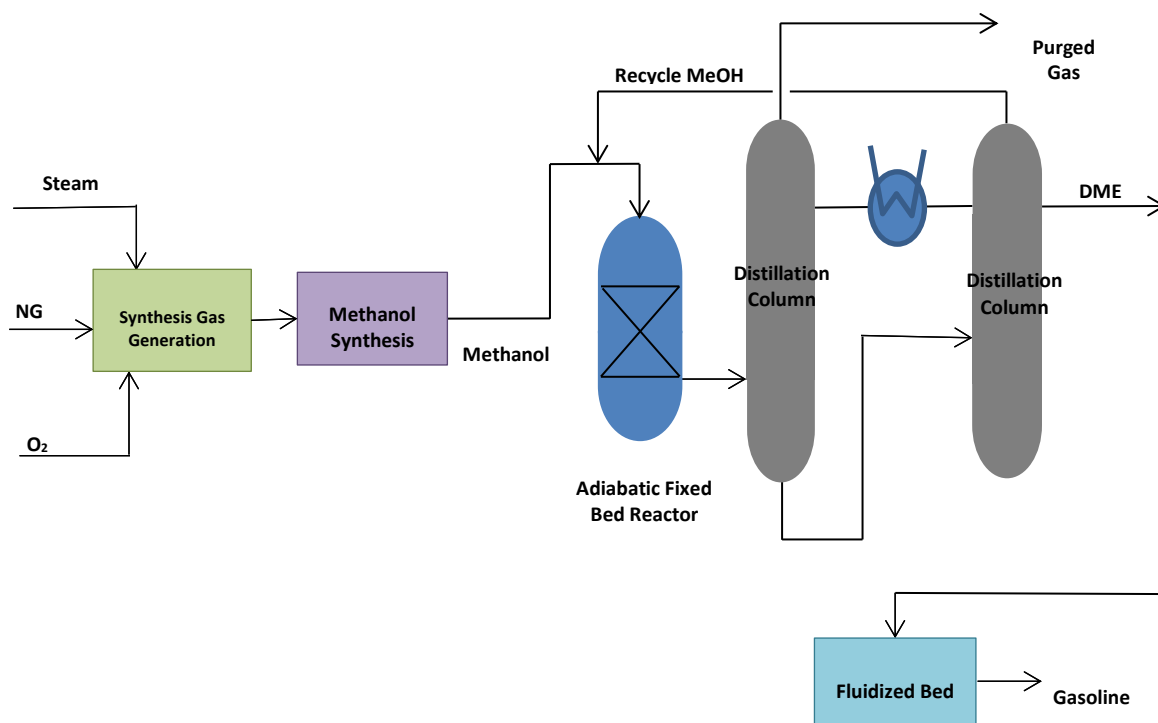
Figure 2-1: Schematic of the DME Process (derived from [7, 42, 43])

In the direct method, MeOH production and dehydration take place in a single bi-catalytic reactor [40]. The catalyst has a great impact on selectivity (the conversion of the reactant to the desirable product over the conversion of the reactant) and DME conversion factors [40, 44]. A zinc-copper alumina catalyst is commonly used for the direct process [44]; however, many studies report that the new catalysts for direct DME improve selectivity and conversion factors of the reaction. Tan et al. [45] modified the Cu-based catalyst and Ge et al. [44] described the characteristics and nature of the two bifunctional catalysts. Sun et al. [46] added ZrO_2 to a Cu-based catalyst and described the new catalyst as achieving improved catalytic activity, high selectivity of DME, and good CO conversion [46].

The direct method has several advantages. The production expenses were 20% lower than those of current industrial methods [40]. Moreover, only one purification unit is required for the direct

process, so this method can reduce both operation and fixed costs. These reduced costs make the one-step method attractive to industry [5, 42-44, 47, 48]. The direct DME plan with a capacity of 37,000 tonne/day is available and another one is being tested by Topsoe Inc. [49].

Generally, DME has been used as an intermediate substance to produce dimethyl sulfate or oxygenated compounds. Also, it can be used in a combustion engine as a fuel (though engine modification is required) and in power plants [11]. It must be mentioned that DME combustion emits less smoke and NO_x than conventional fuel and is considered a clean fuel [11, 47, 49]. In addition; DME has the same properties as diesel, such as a comparable cetane number and ignition temperature [43, 50], and has high quality combustion characteristics [50, 51]. Due to similarities with liquefied petroleum gas (LPG) (see Table 2-1) and lower price than conventional fuel, DME has significant potential to be substituted for LPG. On the other hand, demand for DME will be greater than for LPG in the future, if the price of DME is lower than LPG [50, 52, 53]. The lower heating value of DME (see Table 2-1) and its low lubricity are critical barriers for marketing it. Ohira [5] discussed applying new technologies in synthetic fuel production that can reduce the operating cost of the process and facilitate the expansion of DME market. However, economic considerations in the use of DME fuel due to engine modification, distribution infrastructures (like pipelines and fuel stations), and standards and regulations (environmental issues) have meant that the DME market has been restricted to a few Asian countries [5, 11, 43, 48].

Table 2-1: LPG and DME physical properties

Properties	LPG	DME	Ref.
Chemical formula	C_2-C_4	C_2H_6O	[54]
Liquid density (kg/m^3)-20 °C	540	667	[54]
Vapor pressure kPa	520	530	[54]
Energy per bottle unit GJ/m^3	19	16.3	[54]
Boiling point °C	-42	-25.1	[48]
Lower heating value MJ/kg	46	28.8	[54]
Bottle fill %	80	85	[54]

2.2.3.   Gas to Fischer-Tropsch conversion

The Fischer-Tropsch (FT) reaction was developed between 1902 and 1928 in Germany by Franz Fischer and Hans Tropsch during the conversion of coal-derived syngas to synthetic hydrocarbons [3, 18, 26]. This innovation was a key source for the GTL method [22]. Later, due to the high need for fuel, other companies further developed this method by building up the operating units. Sasol, a South African energy and chemical company, pioneered this process and built the first CTL unit based on the Fischer-Tropsch reactions in 1955 [26]. The first commercial GTL plant was located in Bintulu, Malaysia [55]. It was based on the Fischer-Tropsch technology and operated by Shell in 1988 [55]. The plant's capacity is 14,700 bbl/day of liquid fuel containing diesel [18, 55]. Recently, Qatar Petroleum and Shell presented a GTL plant that can produce 140,000 bbl/day of diesel fuel [56]. In addition, Sasol and Chevron are constructing a GTL plant in Qatar (Oryx-I)

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that will produce 34,000 bbl/day of light olefins and gasoline [57]. Companies like ExxonMobil and ConocoPhillips are investigating new GTL projects at different capacities [21].

Figure 2 shows the process flow diagram of a general Fischer-Tropsch process. After syngas production, syngas reacts over an iron or cobalt catalyst to produce varying products in different chain lengths [7]. The Fischer-Tropsch reaction is shown below [18, 24]:

$$nCO + (2n + 1) H_2 \rightarrow C_nH_{2n+2} + nH_2O \tag{7}$$

$$CO + H_2O \rightarrow CO_2 + H_2 \tag{8}$$

where n is the number of carbons in the hydrocarbon chain in liquid fuels. Product distribution is described by the Anderson-Schulz-Flory (ASF) distribution function [7, 9] as follows:

$$W_n/n = (1 - \alpha)^2\alpha^{n-1} \tag{9}$$

where W_n is the mass fraction of n-carbon chain and α is the chain growth probability to form longer chains [7, 9]. The chain growth probability, α, increases when the reactor temperature decreases. Also, the H_2/CO ratio has an impact on the α value [7]. An increase in α is observed at a lower H_2/CO ratio [7, 9, 35]. H_2 is required for the FT reaction and the H_2/CO ratio varies for different catalysts. For instance, for cobalt-based catalysts, H_2/CO ratio is about 1.8 to 2.1, while for iron-based catalyst it is below 1 [58]. Further, cobalt catalysts are more suitable for natural gas-derived syngas because of their longer lifetime; therefore, these catalysts have both a long life and high efficiency [59] compared to iron catalysts [7]. Long life and high efficiency can compensate for the higher cost of cobalt catalysts. The operating pressure of the FT reactor ranges between 0.1 and 4 MPa [60]. Trippe et al. [7] simulated a plant with an operating pressure between 4 and 8 MPa. They explained that the 8 MPa pressure plant can generate electricity. Van der Laan's data

showed that by decreasing pressure the average chain length decreased and the methane production rate was reduced. Consequently, reaching a high production rate entails low temperature, relatively high pressure, and an H_2/CO around 2 [14, 24].

FT GTL products can be naphtha, diesel, and other co-products such as lubricant base oils, jet kerosene, waxes, and normal paraffin. All of these products have very low sulfur (less than 1 ppm) and aromatic content (less than 1%) [11, 12, 61].

For commercialized FT reactors, the difference between Low Temperature FT and High Temperature FT is an important economic issue, due to the fact that temperature controlling mechanisms and heat removal affect product selectivity and catalyst lifetime. Low Temperature FT (LTFT) reactors operate between 200 and 240°C and are designed to produce diesel and wax; in contrast, the temperature range for the High Temperature FT (HTFT) reactor, designed to produce gasoline and light hydrocarbons, is between 300 and 350°C [18]. Wood et al. considered the reactor temperature (320°C) and pressure (2.5 MPa) carried out in fluidized bed reactors. Trippe et al. [7] modeled a FT-GTL plant with LTFT and HTFT reactors that operated between 220 and 250°C and 330 and 350°C, respectively. In the HTFT reactors the only phase present in the catalyst particle is gas. Gasoline and diesel, which are taken from the Fischer-Tropsch reactor, are treated similarly to petroleum-based fuels [52].
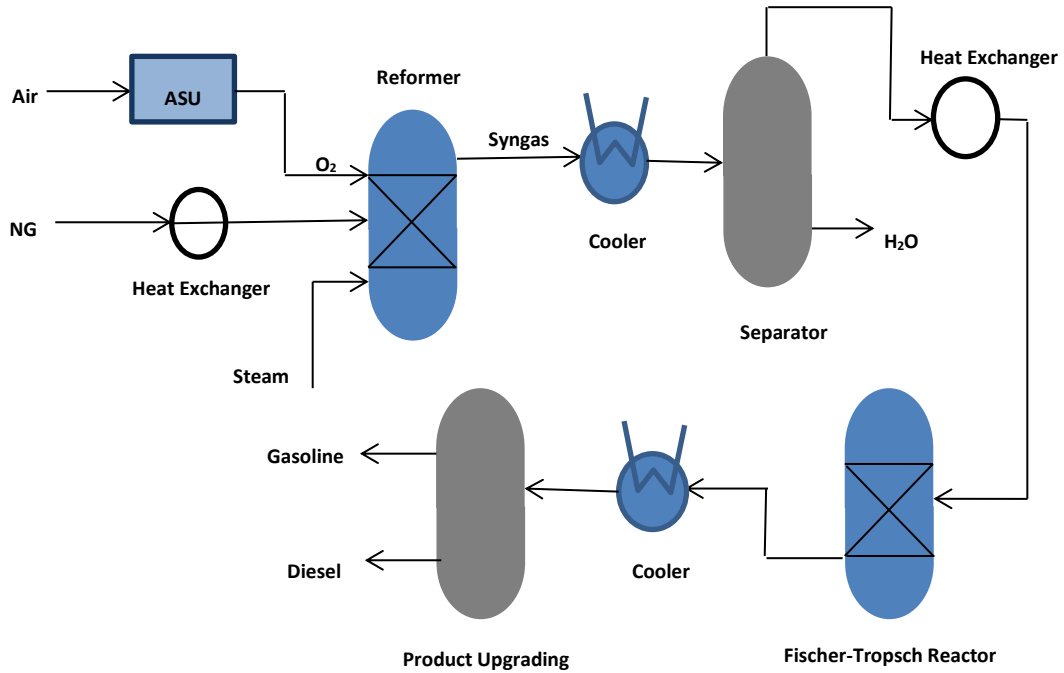
Figure 2-2: Schematic of the Fischer-Tropsch process (derived from [7, 16, 22])

2.2.4.   Gas to Methanol

Methanol production involves two phases. Syngas production phase that is similar to the other gas liquefaction technology. In the second step, syngas is chemically reacted on a cobalt or platinum catalyst to produce methanol at 230°C and 3000 kPa [62]. Gradassi et al. considered 8.28 MPa to be the operating pressure [14]. De Klerk [63] introduced a technique involving Cu-Zn alumina catalyst while, the temperature ranged 200-300°C and pressure accounted for 3.5-5.5 MPa. The Methanol formation reactions are presented by equations 10 and 11:

$$CO + 2H_2 \rightarrow CH_2OH \tag{10}$$

$$CO_2 + 3H_2 \rightarrow CH_2OH + H_2O \tag{11}$$
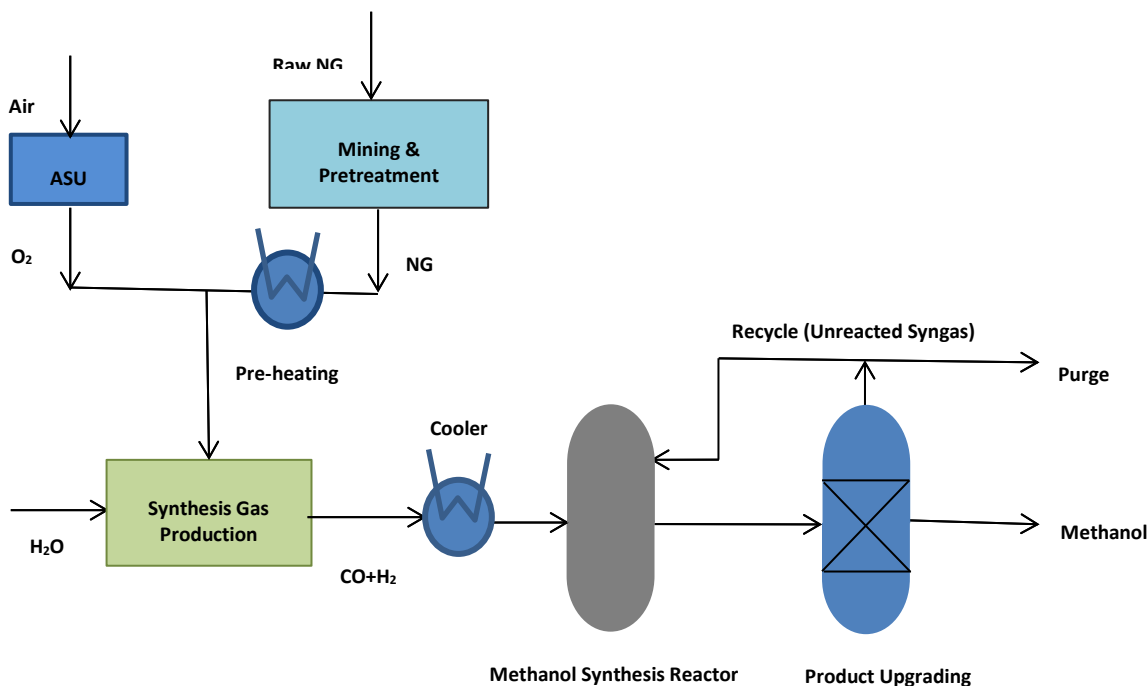
Figure 2-3: Schematic of methanol production process (derived from [41, 64])

Because of the accidental oxidation of syngas (H_2+CO) in the production of CO_2 and H_2O, the methanol production process has a low efficiency and has the lowest profitability compared to the DME and FT processes [12, 23]. Further, the hazardous nature of methanol makes it less desirable in the global market. Methanol production is not the main target of the global market, and it has not been commercialized due to its uncompetitive prices and the environmental issues related to its toxicity. Furthermore, the volumetric energy density of methanol is half as much as the petroleum-based fuels [65, 66]. In spite of this fact, some companies have tried to make a tremendous change and have modified methanol production to obtain beneficial products. ExxonMobil introduced the methanol-to-gasoline (MTG) process in the 1970s [67]. This company conducted research on the conversion of methanol to gasoline and showed that after methanol is produced, hydrocarbon chains form over a synthetic zeolite [64]. It is worth pointing out that the Fischer-Tropsch process can produce a broad range of paraffinic chains in various lengths that

must be upgraded; however, methanol can produce pure gasoline with low sulfur content, low aromatic content, and a high octane number [64, 67]. The result is that an FT plant is a competitive way to produce fuel [67]. If oxidation of methanol is coupled with the downstream processes, methanol will be able to make lighter products like olefins and then can be converted to gasoline. Typically, propylene and ethylene are the products made from methanol and then converted to diesel [65].

Another method for converting methanol to liquid fuel is called gas-to-gasoline (GTG) [66, 68]. The GTG method is a direct method of converting gas to liquid fuel. First, methanol is produced from the gas-derived syngas; then it is dehydrated, vaporized, and fed to a fluidized bed reactor at 380-430°C to synthesize light and heavy gasoline, ethylene, and light hydrocarbons such as propane and butane (C_3/C_4) [66]. Ethylene is recycled in the methanol production plant, C_3/C_4 are entered to the additional unit to produce gasoline, and then heavy gasoline is hydro-treated to upgrade its properties. The methanol-to-gasoline process was first developed by Mobil in 1985 in New Zealand using an adiabatic fixed bed reactor [64]. Later another plant was built in Germany with a fluid bed reactor [65]. A typical methanol to gasoline plant is shown in Figure 2-4.
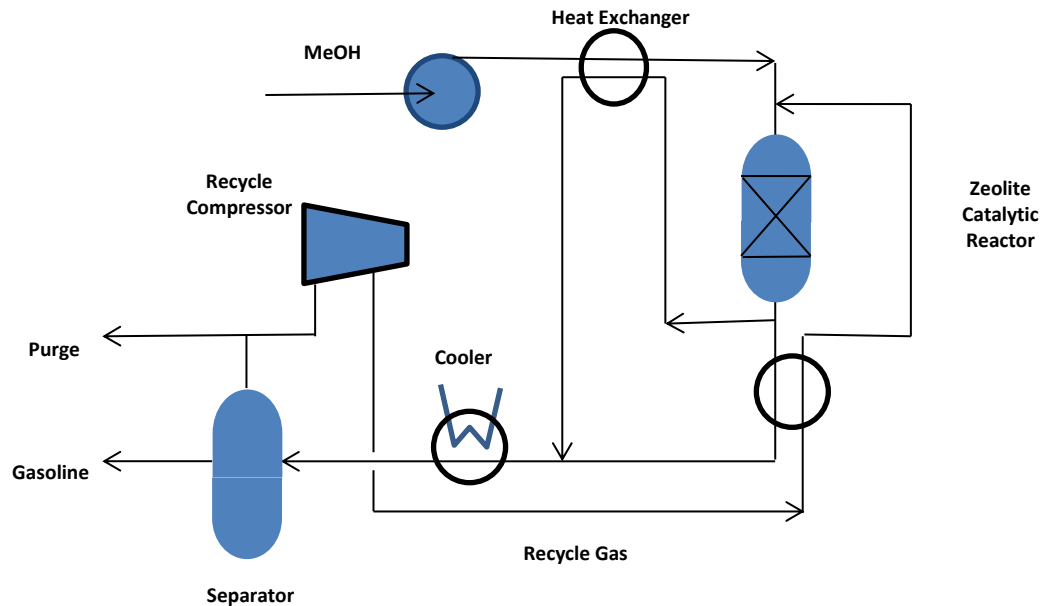
Figure 2-4: Schematic of methanol to gasoline process (derived from [66])

In the future, deploying the GTG method with the other GTL paths will be probable. Currently, the GTG method is still immature [65].

2.3. Coal to liquid process

The coal-to-liquid (CTL) process has three basic approaches: pyrolysis, direct coal liquefaction (DCL), and indirect coal liquefaction (ICL). The basic of all these methods is a hydrogen source like steam combined with a source of carbon (coal). After chemical reactions, hydrocarbon chains of various lengths are fabricated and H/C ratio increased [66].The properties of end products depend on the type of coal used as the feedstock. The available technologies for the coal liquefaction are described below.

2.3.1.   Pyrolysis

Pyrolysis is the oldest method for obtaining liquids from coal. In this method, coal is heated and the heat decomposes the coal. Volatile components are driven away and the carbon content increases during heating. Then the volatile components are quenched and liquid products gathered. The rate of production is low (around 20%) [34, 69], although some modifications to the process can increase the production rate. For instance, the temperature of the pyrolysis process is typically high (around 900°C) [70, 71]. By exposing coal to a mild temperature (between 500 and 600°C) [34, 72] and by pretreating coal in low temperature steam (between 300 and 370°C) [73] or in supercritical steam [74], the liquid production rate can be increased. Another barrier for developing the pyrolysis process is unworthy byproducts. A main byproduct of this process is coal tar [71]. Coal tar is not usable as a fuel, but as insulation and waterproofing. Increasing the quality of coal tar requires further process to reach the commercial fuel grades. In this regard, coal tar enters to the upgrading unit where hydrocracking, reforming, and hydrogenation processes take place. Consequently, the capital costs of the pyrolysis plant increases significantly [34]. Thus, there is a little possibility for pyrolysis products to compete with other synthetic fuels.

2.3.2.   Indirect coal liquefaction

Indirect coal liquefaction (ICL) and direct coal liquefaction are two different means of producing liquid fuel from coal. This paragraph discusses the ICL process. Indirect coal liquefaction consists of four steps: gasification (the mixing of hydrogen and carbon monoxide), purifying the gas, producing synthetic fuel, and upgrading [26] (see Figure 2-5). The final product has the same properties as diesel and can be blended with refining diesel. Producing MeOH from syngas is another alternative, and methanol can be converted to gasoline later [36]. Generally, the aim of the ICL process is to increase the H/C ratio to 2 (molar basis) [36]
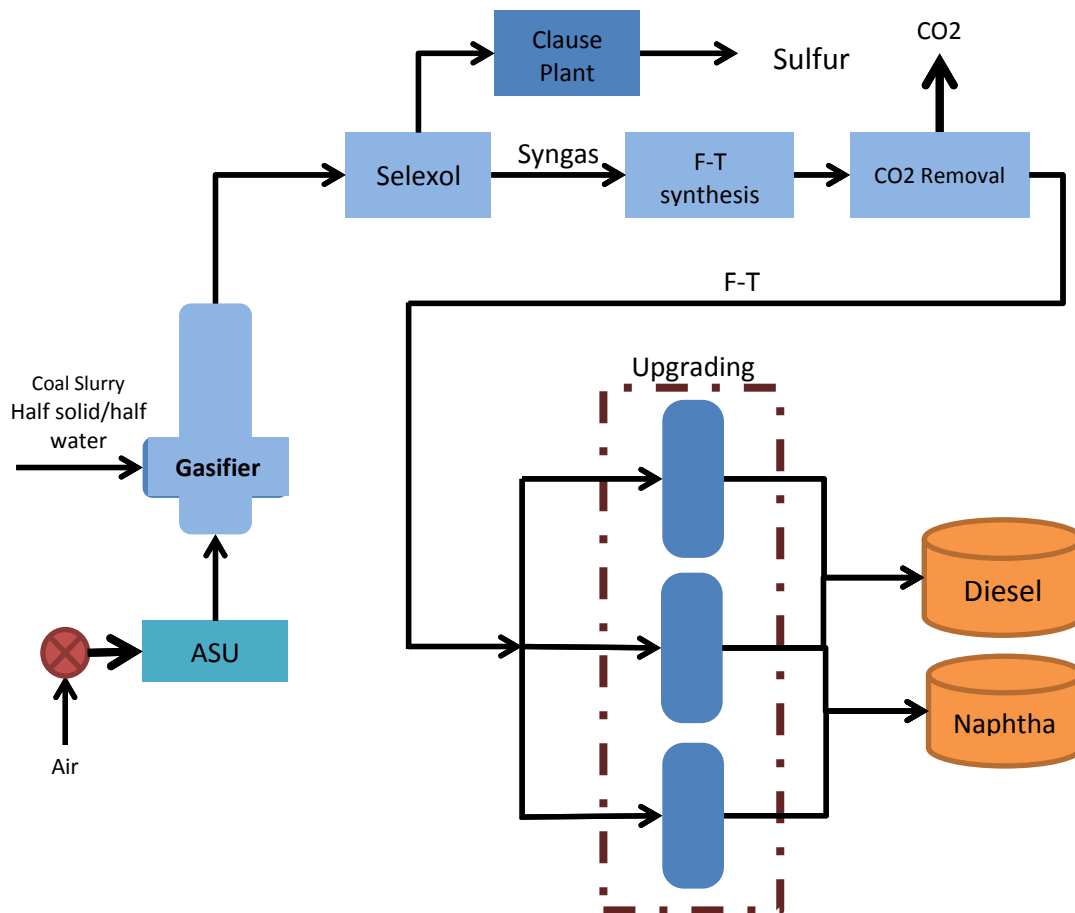
Figure 2-5: Schematic of the CTL process with the Fischer-Tropsch reactor

As with GTL (described above), the Fischer-Tropsch process is used for liquefaction after the gasification of coal (see Eq. 12). Oxygen or steam is added to the reaction to obtain a suitable combination of carbon monoxide and hydrogen. As mentioned in section 2.2, syngas undergoes a catalytic reaction which results in the production of different hydrocarbon chains (see Eq. 4). The catalyst has an impact on the efficiency of the process and also determines the type of products. Common catalysts are cobalt, ruthenium, and iron. Furthermore, as shown in Eq. 8, CO_2 is a byproduct of the Fischer-Tropsch process, and many catalysts are notoriously sensitive to carbon dioxide, which requires special treatment and separation units to prevent catalyst poisoning. Researchers face challenges selecting appropriate catalysts and optimizing the Fischer-Tropsch

process. The product types depend on the catalysts used and the temperature of the reactors. Mainly, HTFT reactors result in gasoline and LTFT processes produce diesel. The energy efficiency of the indirect CTL plant is estimated to be between 40 and 44% [75].

$$C + \frac{1}{2}O_2 \rightarrow CO \tag{12}$$

There are two configurations for FT-CTL relating to unconverted gas: liquid-only and co-production. In a liquid-only configuration, unconverted syngas is recycled back to the reactor (see Figure 2-6).
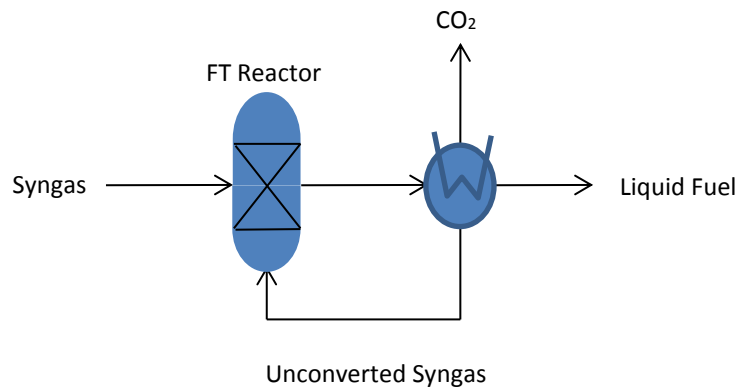
Figure 2-6: Schematic of the CTL plant with liquid-only Configuration (derived from [16, 18, 22, 76])

However, in a co-production configuration, unconverted syngas is combusted in a gas turbine to generate electricity power (Figure 2- 7).
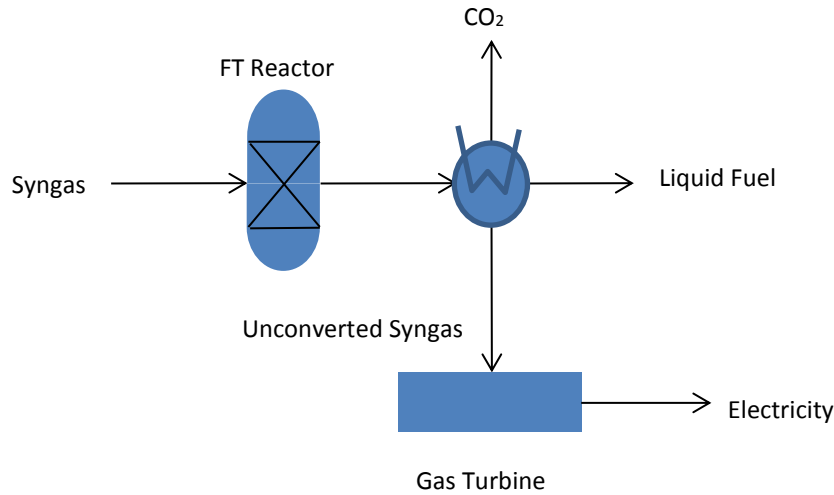
Figure 2-7: Schematic of the CTL plant with co-generation configuration (derived from [18, 76, 77])

2.3.3.   Direct coal liquefaction

In 2002, primitive pilot plants were tested in China by the Shenhua Group Corporation. The direct method is like the hydro-cracking of crude oil. The basis of direct liquefaction is the Bergius equation (see Eq. 13) [34]. The process includes splitting coal into shorter chains by adding high pressure and high temperature hydrogen through a catalyst. Consequently, syngas as an intermediate substance is eliminated from the process and coal directly provides liquid fuels [23, 26, 36]. These liquid products are of a higher quality than those produced through pyrolysis. The liquid product can be categorized as syncrude, and therefore further treatments and upgrading are required to convert the liquid product to usable fuel [26, 78]. Finally, gasoline, diesel, propane, and butane can be produced as final products of a full process chain. The Berguis equation is shown below:

$$nC + (n + 1)H_2 \rightarrow C_nH_{2n+2} \tag{11}$$

Temperature is 427-455 °C and pressure is 17 MPa [79]The energy efficiency of the plant is in the range of 45-55% [75]. The DCL needs less equipment than does FT-CTL, since syngas is not being produced. The other key aspect is that ICL has a lower GHG emission footprint than DCL. In fact, coal has different unwanted toxic, noxious, sulfuric, and other components that must be separated and can poison the catalyst if they enter the reactor. Moreover, fuels from Fischer-Tropsch CTL are cleaner than those from direct coal liquid. Consequently, the direct method is less economically proven than indirect coal to liquid [36].

All types of natural gas and coal liquefaction processes and their characteristics are summarized in Table 2-2:

Table 2-2: Summary of the GTL and CTL available technologies

Feedstocks	Process		Product types	Operation conditions	Technology readiness level
Natural gas	GTM (Gas-to-Methanol)		Methanol	200-300°C, 3.5-5.5 MPa	Under development
	Fischer-Tropsch	LTFT	Gasoline, light hydrocarbons	200-250 °C, 0.1 – 4 MPa	Commercialized
		HTFT	Gasoline, diesel	300-350 °C, 0.1 – 4 MPa	Commercialized
	Gas-to-DME		Dimethyl ether	230 °C, 3 MPa	Under development

	GTG	Gasoline	280-430 °C	New
Coal	Pyrolysis	Various products include: gasoline, naphtha, and diesel	850-950 °C, Atmospheric pressure	Non-economical
	Indirect CTL	Different products include: gasoline, naphtha, and diesel	1316-1427 °C, 4.3-5.6 MPa for gasification unit	Commercialized
	Direct CTL	Different products include: gasoline, naphtha, and diesel	425-455°C, 17 MPa	Under development

2.4. Life cycle greenhouse gas (GHG) emissions

Alternative CTL and GTL fuels have the potential to decrease climate change emissions from engine combustion of vehicles. The magnitude of Greenhouse gas (GHG) emissions can be determined using the LCA method. To understanding the results of LCA depicted in the literature, basic concepts requires to be explained in this regards. First, CO_2 gas is less harmful than methane, and the global warming potential of methane is 25 times greater than that of carbon dioxide over a 100-year period [27]. However, lack of concern regarding less emitted gaseous emissions such as CO_2, N_2O, and CH_4 might have irrecoverable consequences to the environment. Second, the weight of CO_2 per unit of heat trapping of the fuel (lb CO_2/MMBtu or g CO_2/MJ) is used as the parameter to show GHG emissions. This dissertation, same as other studies, reported N_2O and

methane as CO_2 equivalents. Third, the first part of the LCA called "well-to-tank" and deals with gathering resources, fuel production, and fuel delivery. The next part considers the efficiency of fuel consumption in vehicles and is called "tank-to-wheel" [19, 80]. Consequently, the entire life cycle analysis is known as "well-to-wheel" [80].

2.4.1. Life Cycle GHG Emissions of GTL plant

There have been few studies focused on LCA of a gas-to-liquid plant. Burnham et al. [81] examined the CH_4 emission from different fossil fuel sources like shale gas, natural gas, coal, and conventional crude oil and updated and revised the GHG emissions estimation by using the GREET model. The results show that natural gas emissions are lower than conventional crude oil and coal emissions over the life cycle. Elia et al. [82] studied a plant with the co-feeding (hybrid feedstock system) of coal, natural gas, and biomass and analyzed the GHG emissions from different sections of the plant. The authors showed that emissions reduce by about 50% when a hybrid system is used instead of a petroleum-based feedstock alone. Bengtsson et al. [19] conducted a LCA of liquefied natural gas (LNG) and compared it with an LCA of three other fossil fuels. Jaramillo et al. [16, 27, 83] estimated the GHG emissions of Fischer-Tropsch liquid fuels for different scenarios. They assumed two different sources for electricity, one is from low emissions sources such as solar energy and the other is from high emission sources like fossil fuels. Forman et al. [61] evaluated the GHG emissions of GTL fuel. All these studies are reviewed in further details in this section. In addition, these studies are not jurisdiction- specific, therefore, the LCA results can be expanded for a generic GTL plant.

Generally, for GTL fuel, the life cycle starts with natural gas production, followed by NG transition and storage, gas pretreatment, GTL processing, and fuel transition, and combustion in vehicles. The schematic of GTL life cycle is shown below:
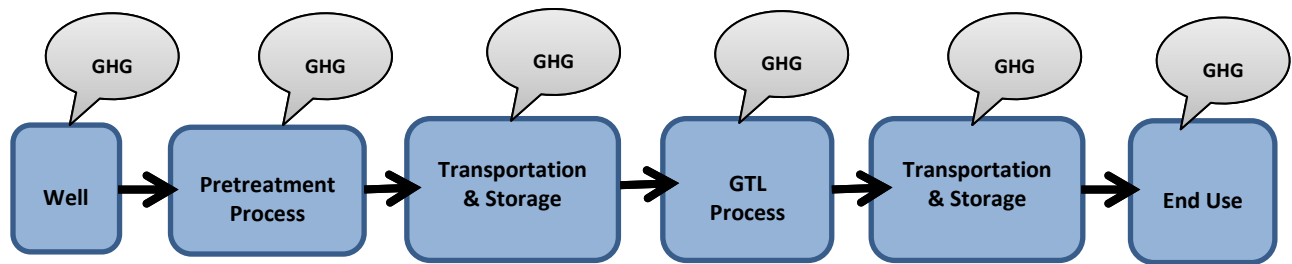
Figure 2-8: Liquid fuel life cycle (derived from [4, 84])

The first step of the life cycle is the natural gas production. Natural gas production requires large equipment that consumes diesel for mining, drilling, and extracting. Methane is intentionally vented as part of operations or leaks from equipment such as like pipelines, valves, and flanges. However, in some cases, methane is flared rather than vented directly. N_2O and methane are also emitted during the combustion and processing of natural gas. In addition, 0.4% of raw natural gas is vented during different stages of production for safety and the prevention of over-pressuring, and 0.2% of raw natural gas is flared to the atmosphere [61]. Forman et al. [61] considered 12.1 (gCO_2e/MJ) for net emissions of natural gas from offshore extraction.

Sweetening and compression are types of pretreatment processes in the natural gas production. Storage and transportation from the well to the GTL plant required fuel consumption which is associated with CO_2 emissions. Production steps accounted for emission of 0.38% of natural gas in North America [83]. According to the Environmental Protection Agency, 1.07% of natural gas produced is lost in production, gas pretreatment, storage, and transition [85]. Burnham et al. [81] considered 0.06-0.23 % of natural gas leaked or vented during the process time equaling to 0.583-1.081 gCO_2e/MJ. Jaramillo et al. estimated that upstream use emissions from domestic natural gas are between 6.5 and 8.6 g CO_2e/MJ [16]. In some countries without domestic natural gas, emissions from the delivery of synthesis fuels from foreign countries must be added to the total calculation. Forman et al. [61] evaluated the net GHG emissions of natural gas transportation (47

miles by pipeline) and gas pretreatment to be 0.5 gCO_2e/MJ and 7.7 gCO_2e/MJ, respectively. Burnham et al. used the range of 0.29-1.05 % natural gas for transmission and distribution leakage and venting [81].

Life cycle emissions include those from the electricity used in the plant, transporting the synthesis fuel, and the liquid fuel combustion. To estimate emissions from a GTL plant, different assumptions are used. Product ratio, energy efficiencies, energy balance, and carbon dioxide mass balances have impacts on the amount of GHG emissions. Generally, energy efficiency is defined as the fraction of internal energy in the raw gas that is present in the synthetic fuel.

Input and output mass and energy are necessary to study a life cycle assessment on GTL. Products from commercial GTL plants are 70% diesel, 23% naphtha, 4% LPG, and 2% wax [86]. Jaramillo et al. [16] assumed a plant produced 62% diesel, 35% gasoline, and 3% propane. Typically, GTL plants produce more diesel than other products (40-80%) [87]. Forman et al. [61] assumed that GTL plants produce 8.4% LPG, 17.8% condensate, 23% GTL naphtha, 40.7% GTL diesel, and 10% normal paraffin and lubricant base oils. The energy efficiency of GTL plants is 53-67.6% [16, 61, 80].

There are two assumptions for electricity consumption in the GTL process – one, that electricity is purchased from low-emission sources such as solar energy and two, that power comes from high-carbon sources like coal and natural gas. In both assumptions, the amount of CO_2 that is produced from electricity generation might be added to the total emissions from the plant [16]. Electricity generated at the GTL plant (without CCS) can be sold [16, 83]. Therefore, this electricity can be considered an emission offset. Through combinations of CCS and the use of low and high energy sources, GTL plant products can compete economically with petroleum-based products. GHG emissions from gasoline and diesel produced from natural gas are higher than those

from petroleum-based products, assuming a common source for electricity generation and a plant without CCS. By applying CCS and low carbon sources for power generation, GHG emissions from GTL gasoline and diesel are relatively equal to those from petroleum bases [16]. GTL diesel can be blended with petroleum-based products[61]. Using GTL diesel as the blending component can reduce the energy consumed and GHG gases emitted during desulfurization, denitrogenation, hydrogenation, and dearomatization of petroleum-based diesel that has high sulfur and aromatics [61]. The net GHG emissions of a GTL diesel plant is 35.1 gCO_2e/MJ [61]. In this study, the impact of GTL coproduction of products such as lubricants and LPG is considered. Coproduction reduces the total GHG emissions of the liquid fuel.

For estimating the Well-to-Wheel emission factor, emissions from transportation and fuel combustion should be added to the above calculations. The synthesis fuel is carried by pipeline, tanker, barge, rail, or truck. The distance traveled determines the type of transportation and the emissions factor. For example, in the U.S, pipelines transport just 20% of the diesel cross-country; the rest is transported by rail and truck. Natural gas, on the other hand, is only transported by pipeline in the U.S. [61]. So, to estimate the GHG emissions in the transportation of liquid fuels, the method of transportation must be considered.

Another defined parameter for transportation emissions factor is energy intensity (kJ/metric ton-km). Energy intensity can be taken from transportation data books or calculated from the GREET model.

The carbon content of gasoline and diesel from GTL are 18.90 and 20.20 g/MJ, respectively [88]. The net GHG emissions of diesel fuel for 7200 nautical miles by tanker ship transportation and 50 miles of road transportation is 2.8 gCO_2e/MJ [61]. Values for transmission and distribution of natural gas range between 0.29 and 1.05 % of natural gas produced [81].

The total GHG emissions of natural gas are estimated by adding all emission factors from the life cycle of NG to liquid fuel. There are two methods for reporting the total Well-to-Wheel GHG emissions of GTL diesel [61]. The first is by excluding the emissions of the co-product from net GHG emissions of diesel production (substitution method); the second is by using allocation method. The results are 86.2 gCO_2e/MJ and 103.1 gCO_2e/MJ, respectively [61]. This evaluation compared to the GHG emission of ULSD (Ultra Low Sulphur Diesel) of 91.1 gCO_2e/MJ showed that the methodology for calculating has a vital impact. To draw a conclusion, without considering the downstream emissions and co-product impacts, the estimation of total GHG emissions might be imprecise. Table 2-3 summarizes the life cycle GHG emissions from different steps in the GTL process.

Table 2-3: Summary GHG emission and life cycle analysis of GTL process

Study	GHG emissions	Description	Comments	Ref.
Forman et. al. 2011	0.4% of NG	Natural gas is produced offshore and processed onshore on the gas units.	Vented	[61]
Forman et. al. 2011	0.2% of NG	Natural gas production	Methane Flared	[61]
Jaramillo et. al. 2007	0.38% of NG	Natural gas production includes: combustion of natural gas during extraction, processing, transmission and storage	Emitted	[83]

Study	GHG emissions	Description	Comments	Ref.
Jaramillo at. al. 2007, Harrison et. al. 1996	1.07% of NG	Natural Gas Production includes: 62% fugitive emissions, 8% combustion, and 30% vented.	Lost in Production	Environment Protection Agency (EPA) [83, 89]
Burnham et. al. 2011	0.06-0.23% of NG (0.583-1.081 gCO2eq/MJ)	Natural Gas Production	Leaked or Vented	[81]
Burnham et. al. 2011	0.29-1.05%	Transition& Distribution		[81]
Jaramillo at. al. 2007	1.54-3.35 gCO2/MJ	Transmission and Storage in underground facilities such as reconditioned gas reservoirs or salt caverns.	-Emitted -Fugitive emissions	[83]
Forman et. al 2011	12.1 gCO2/MJ	Extracted offshore and processed onshore. Sulphur is recovered.	Vented	[61]

Study	GHG emissions	Description	Comments	Ref.
Forman et. al. 2011	0.5 gCO2/MJ	Raw gas is transported 47 miles by pipelines to gas process unit	-Emitted -Fugitive	[61]
Forman et. al. 2011	7.7 gCO2/MJ	Gas Treatment	Efficiency 98%	[61]
Jaramillo et. al 2007	35.1 gCO2/MJ	Fischer-Tropsch GTL Plant	Well-to-Plant Emission, energy efficiency:67.6 and carbon efficiency 81.8%	[83]
Forman et. al. 2011	2.8 gCO2/MJ	Fuel transportation	Leaked and vented, 50miles road + 7200 Nautical Miles	[61]
Forman et. al. 2011	86.2 gCO2/MJ	FT- GTL WTW	Substitution Method	[61]
Forman et. al. 2011	103 gCO2/MJ	FT- GTL WTW	GREET	[61]

2.4.2. Life Cycle GHG emissions of CTL plant

Conceptually, the coal life cycle is similar to the natural gas life cycle in that both life cycles include mining and pretreatment, transportation, conversion to liquid, distribution, and combustion. Therefore, all of the above calculation methods apply to coal. Coal is extracted by two types of mining: surface mining and underground mining. Greater amounts of coal are mined from surface mining. For instance, in the U.S. 67% of coal is produced from surface mines [83]. Mining operations also produce CO_2. In 1997, 75 million tons of CO_2e methane were emitted from coal mining, according to the U.S. Environmental Protection Agency (EPA) [90]. In total, coal mining and pretreatment processing emissions range from 1.7-15 gCO_2e/MJ [81, 91].

Mining and transportation make up the upstream life cycle stages for coal. After the removal of impurities, coal is transported to the CTL plant. Generally, coal is transported by rail, barge, or truck. The emissions factor for coal transportation is between 1.3 and 3.2 gCO_2e/MJ [91]. Once at the CTL plant, coal is fed into it. In this stage of the coal life cycle, as with GTL plants, efficiency and plant configuration are critical parameters. Coal is rich in carbon, while liquid fuels are high in hydrogen. Therefore, through the CTL process the H/C ratio increases from 1 to 1 in coal (compared to the 2 to 1 in liquid fuels) and excess carbon is converted to CO_2 [3]. The CTL plant energy efficiency is 55% [16]. In contrast to the GTL process, there is no electricity generated and so it must be purchased. In addition, using the CCS system increases expenses due to increased power demand. The electricity life cycle emissions factor is 600-620 gCO_2e/MWh for Illinois number 6 coal [16]. Gasoline and diesel produced from a CTL plant emit two times more GHGs than the same fuels produced at a GTL plant by using that uses its own resources for electricity generation. Typical CTL plants produce 53% diesel, 44% gasoline, and 3% propane [92]. As

described in previous section, downstream emissions and co-products should be considered in calculations.

Carbon capture and sequestration (CCS) unit involves capturing and compressing of CO_2 that is emitted from a process [16, 83, 93]. This unit helps to reduce CO_2 emissions significantly; Adding the CCS unit to the CTL plant reduces CO_2 emission, however, production cost is increased due increase in capital cost. It is possible for FT-CTL to be considered in the energy mix in the future but with current technology, using of coal requires more development. Table 2-4 summarizes the life cycle GHG emissions from different steps of the CTL process.

Table 2-4: Summary GHG emission and life cycle analysis of CTL process

Study	GHG Emissions	Description	Comments	Ref.
Burnham et. al. 2011, Venkatesh et. al. 2012	1.7-15 gCO2eq/MJ	Coal Production:17% of total upstream is energy use coal production and 51% methane emission 32% coal transport.	-In surface and underground coal mining methane is vented. -Pretreatment	[81, 91]
Burnham et. al. 2011	1.3-3.2 gCO2/MJ	Transmission, 32% of total upstream emissions.	Leaked and vented	[81]
Jaramillo et. al. 2007	100-120 gCO2/MJ	Fischer-Tropsch CTL Plant	Well-to-Plant Emission	[83]
Jaramillo et. al. 007	0.6-0.7 kgCO2/liter	FT- CTL Plant	Well-to-Wheel Emission	[83]

Chapter 3. Methodology for techno-economic assessment of GTL/CTL plant[2]

3.1. Background

Fossil fuels such as coal and natural gas are widely used as major source of energy for various industrial and manufacturing processes. The total global commercial energy use indicated that coal consumption was 28%, ranking second after oil as one of the major sources of primary energy and natural gas (at 21%) ranked third [94]. On a global scale, the consumption of coal is approximately 41% and gas 22% [94]. This strongly indicates that coal and natural gas have the largest share in the energy mix, particularly for electricity generation [95]. However, the huge amounts of greenhouse gases (GHG) and trace element releases during utilization of coal and other fossil fuels have drawn much more attention, due to their adverse impacts on the ecological environment and human health [96]. For these reasons, reducing GHG emission and promoting a clean energy economy have initiated several environmental regulations. A recent development is to phase out coal-based plants [97]. This has prompted the search for alternative means by which coal and other fossil fuels can be utilized in a more environmentally friendly way. In view of this, alternative pathways such as converting natural gas to liquid (GTL) and coal to liquid (CTL) fuels are being considered globally. These processes offer advantages over competing technologies in the processing of varieties of feedstocks into a diverse range of desirable liquid fuels such as diesel

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[2] A part of this chapter has been submitted as Mohajerani, S., Kumar, A., Oni A. A techno-economic assessment of gas-to-liquid and coal-to-liquid plants through development of scale factors, *Energy*, 2016.

and gasoline, and other liquid chemicals products (methanol and dimethyl ether). The advantages of producing these synthetic liquid fuels are well established, revolving around the huge deposit of coal and natural gas in some region of the world such as Canada, United States, etc. However, it is important to ascertain that the development of these alternative pathways depict a resourceful and a realistic projection of how it is likely to unfold the associated economic benefits for coal and natural gas utilization. Therefore, the global shift toward the production of synthetic liquid fuels from these conventional feedstocks must be adequately investigated to ascertain their economic benefits as an alternative method for liquid fuel production.

The increased interest in the production of synthetic liquid fuels is expected to reduce dependency on crude oil and other conventional fuels. However, the investment in the production of synthetic liquid fuels still remains a subject of discussion as production cost of crude oil dwindles between $28 and $110 per barrel [98-100]. The production cost of crude oil remains a highly competitive factor for synthetic liquid fuel production from the established processes such as the GTL and CTL. This has made some operators, governments and willing sponsors reluctant to progress with a large number of new plants. A number of studies have also reported that the investment cost on synthetic liquid fuels produced from CTL and GTL are relatively high when compared with the crude oil price. For example, a study conducted by Jaramillo et al. [16] showed that the production cost of liquid fuels from a GTL plant are not economic at low oil prices ($40/bbl), especially if these fuels are produced in the high-emissions scenario and the carbon tax is high ($130/metric ton CO_2). Even if oil prices are high ($120/bbl) and the carbon tax is low, natural gas prices would only have to reach $550/1,000 m^3 or $15/MCF (not unrealistically high) for GTL fuels to become more expensive than petroleum-based fuels. Vliet et al. [93] also reported that the costs of liquid fuels (such as diesel) depend in large part on feedstock prices and conversion plant efficiency. The

break-even point for a GTL oil-based diesel product was at an oil price equivalent of $34/bbl. Hansen et al. [101] reported that the GTL plant is complex, expensive and its energy-consuming stage accounts for up to 60% of the total expenditures and operating costs. Investigation into the investment cost of CTL plant also shows similarly observation. Mantripragada and Rubin [30, 76] estimated the capital cost of a CTL plant with production capacity of 50,000 barrels per day capacity to range between $4.5-6.0 billion. They also showed that depending on the coal type, gasifier type and CO_2 constraint, the product cost is $55 - $97/barrel for a plant without CCS and $62 - $105/barrel for a plant with CCS. Jaramillo et al. [16] also reported that CTL fuels produced without CCS are not economically feasible at low oil prices ($40/bbl), regardless of the carbon price. However, at high oil prices ($120/bbl), CTL becomes economically feasible. The study conducted by Vliet et al. [93] also showed that the break-even point for a CTL oil-based product was at an oil price equivalent of $60/bbl. Further advances in the GTL and CTL processes are also focused on capital expenditures and improving operating and energy efficiencies. Establishing economies of scale with the aim of driving down the production costs of the GTL and CTL plants can provide a break-even point at a favourable oil price equivalent.

Several studies on the use of economies of scale for the capital cost evaluation are available [102-104]. The application of this concept to the GTL and CTL processes are limited to specific plant size, components, or location and are not developed to search for optimum point or to achieve a break-even point. For example, Hamelinck et al. [96, 105, 106], calculated the total capital investment (TCI) of a Fischer–Tropsch (FT) diesel derived from biomass via gasification plant using the factored estimation method, based on known costs for major equipment as found in literature and given by experts. Tijmensen et al. [107], reviewed the technical feasibility and economics of biomass integrated gasification–Fischer Tropsch (BIG-FT) processes in general, identifies most promising system configurations and identifies key R&D issues essential for the

commercialization of BIG-FT technology. The costs of the BIG-FT components are based on cost data on component level, which were obtained from literature, vendor quotes and personal communication with experts. Mantripragada and Rubin [3] have also focused on the technical and economic effects of CCS options on the CTL process using economies of scale for capital cost estimation. With the exception of a few limited studies, relatively little has been reported on the development of scale factors for the GTL and CTL. The advantages of providing a scale factor that adequately represent capital investment cost of GTL and CTL can provide opportunity for developing a plant with a break-even point equivalent to the relatively low oil price.

The objective of this research is to conduct a comprehensive techno-economic assessment of CTL and GTL pathways for Canada using a data-intensive bottom-up methodology. The specific objectives are to:

- Develop a techno-economic model for estimation of cost of liquid fuel production from coal using the CTL pathways;

- Develop scale factors for the key equipment for the CTL plants;

- Develop a techno-economic model for estimation of cost of liquid fuel production from natural gas using the GTL pathways;

- Development scale factors for the key equipment for the GTL plants;

- Conduct a comprehensive sensitivity analysis to assess the impact of various inputs parameters on the cost of production of liquid fuel;

- Conduct a case study for western Canada with respect to development of GTL and CTL plants.

3.2. Methodology and approach

Syngas production, F-T synthesis, and upgrading are analysed in terms of capital and operation costs. A bottom-up techno-economic model is developed to calculate the capital cost. This approach is used extensively by industry to estimate total investment and production costs [108]. To evaluate the plant's capital cost the major equipment in each unit process is identified. After which the plant's equipment and their corresponding sizes are mainly developed from literature and in discussion with the experts [25]. The capacity of the selected GTL and CTL plants are 50,000 bbl/day. The overall capital costs are estimated as the sum of the plant's equipment costs. Direct cost of the plant such as, instruments and control, piping, utilities, and buildings, and the indirect costs of the plant such as, engineering and head office, start-up, and contingencies are also considered alongside the with total capital cost. To develop the scale factors for the entire plant, the equipment cost in the liquefaction plants are calculated based on the data obtained from previous studies. The cost values obtained are plotted against their corresponding sizes to develop the equipment scale factors. The cost of equipment with capacity C_r is determined as follows:

$$\textbf{Cost}_r = \textbf{Cost}_b \cdot [\frac{Cr}{Cb}]^f \tag{14}$$

C_b: The base capacity refers to a particular capacity size

C_r : The required capacity

C_b : The cost of base case capacity

C_r : The cost of the required equipment

where f is the scale factor and ranges between 0 and 1 [109]. The scale factor is used to determine the cost of equipment form one capacity to another. Each piece of equipment is grouped based on a specific category such as vessels, reactors, etc. Using Eq. 14, scaling exponent is derived for all

the equipment. The location factor and capital cost inflation are also taken into account. The discounted cash flow analysis is applied to estimate the final product cost.

3.3.   Inputs and assumptions

The base case production capacity chosen for the GTL and CTL plant in this study is 50,000 barrels per day of liquid product. The required coal input as feedstock for the CTL is 24,533 tonne/day. The study also considered the application of CCS unit to the CTL plant. This was necessary in order to account for the economic effect of capturing CO_2 emissions. The basic economic assumptions used in this study are shown in Tables 3-1 and 3-2. The interest rate is 12%, the plant is assumed to have a 20-year lifetime, and the installation period is 3 years. The loading factor for the first year of operation is 80%; for both the second and third years, 85% is assumed. The maintenance cost is taken to be 4% of the capital cost [9, 16] and the plant capacity factor 90% [25]. The location factor for Canada is chosen and was assumed to be 1.14 [110].

Table 3-1: *GTL plant economic assumptions*

Plant output (bbl/day)	50,000		Assumed the final liquid fuel product capacity of the GTL plant.
Gasoline (% of total product)	30	[25]	Assumed 30% of output (50,000 bbl/day) is gasoline.
Diesel (% of total product)	70	[25]	Assumed 70% of output (50,000 bbl/day) is diesel.
Natural gas feed (1000 lb/hr)	780	[25]	Feedstock flowrate based on the Aspen plus simulation.
Natural gas price	4.89	[111]	Price of natural gas at Henry Hub 2014 ($/Kcf)
Utilities (% of capital cost)	12%	[112]	Utilities include electricity, steam, fuel for combustion, water, and compressed air. There are required for plant construction.
Instrumentation and control (% of capital cost)	20%	[7, 105]	All the equipment and instruments related to plant control and to keep the plant in the stable status.
Building (% of capital cost)	12%	[7, 105]	Included construction cost of all the building in the plant such as, control room and etc.
Piping (% of capital cost)	4%	[105, 108]	Included pipes are required to carry the flows.
Contingencies (% of capital cost)	20%	[78]	An allowance for unforeseeable costs.
Engineering and head office (% of capital cost)	15%	[7, 9]	Represented the cost of head office and engineering design and etc.
Start up (% of capital cost)	4%	[9, 105]	Cost associated with the implementation of the plant.

Table 3-2: *The CTL plant economic assumptions*

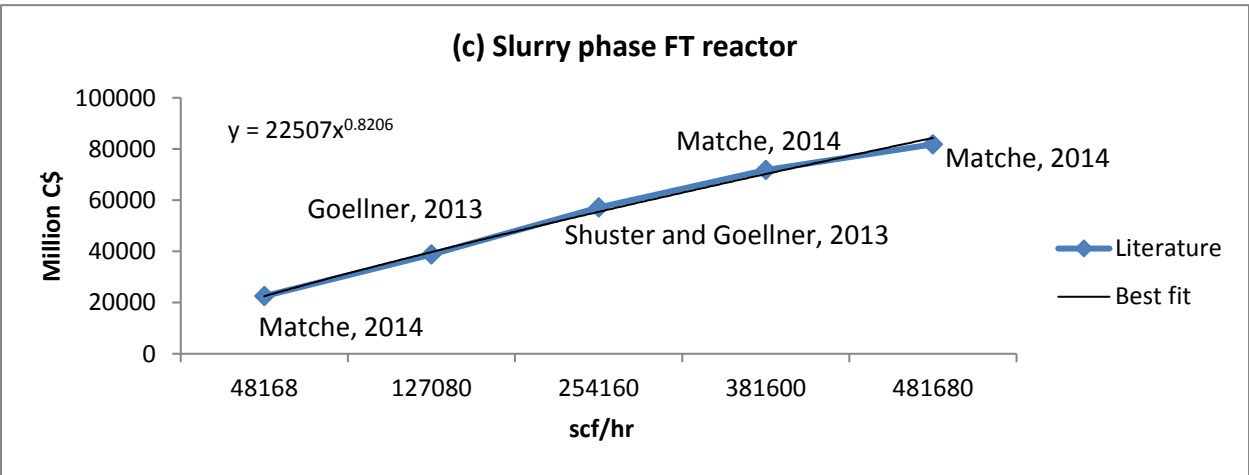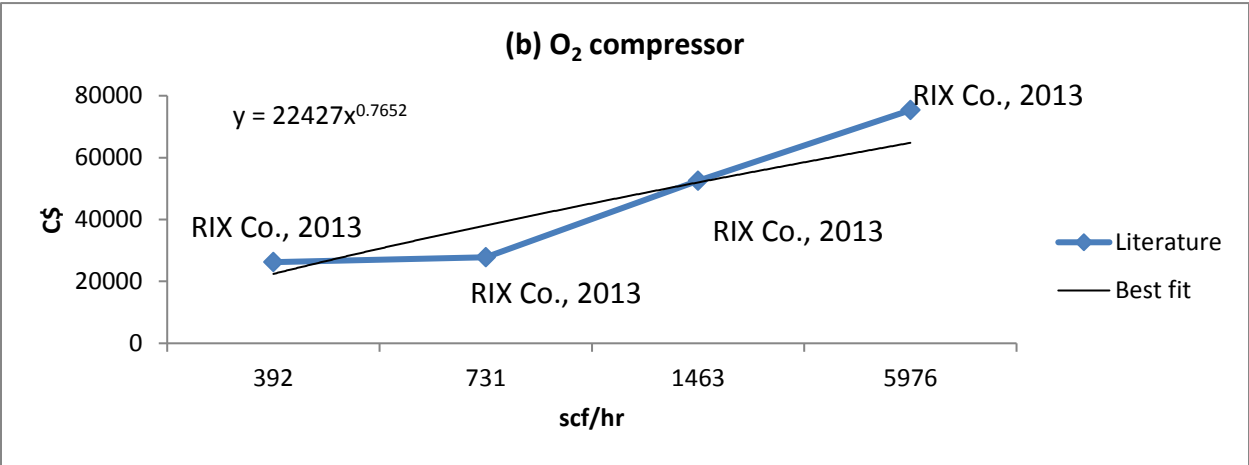|			
Plant output (bbl/day)	50,000	[20]	Assumed the final liquid fuel product capacity of the CTL plant.
Naphtha (% of total product)	56	[20]	Assumed 56% of output (50,000 bbl/day) is naphtha.
Diesel (% of total product)	44	[20]	Assumed 44% of output (50,000 bbl/day) is diesel.
Coal feed (tonne/day)	24,533	[20]	Feedstock flowrate based on the Aspen plus simulation.
Coal price from Western Canada 2015 ($/tonne)	10	-	Assumed based on the lower price.
Utilities (% of capital cost)	12%	[112]	Utilities include electricity, steam, fuel for combustion, water, and compressed air. There are required for plant construction.
Instrumentation and control (% of capital cost)	20%	[7, 105]	All the equipment and instruments related to plant control and to keep the plant in the stable status.
Building (% of capital cost)	12%	[7, 105]	Included construction cost of all the building in the plant such as, control room and etc.
Piping (% of capital cost)	4%	[105, 108]	Included pipes are required to carry the flows.
Contingencies (% of capital cost)	20%	[78]	An allowance for unforeseeable costs.
Engineering and head office (% of capital cost)	15%	[7, 9]	Represented the cost of head office and engineering design and etc.
Start up (% of capital cost)	4%	[9, 105]	Cost associated with the implementation of the plant.

Chapter 4.   Economic assessment of the Gas-to-Liquid plant using scale factor[3]
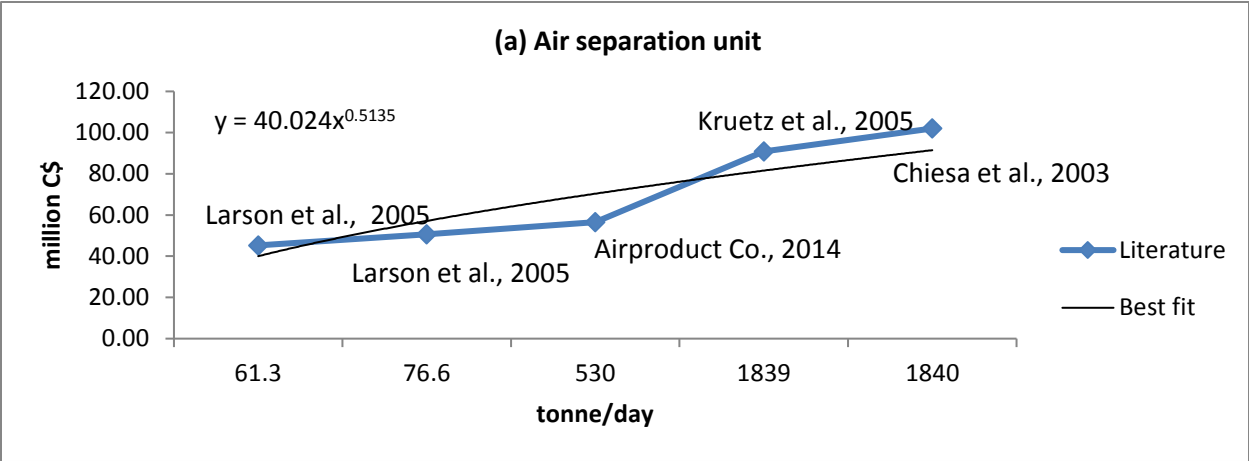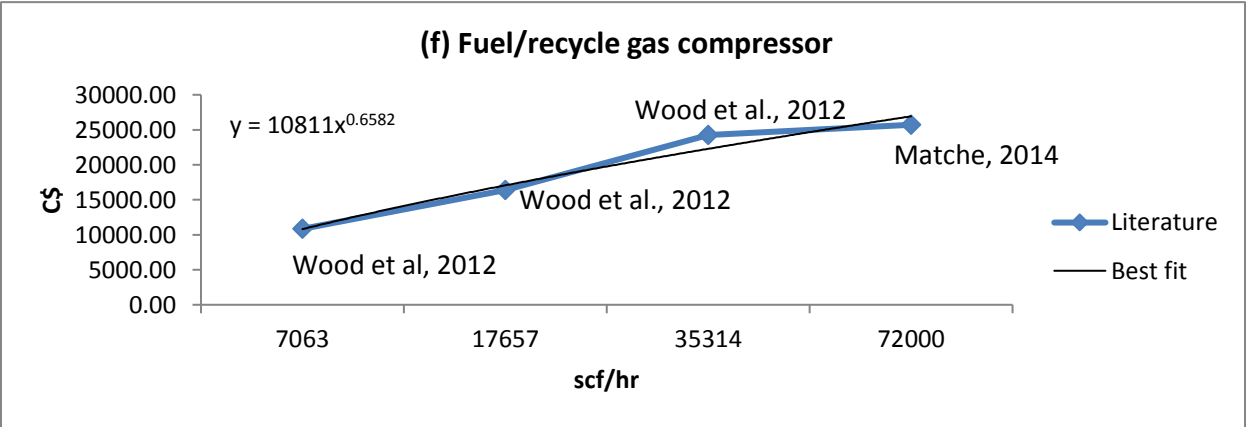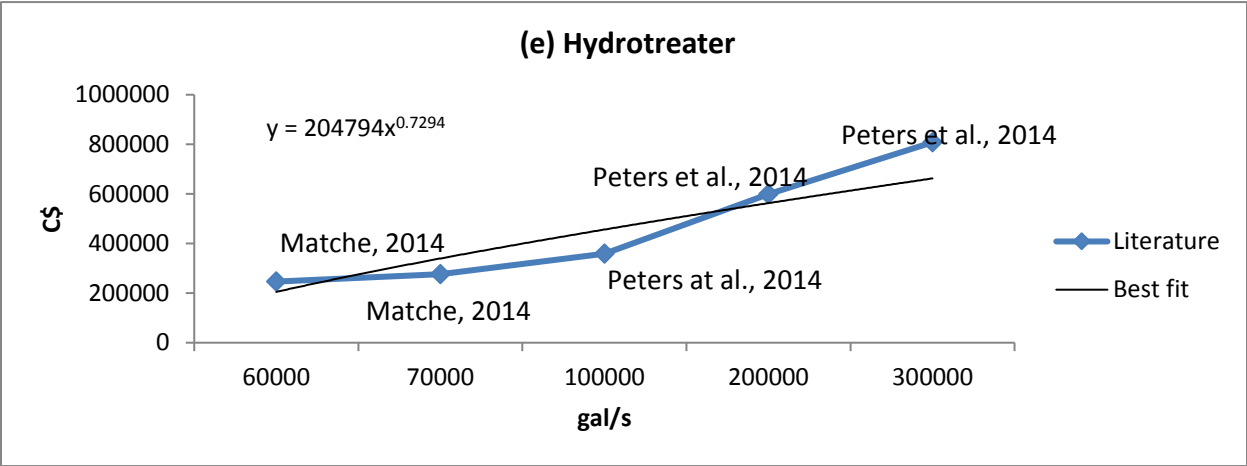
4.1.   GTL plant cost analysis

To estimate the cost of equipment in a GTL plant, scale factors for the equipment are calculated based on the methodology described in section 3.1. If the scale factor = 1, means capital cost increases proportionately with capacity. This indicates there is a constant rate to scale. A scale factor <1, means the capital cost increases at a rate less than the capacity, so, there is an increasing return to scale.

The calculated scaling factors for the equipment are shown in Table 4-1. Figure 4-1 (a) shows that the capital cost of ASU at various capacities are as reported earlier [109, 113]. Based on these figure, the calculated scale factor for ASU is 0.51. Figure 4-1 (b) shows the capital cost of oxygen compressor at different sizes taken from industrial quotes [114]. The scale factor for compressor derived from the Figure 4-1 (b) is 0.76. This estimate is lower than that found in various literatures. Hamelinck et al. considered it to be 0.85 [106]. Figure 4-1 (c) shows the capital cost of slurry phase reactor at different sizes [115]. Based on Figure 4-1 (c) the estimated scale factor for slurry phase reactor is 0.82. The scale factor reported in other studies is 0.72 [106]. The main reason for this variation in values is that cost was estimated for different years and locations. The range of capital

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[3] A version of this chapter has been submitted as Mohajerani, S., Kumar, A., Oni A. A techno-economic assessment of gas-to-liquid and coal-to-liquid plants through development of scale factors, *Energy*, 2016.

cost for PSA unit is shown in Figure 4-1 (d) [105, 109]. The derived scale factor from Figure 4-1

(d) is 0.82. The scale factor derived for hydrotreater considered for this model is 0.72. Figure 4-1

(e) shows the capital cost of hydrotreater of different sizes [115, 116]. The scale factor calculated

for the fuel/ recycle gas compressor is 0.65. This is based on the data for gas compressor given in

Figure 4-1 (f) [115, 116]. Figure 4-1 (g) the scale factor for reformer/ATR is 0.84 [115]. This value

is higher than the value used in earlier study [106] for biomass to liquid. The estimated scale factor

for isomerization is 0.62 based on data in Figure 4-1 (h) [109, 115]. Calculated scale factor for the

storage tanks is 0.50 based on different capacities shows on Figure 4-1 (i) [115]. Some of the scale

factors calculated in this chapter do not have a same value as those in the literature. This is because

the estimated cost was in different years and location.

(a) Air separation unit

$y = 40.024x^{0.5135}$

Larson et al., 2005

Larson et al., 2005

Airproduct Co., 2014

Kruetz et al., 2005

Chiesa et al., 2003

(b) O$_2$ compressor

$y = 22427x^{0.7652}$

RIX Co., 2013

RIX Co., 2013

RIX Co., 2013

RIX Co., 2013

(c) Slurry phase FT reactor

$y = 22507x^{0.8206}$

Goellner, 2013

Matche, 2014

Shuster and Goellner, 2013

Matche, 2014

Matche, 2014

(d) PSA unit

$y = 10.717x^{0.814}$

Carbotech Co., 2014

Larson et al., 2005

Larson et al., 2005 &
Kruetz et al., 2005

Hamelinck et al., 2002

Larson et al., 2005

Literature
Best fit

million C$

Kmol/s

(e) Hydrotreater

$y = 204794x^{0.7294}$

Peters et al., 2014

Peters et al., 2014

Matche, 2014

Peters at al., 2014

Matche, 2014

Literature
Best fit

C$

gal/s

(f) Fuel/recycle gas compressor

$y = 10811x^{0.6582}$

Wood et al., 2012

Wood et al., 2012

Matche, 2014

Wood et al, 2012

Literature
Best fit

C$

scf/hr

49

(g) Reformer/ATR

$y = 21366x^{0.8459}$

Matche, 2014

Goellner, 2013

Matche, 2014

Hamelinck et al., 2004

Matche, 2014

(h) Isomerization

$y = 1.0432x^{0.7328}$

Matche, 2014

Matche, 2014

Goellner, 2013

Matche, 2014

(i) Storage tank

$y = 1E+06x^{0.5063}$

Matche, 2014
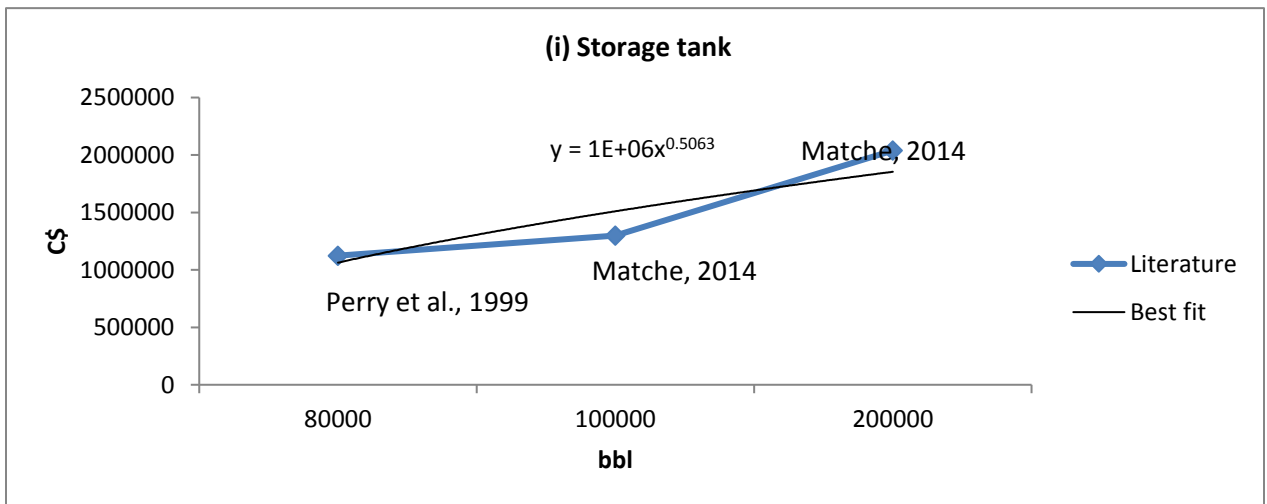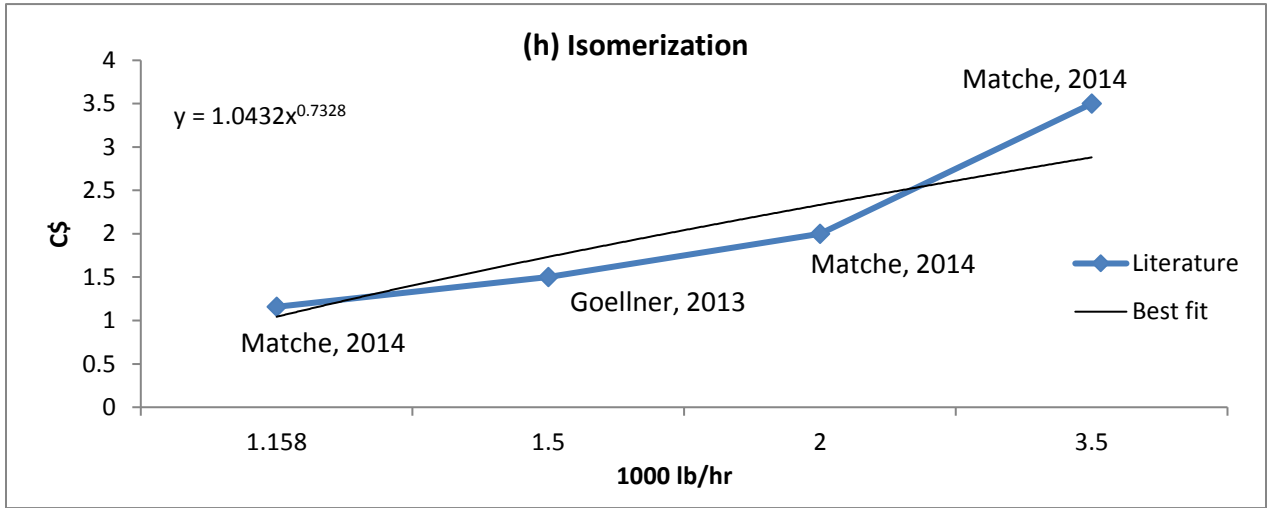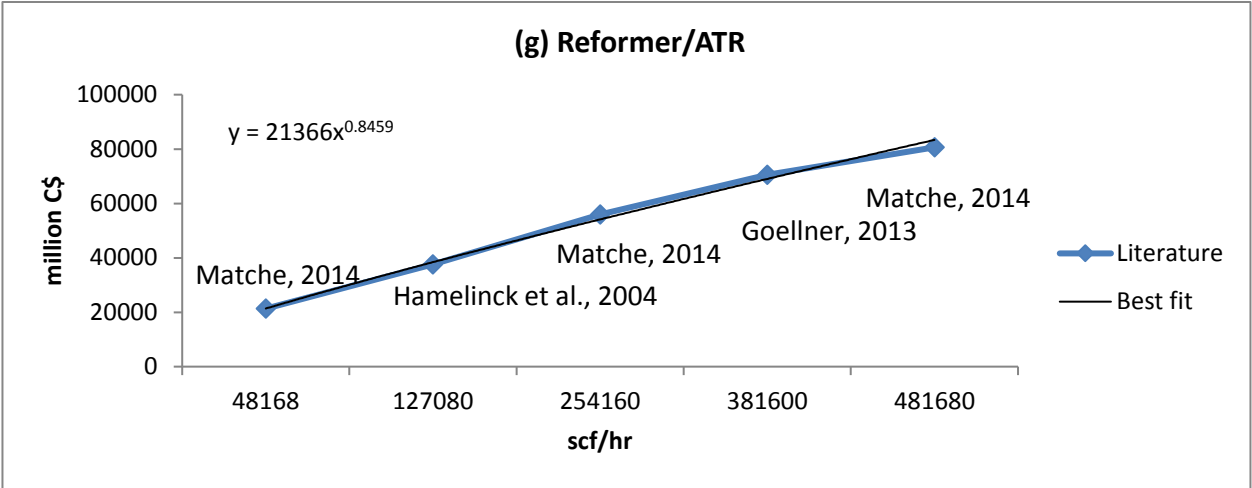
Matche, 2014

Perry et al., 1999

Figure 4-1: Scale factors for key components of a GTL plant

Table 4-1: Calculated scale factors for key equipment in a GTL plant

Process equipment	Calculated scaling factor	Sources used for calculation
Air separation unit (ASU)	0.51	[109, 113, 117, 118]
O_2 compressor	0.76	[114]
FT- Slurry phase reactor	0.82	[25, 77, 115]
PSA unit	0.82	[105, 109, 113, 119]
Hydrotreater	0.72	[115, 116]
Fuel/ recycle gas compressor	0.65	[11, 115]
Reformer/ATR	0.84	[77, 106, 115]
Isomerization	0.62	[25, 115]
Storage tank	0.50	[110, 115]

Figure 4-2 shows the variation of the unit capital cost of the GTL plant with production capacity. There is economy of scale benefit as plant sizes increases. The scale factor for the plant is found to be 0.7. A scale factor of 0.7 implies that one percent increase in the plant size, increases capital cost by 0.7%. The capital cost of the GTL plant per unit of output decreases with increase in capacity due to economy of scale. For plant production capacity higher than 20,000 bbl/day, the change in unit capital cost is not significant.

The total capital investment cost for a 50,000 bbl/day plant is estimated to be C\$ 4.3 billion. The main cost-driving equipment in the GTL plant is the natural gas pre-reformer and reformer units, they accounted for about 41% of the overall plant. The complexity of design of these units makes them cost intensive. These processes are designed to withstand high pressure and temperature. The pre-reformer plant is added to reduce energy intake into plant. Pre-reforming often occurred in low temperature compared to the reformer unit [120]. Table 4-2 shows the capacity and the calculated cost of the equipment. ASU and FT reactor are 30% and 9% of total investment cost of the GTL plant respectively. Upgrading unit is another major unit operation in the GTL plant, its accounted

for 20% of overall capital cost. The cost of the storage tanks is relatively small, they accounted for about 0.14% of the overall capital cost of the GTL plant (Figure 4-3).

The natural gas available as feedstock is priced at C$ 5.9 per GJ [111]. This price corresponds to the Henry Hub price for natural gas [111]. The total cost of the plant is the sum of the amortized total equipment cost and the operation and maintenance costs. The cost distribution of different process units for a 50,000 bbl/day of the GTL plant is shown in Figure 4-4 shows the yearly operation costs. The cost of natural gas is the most cost intensive parameter, its accounted for 42% of the entire production cost. The capital, electricity, labour, catalyst, maintenance, and water costs accounted for 29.0%, 14.0%, 11.0%, 1.4%, 1.3%, and 1.1%, respectively of the entire production cost. The cost of the cobalt catalyst and the unit's lifetime are assumed to be C$593 / bbl /day and 5 years, respectively [25].
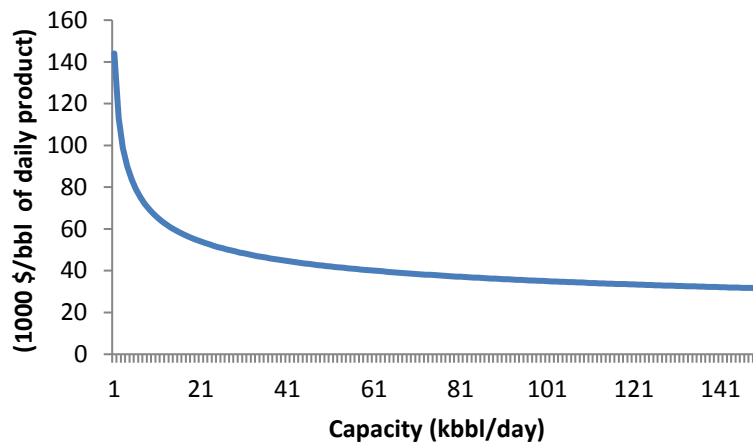

Figure 4-2: Unit capital cost of the GTL plant versus capacity

Table 4-2: The GTL plant size and cost

Process equipment	Capacity (tonne/hr)	Cost (million C$)
Natural gas pre-reformer	750	223.9
Auto-thermal reactor (ATR)	1543	524.8
ASU	237	471.3
O_2 compressor (MW)	10	82.1
F-T reactor	1211	170.9
Hydrocarbon recovery	240	68.6
Naphtha hydrotreater	37	12.4
Naphtha reformer	34	48.4
C5/C6 isomerization	27	12.6
Diesel hydrotreater	56	35
Wax hydrotreater	142	97.5
PSA unit	52	11.2
Steam methane reformer	52	40.8
Gasoline storage tank (bbl/day)	35000	0.97
Diesel storage tank (bbl/day)	15000	1.5

Figure 4-3 shows the total production cost versus capacity of the GTL plant. X-axis demonstrates the plant capacity ranging from 10,000 to 100,000 bbl/day. Figure 4-3 indicates that production cost decreases by increasing the capacity. The decrease in the cost of fuel production is significant up to a capacity of 50,000 bbl/day indicating the strong economy of scale up to this size.
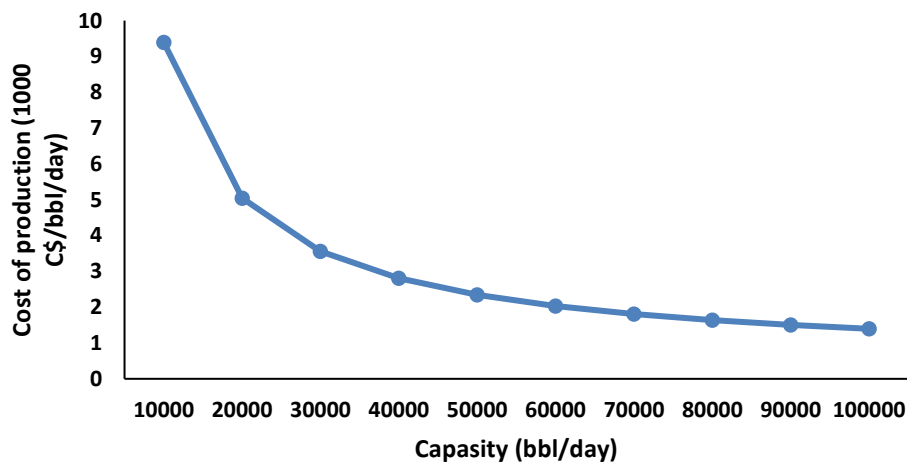

Figure 4-3: Unit production cost of the GTL plant versus capacity
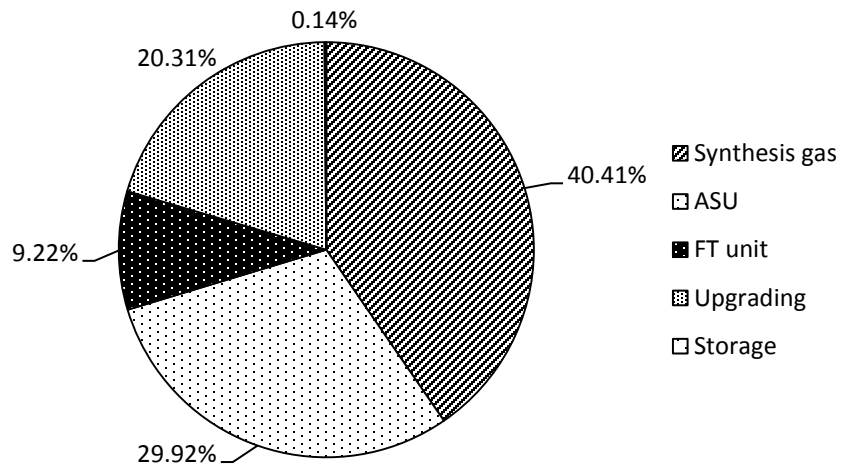
Figure 4-4: Cost distribution in a GTL plant for different unit operations
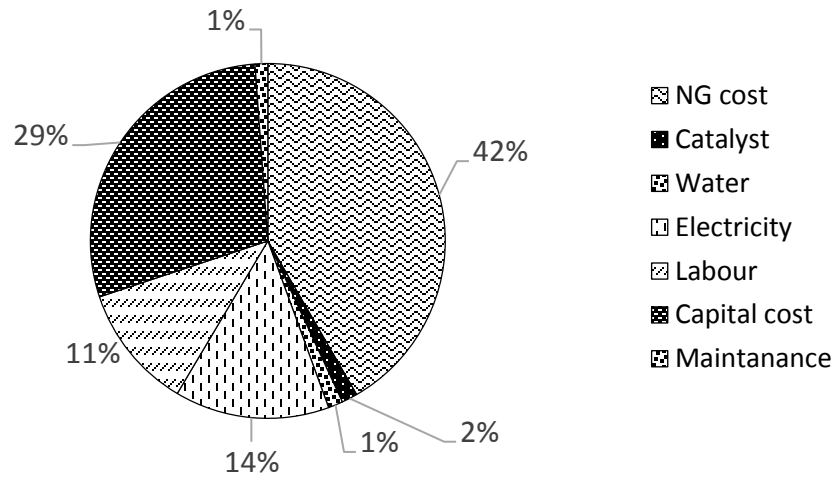
Figure 4-5: GTL plant production cost distribution

The capital cost of GTL plants found in the literature is presented in Table 4-3. These results are compared with the values obtained in this study. The difference in the estimated values reported in the literature varies widely. The variations might be due to the various assumptions made such as location factors, base year and plant consideration window. For example, the cost values

reported by Shuster and Goellner [25] for 50,000 bbl/day capacity included electricity generation and mercury removal unit which was not considered in this study.

Similarly, the production costs of the GTL plants presented in literature are compared with this study. The production cost reported by Rafiee et al. [17] is 55 cent/liter, this value is close to the value reported in this study. The variation in the results might be due to the difference in the cost of natural gas assumed. In addition, Rafiee et al. [17] used the module costing technique, which is different from the discounted cash flow analysis used in this work. Gardassi et al. calculated the production cost of the GTL plant to be 41.82 cent/liter [14]; they assumed that all final products are gasoline grade. The variation in the results presented by Gardassi et al. and this study might be due to differences in plant capacities and the final product type.

Table 4-3: GTL cost on the literatures

Name	Capacity (bbl/day)	Cost (billion C$ 2014)	Cost/Capacity (C$/bbl/day)	Reference
Shuster and Goellner	50,000	4.8	96,000	[25]
Bao et. al.	118,000	9.7	82,203	[18]
Lee	31,787	3.02	95,000	[12]
Chedid	140,000	5.67	40,500	[21]
Foster Wheeler	100,000	3.44	34,400	[112]
Present study	50,000	4.3	86,000	

Chapter 5. Economic assessment of the Coal-to-Liquid plant using scale factor[4]
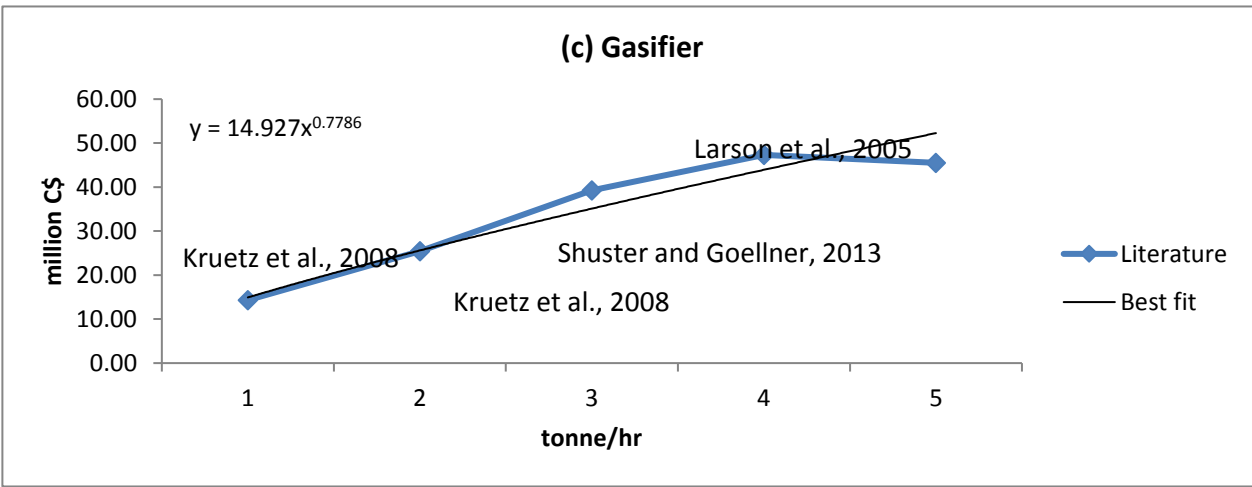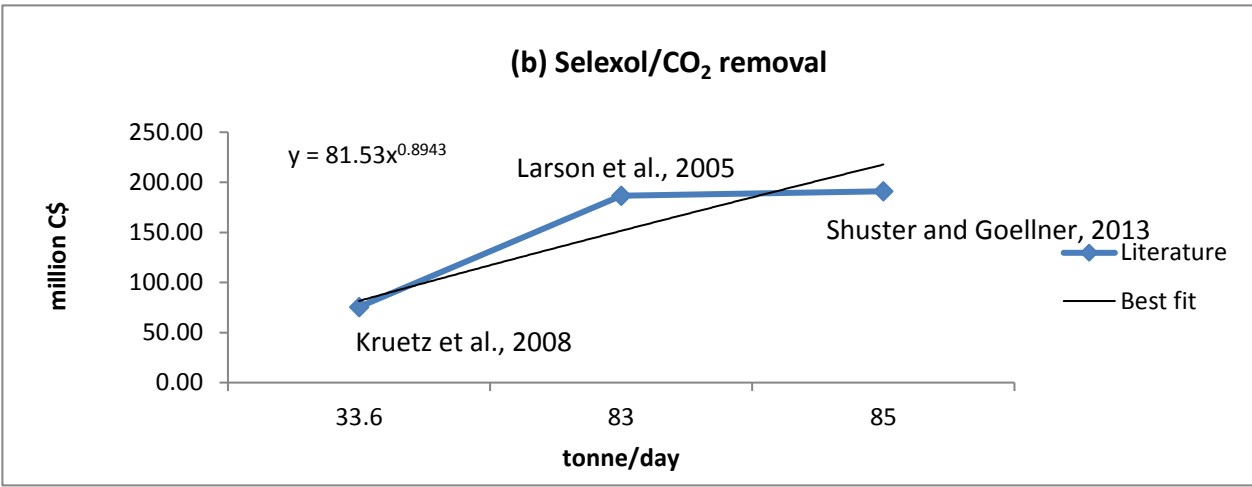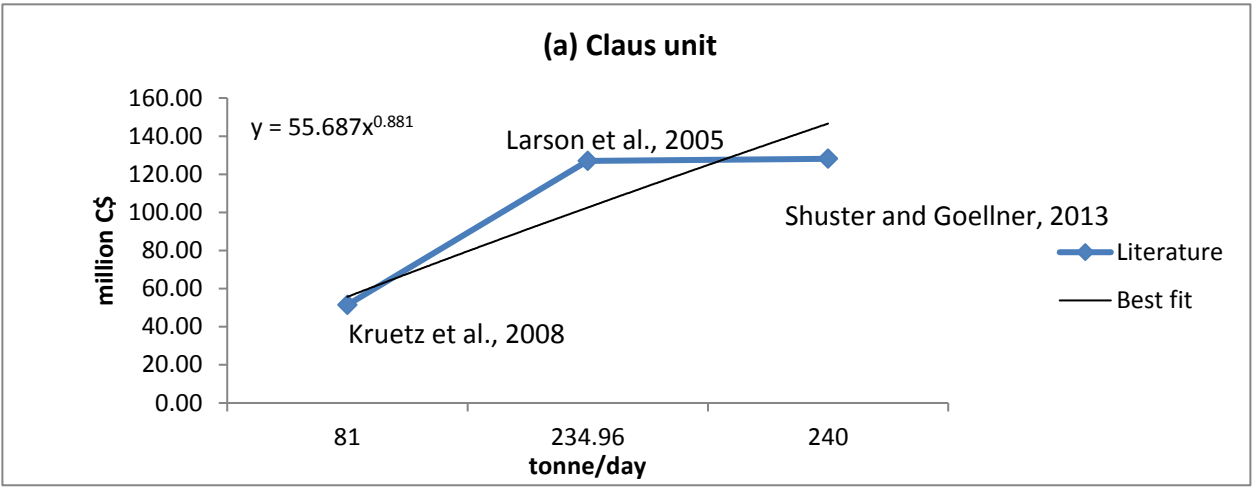
5.1. CTL plant cost analysis

5.1.1. CTL plant without CCS

Figure 5-1 shows the developed scale factors for the main components for the CTL plant. The CTL and GTL have similar equipment in common, for the equipment in this category, the scale factors developed in section 4.2 was used to determine their corresponding cost for the CTL plant. For this reason, they are not repeated here. Table 5-1 shows the developed scale factors for the equipment in the CTL plant.

Figure 5-1 (a) shows the capital cost of Claus unit at various capacities, as reported in literature [109, 113, 115]. Based on these figure, the calculated scale factor for Claus unit is 0.88. Figure 5-1 (b) and (d) shows the capital cost of H_2S/CO_2 selexol removal units at different sizes reported in literature [109, 113]. The scale factor for selexol unit derived from the Figure 5-1 (b) and (d) is 0.89. This estimate is higher than that found in the literature. Hamelinck et al. considered it to be 0.7 [106]. Figure 5-1 (c) shows the capital cost of gasifier at different sizes [106, 113]. Based on Figure 5-1 (c) the estimated scale factor for slurry phase reactor is 0.77. The scale factor reported is 0.65-0.7 [105, 106, 121].

(a) Claus unit

$y = 55.687x^{0.881}$

Larson et al., 2005

Shuster and Goellner, 2013

Literature

Best fit

Kruetz et al., 2008

million C$

tonne/day

81   234.96   240

(b) Selexol/CO_2 removal

$y = 81.53x^{0.8943}$

Larson et al., 2005

Shuster and Goellner, 2013

Literature

Best fit

Kruetz et al., 2008

million C$

tonne/day

33.6   83   85

(c) Gasifier

$y = 14.927x^{0.7786}$

Larson et al., 2005

Kruetz et al., 2008

Shuster and Goellner, 2013

Kruetz et al., 2008

Literature

Best fit

million C$

tonne/hr

1   2   3   4   5

(d) Selexol/CO₂ removal
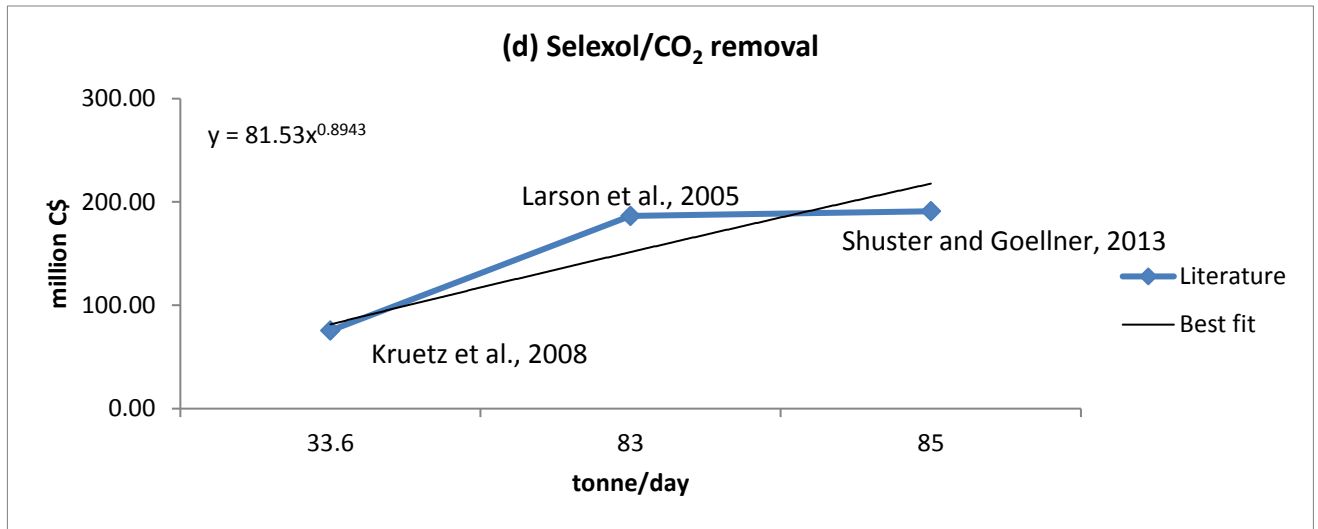
$y = 81.53x^{0.8943}$

Figure 5-1: Scale factors for key components of a CTL plant

Table 5-1: Calculated scale factors for key equipment indirect CTL

Unit operation	Calculated scaling factor	References needed for calculation
Air separation unit	0.51	[109, 113, 117, 118]
O₂ compressor	0.76	[114]
FT- slurry phase reactor	0.82	[25, 77, 115]
Hydrotreater	0.72	[115, 116]
Storage tank	0.50	[110, 115]
Gasifier	0.77	[25, 109, 122]
Selexol/H₂S removal	0.89	[25, 109, 122]
Selexol/CO₂ removal	0.88	[25, 109, 122]
Clause unit	0.88	[25, 109, 122]

Figure 5-2 shows how the unit capital cost of the whole plant changes with capacity. The scale factor for the entire plant is estimated to be 0.65. The capital cost of the CTL plant per unit of output decreases with increase in capacity due to economy of scale. For plant capacity higher than 20,000 bbl/day, the change in unit capital cost is not significant.

The capital investment cost for a basic indirect coal liquefaction plant with a 50,000 barrel/day capacity estimated to be C$7.4 billion. The coal available as the feedstock is priced at C$10 per tonne. The plant cost is the sum of the amortized total equipment cost and the operation and maintenance costs. The total amortized investment is calculated to be C$ 987 million. The cost distribution of different process units in the indirect CTL plant is shown in Figure 5-3. The gasification unit, including the gasifier and the air separation unit, is the most cost-intensive equipment of a CTL plant with 23% of the total capital equipment. The next major components include gas clean-up unit and FT reactor 24% and 23% respectively. ASU unit is 18% of the total capital cost. The cost of storage is negligible compared to other costs. Figure 5-4 shows the yearly operation costs. The operating cost accounted for feedstock, labor, water, electricity, maintenance, and catalysts are 7%, 7%, 5%, 4%, 2% and 0.05% respectively. The capital cost accounted for 75% of the total production cost of the CTL plant. It shows that the CTL plant is cost-intensive (see Table 5-2). Coal and labour cost each is attained the 7% of the plant cost. The total cobalt catalyst consumption is 226,251 kg and a daily consumption of 123 kg [20].
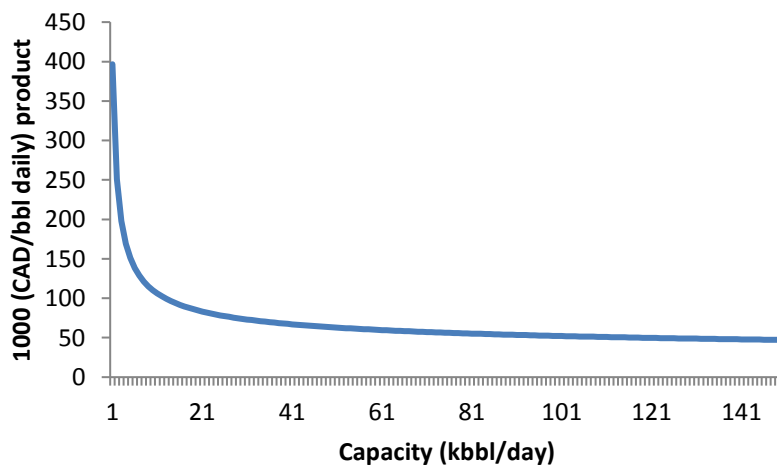

Figure 5-2: CTL plant capital cost versus daily product cost

59

Figure 5-2 shows the total production cost versus capacity of the CTL plant. The X-axis demonstrates the plant capacity ranging from 10,000 to 100,000 bbl/day. Figure 5-3 indicates that production cost decreases by increasing the capacity. Beyond the capacity of 50,000 bbl/day, variation in the cost of production is low due to low economy of scale benefits.
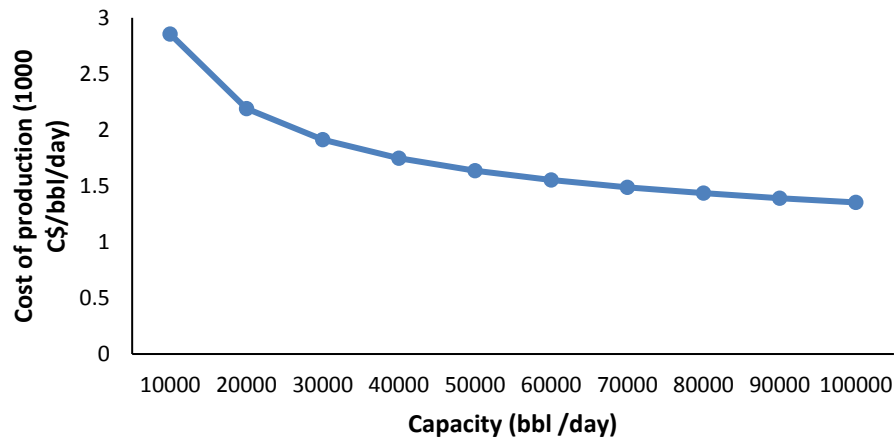
Figure 5-3: CTL plant production cost versus capacity

Table 5-2: The CTL plant equipment cost and size

Process equipment	Base case capacity	Base case cost (million C$)
Gasifier	14,573 (kg/hr feed gas)	717.9
Air separation unit	769,592 (kg/hr pure O_2)	392.9
O_2 compressor	50,872 (KW)	69.3
Slurry phase reactor	1,118,843 (kg/hr feed)	604
Wax hydrotreater	1,461 (tonne/hr)	133.8
Distillate hydrotreater	47 (tonne/hr)	47
Naphtha hydrotreater	46 (tonne/hr)	17
Selexol/H_2S removal	23,142 (kg/hr pure H_2S)	177.3
CO_2 removal	612 (tonne/hr)	248.2
Clause unit	23,142 kg/hr	118.2
Naphtha storage tank	27,819 (bbl/day)	0.97
Diesel storage tank	22,173 (bbl/day)	1,1.5

60

Figure 5-4: Capital cost distribution of the CTL plant for different unit operations

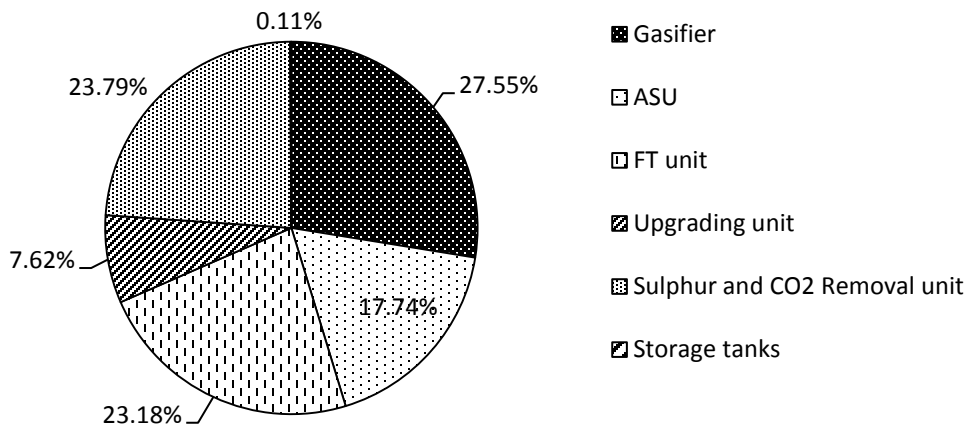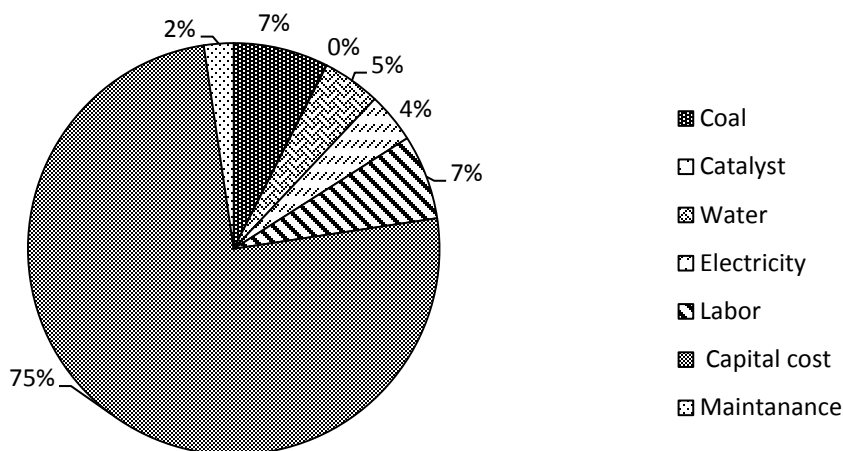*Figure 5-5: CTL plant operation cost distribution*

5.1.1. CTL plant with CCS unit

Carbon capture and sequestration (CCS) is a key pathway to mitigate high CO_2 levels. CTL plants are a suitable choice for CCS implementation. In CCS, CO_2 is separated from the gas stream using amine as solvent before the CO_2 passes into the F-T reactor. Adding a CO_2 compression unit to the plant is the only requirement for CCS [30, 32]. The compression of CO_2 is carried out at high pressure ratio, thus, energy consumption due to electricity is high. The amount of electricity is required for compression ranges from 80 - 140 kWh per tonne of CO_2 compressed [16]. The estimated emission of CO_2 per day is found to be 29,233 tonne for the capacity of 50,000 bbl/day. In addition, the plant produces methane. The CO_2-eq per tonne of product is calculated to be 7.52.

The scale factor for the CCS unit is estimated to be 0.6. Using this value, the capital and production cost of the CTL plant with CCS are estimated to be 8.4 billion Canadian dollars and 67.54 cent/liter respectively. The addition of CCS increases the capital cost and production by $1.0 billion dollars and 10 cent/liter respectively. The inclusion of the CCS and sulphur removal unit increases the

complexity and overall cost of the plant, they accounted for about 24% of the production cost. The production cost evaluated in this study for the CTL plant with and without CSS was compared against the value from Jaramillo and Rubin [16] which was C$61.67 and C$49.56 and, Mantripragada et al. [3] C$67.94 and C$ 62.7 respectively. The variations may be due to the differences in plant configuration, cost of coal and other operating costs.

5.1.2.Direct Coal liquefaction

By elimination of syngas production step from indirect coal liquefaction, direct coal liquefaction (DCL) process is determined. DCL is a hydrocracking process in which the coal is partially broken into smaller molecules under high hydrogen pressure and temperature. This operation is carried out in the presence of a solvent (CRC II) and catalyst(s) [123]. The partially detached smaller molecules remain mostly on aromatic molecules and therefore need further upgrading to convert to final products. The process flow diagram is shown in Figure 5-5.
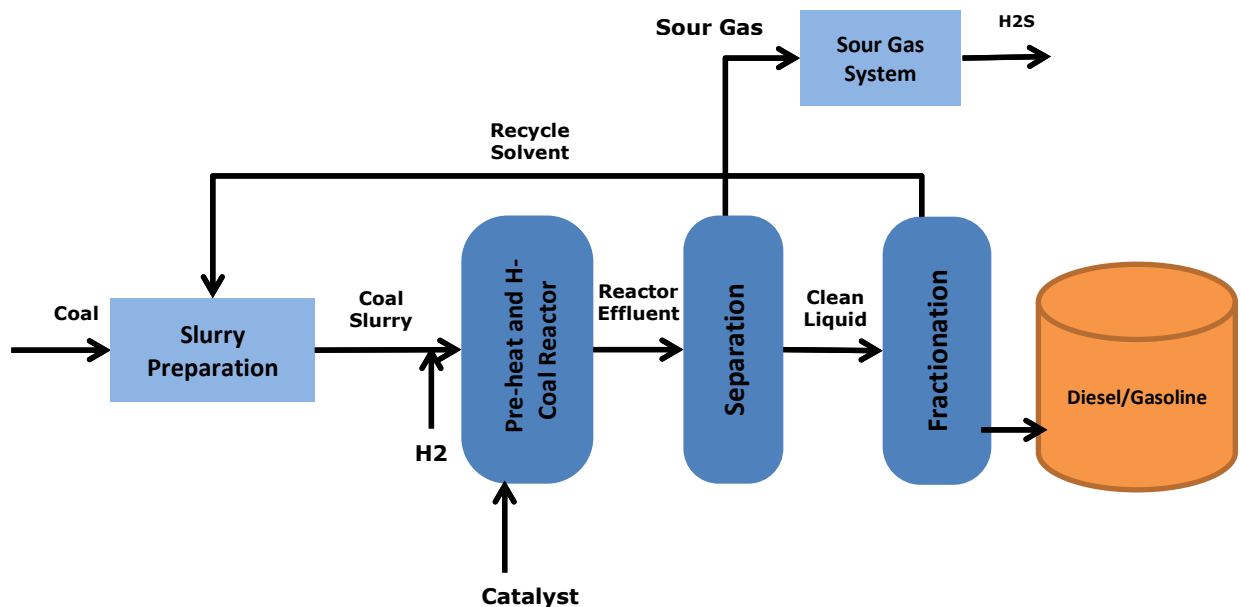
Figure 5-6: Schematic of the direct liquefaction plant

Due to the limited number of literature on the economic assessment of the DCL technology, it was difficult to compare the variations in the different cost data for each component of the plant. Table 5-3 shows the data obtained from a couple of literature [28, 124] for the economic model. Data are updated to 2014 for Canada and production cost is calculated by discounted cash flow analysis. Capital cost is 10.836 billion C$ while, production cost of the plant is calculated to be 63.50 cent/lit. Location factor for Canada and coal price are considered.

Table 5-3: Inputs and assumptions for the base DCL plant

Plant Capacity, bbl/day	50,000
Coal Feed tonne/day	26,370
Coal Cost $/tonne	10

Chapter 6.   Sensitivity analysis and uncertainty analysis[5]

6.1.   Sensitivity analysis

The sensitivity analysis was conducted to investigate the effect of variability in the key operating cost parameters. The probability distributions and ranges of the parameters of the model corresponding to the GTL and CTL are presented in Table 6-1. The Monte Carlo simulation technique is used to conduct the sensitivity analysis. That is implemented using the ModelRisk

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[5] A version of this chapter has been submitted as Mohajerani, S., Kumar, A., Oni A. A techno-economic assessment of gas-to-liquid and coal-to-liquid plants through development of scale factors, *Energy*, 2016.

software for the GTL and CTL plant costs. The Monte Carlo method is an algorithm which uses repeated random samplings to obtain the results [125-127]. It is a widely used concept for probability distributions [128, 129].

The results of the sensitivity analysis for the GTL and CTL plants generated by ModelRisk are depicted in Figures 6-1 and 6-2 respectively. The figures examine the impact of the cost parameters on the production cost. It is observed that the cost of natural gas and capital investment accounted for 42% and 75% of the total production cost of the GTL and CTL respectively. The correlation rank in the x-axis of the plot, ranging between -1 to +1, indicates negative and positive correlations respectively. As illustrated in the Figures 6-1 and 6-2, the most effective variable on the product cost of the GTL and CTL are the natural gas and the capital cost respectively. Although, these figures did not demonstrate how much the final product changes these cost variables, further illustration is shown in Figures 6-3 and Figure 6-4. Figures 6-3 shows the relationship between natural gas price and final product cost of the GTL plant. It can be seen that the cost of the GTL product is sensitive to natural gas cost. A variation of about ±30% of natural gas cost changes the product cost from 64 to 84 cent/lit. Similarly, for the CTL plant, Figure 6-4 shows that product cost is less sensitive to electricity price, coal price, and water price, and more sensitive to capital cost. A variation of about ±20% of capital cost changes the product cost from 48 to 67 cent/lit.

Table 6-1: Assumed range of variation in selected cost parameters

Process	Parameters	Base case	Distribution
GTL	Capital cost (million C$)	575	Triangular (5.0×10^8, base case, 6.50×10^8)
	Electricity price (cent/kWh)	10.345	Triangular (8.276, base case, 12.414)
	Natural gas price (C$/GJ)	4.89	Triangular (0.5, base case, 8)
	Water Price (C$/m³)	2.0705	Triangular (1.65, base case, 2.48)

CTL	Capital cost (million C$)	987	Triangular (7.9×10^8, base case, 11.8×10^8)
	Electricity price (cent/kWh)	10.345	Triangular (8.276, base case, 12.414)
	Coal price (C$/tonne)	10	Triangular (7, base case, 13)
	Water Price (C$/m^3)	2.0705	Triangular (1.65, base case, 2.48)

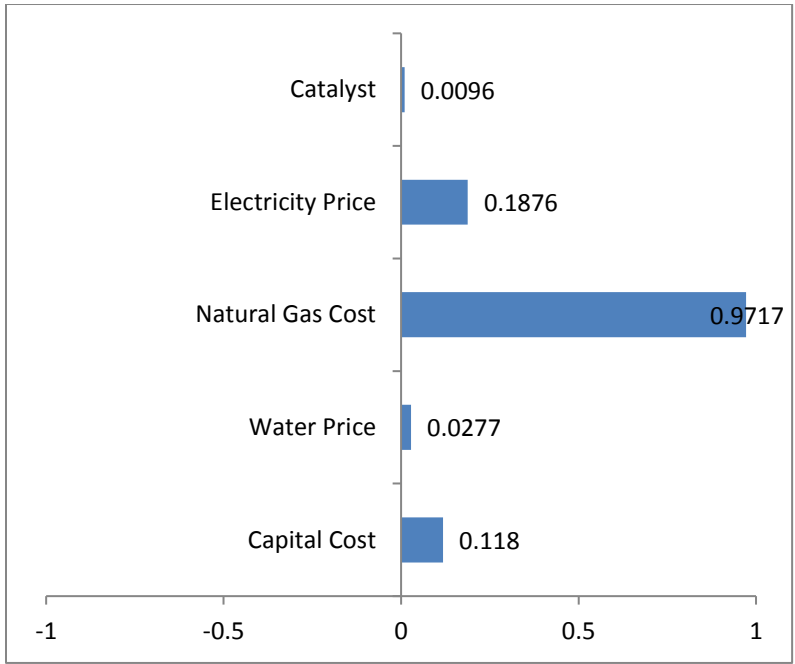*Figure 6-1: Tornado plots of GTL plant-Sensitivity of product cost to capital cost and operating cost using ModelRisk software*
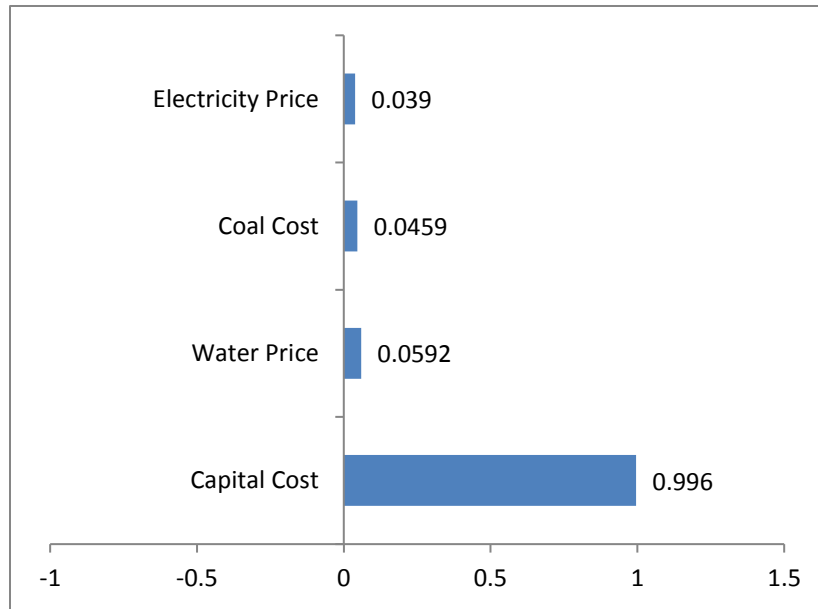
Figure 6-2: Tornado plot of CTL plant- Sensitivity of product cost to capital cost of the GTL plant using ModelRisk software
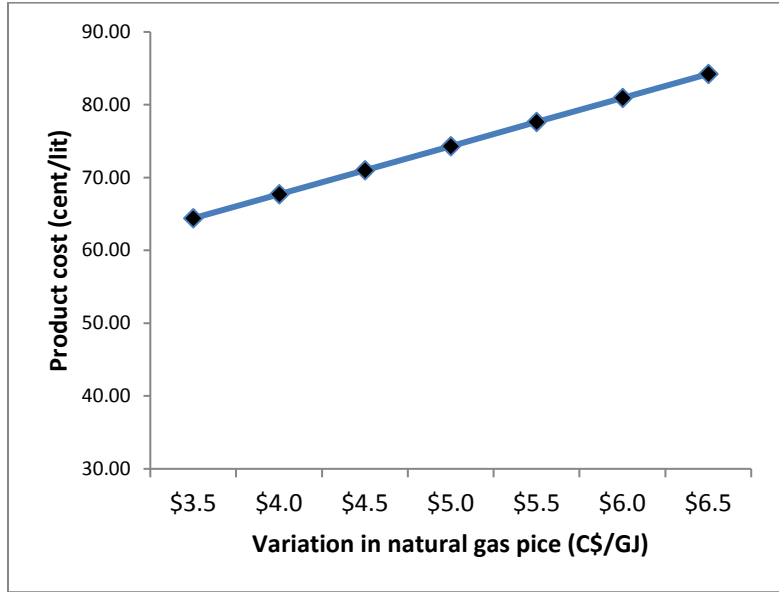
Figure 6-3: Sensitivity of product cost (cent/lit) of the GTL plant to natural gas price
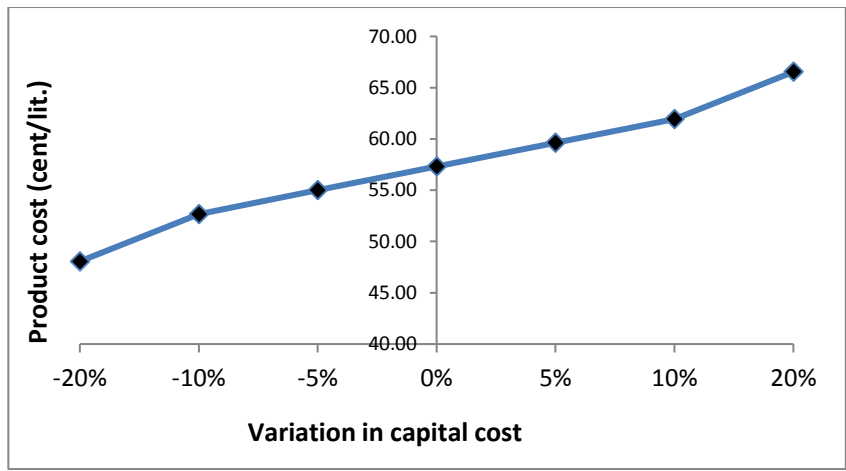
Figure 6-4: Sensitivity of product cost (cent/lit)of the CTL plant to capital cost

6.2. Uncertainty analysis

Uncertainty analysis is performed with the purpose of describing the range of possible outcomes if all the parameters change altogether. The findings of the techno-economic model and sensitivity analysis show that the cost of some parameters including the electricity price, feedstock cost, capital cost, water and catalyst expenses are the major contributor to final product cost of both GTL and CTL model. Therefore, an uncertainty analysis was conducted to assess the impact of these variables on final product cost of both GTL and CTL plant. Figure 6-5 demonstrates that with 90% probability final product cost will change between 75 to 120 C$/bbl if all the main parameters changed altogether. Figure 6-6 shows that with considering variation in the key parameters of the CTL plant possible outcome will be between 50 to 65 C$/bbl.

Figure 6-5: Ascending cumulative plot for production cost (C$/bbl) of the GTL plant

Figure 6-6: Ascending cumulative plot for production cost (C$/bbl) of the CTL plant

Chapter 7.   Conclusions and future works

7.1.   Conclusions

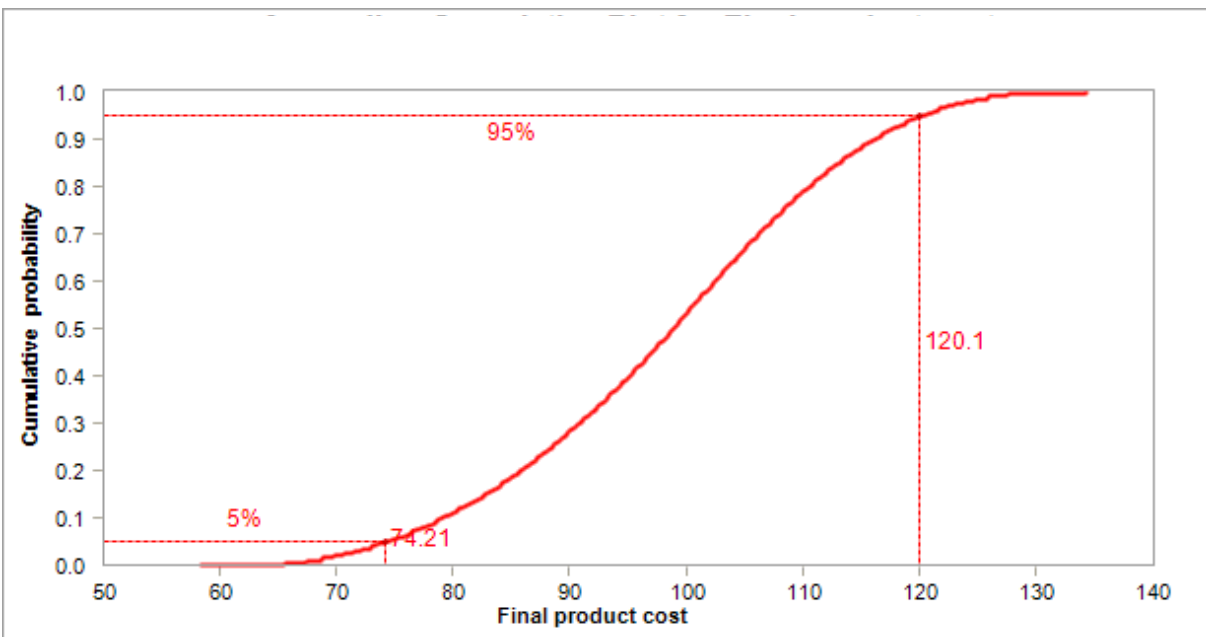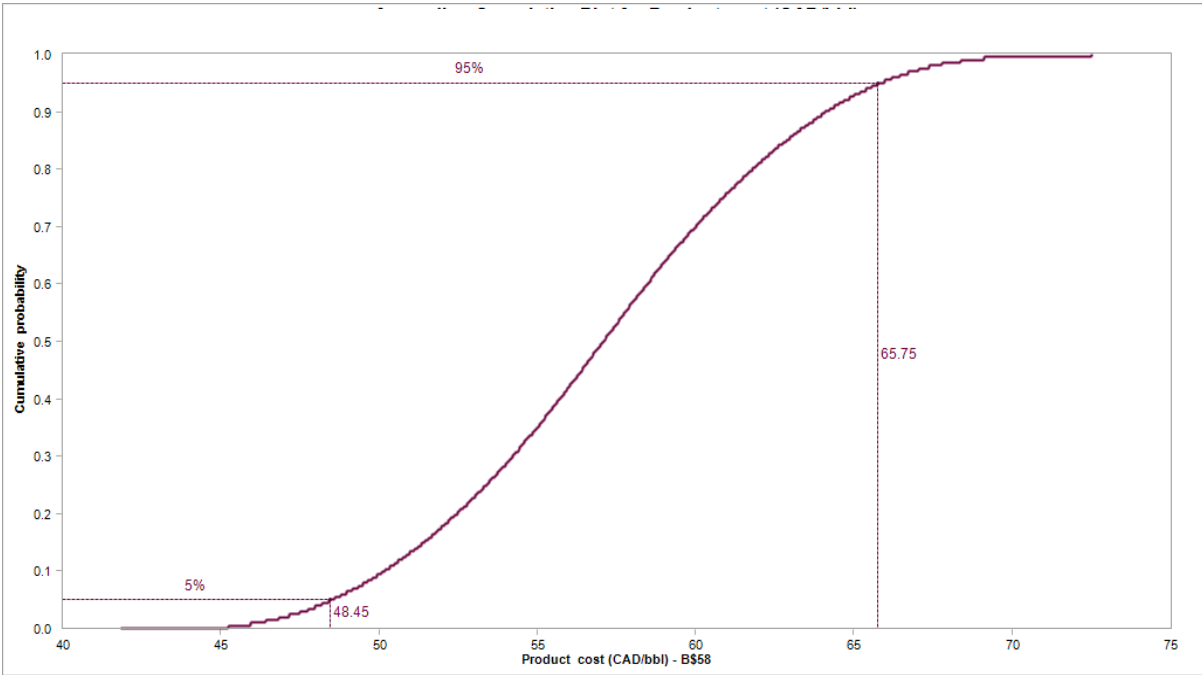The main objective of this work is to develop a data intensive techno-economic model for the assessment of GTL and CTL pathways for Canada. The aim was to estimate capital cost and production cost of liquefaction plants, which could provide useful information for decision makers on regulation policies. Scale factors for the key equipment of these plants are developed to estimate capital cost of liquefaction processes. In addition, the production cost for the liquid fuel from the GTL and CTL are evaluated. It was shown that capital cost of the GTL and CTL plant per unit of output decreases with increase in capacity due to economy of scale. For plant capacity higher than 20,000 bbl/day, the change in unit capital cost is not significant for both plants. This implies that the search for optimum capacity which provides a favourable price equivalent to the conventional oil price can be obtained. In this model, a conceptual plant design along with cost estimation was developed for a Fischer-Tropsch GTL and CTL plant with 50,000 bbl/day capacity. The capital cost of the GTL and CTL plant is estimated at 4.3 and 7.4 billion dollars respectively while, the production cost is 73.59 and 57.30 cent/lit respectively. The sensitivity analysis was performed to investigate the effects of changes in critical input parameters of the techno-economic model. Sensitivity analysis showed natural gas price had major effect on the cost per unit of GTL product. Also, production cost of the CTL plant is most sensitive to the capital cost.

Furthermore, this dissertation reviewed different technologies for GTL and CTL, and made deductions based on the liquefaction mechanism, characteristics, and technology readiness level. In addition, to understand the trend and variations of GHG emissions from the CTL and GTL processes, reports on the life cycle assessment were reviewed. The deductions from various reports

showed that the production of liquid fuels from the CTL is more emissions intensive when compared with the GTL and conventional process. However, the addition of the CCS to the GTL and CTL units reduces CO_2 emissions. These processes can be considered an alternative for producing fuel in Canada due to the abundances of their feedstocks in its reservoirs and other benefits. However, economic profits can be achieved in higher capacities due to the economy of scale. In addition, reducing the dependency on conventional crude oils is a strong motivation to develop new technologies to produce alternative fuels. Therefore, evaluating the GHG emissions of a new process is a critical factor due to associated environmental issues.

7.1.1. *Recommendations for future studies*

The research carried out in this study is comprehensive, further improvements in the techno-economic model can be made. Recommendations are presented below:

1. *Liquefaction plant process simulation:* The liquefaction process is highly dynamic with changes in natural gas and coal composition, pressure and temperature profiles, etc. Moreover, as found in the current study, the syngas unit and the gasification unit contribute to the majority of the costs incurred in the liquefaction of natural gas and coal respectively. Therefore, it is imperative to develop a process simulation model using simulation software such as Aspen Plus or HYSYS for a better command on the liquefaction process and to optimize it.

2. *Direct coal liquefaction plant simulation:* due to lack of data on direct liquefaction, it is vital to develop a process simulation model using Aspen Plus or HYSYS.

3. *Co-generation and co-products:* In this study, it is assumed either GTL or CTL plant produced only liquid fuels as final products. But, different configurations can be considered

as a future study. For example, adding a power plant unit decreases the energy intensity and it is a way to save energy in addition, electricity generation would pay off a portion of the operating cost. The current scope of economic assessment model for the estimation of liquefaction involved only diesel, gasoline and, naphtha as products produced during natural gas and coal processing. However, there are other products such as natural gas liquids that are co-produced during the gas and coal processing. An economic assessment of these co-products can be useful in evaluating their competitiveness with other conventional pathways. Consequently, the presented model can be modified to estimate the production cost of various GTL and CTL plant configuration.

4. *Hybrid liquefaction techno-economic assessment:* different sources of energy can be mixed with natural gas and coal as the feedstock for GTL and CTL plant. Biomass is one of the options for mixing with natural gas and coal. Therefore, CBTL (coal and biomass to liquid) or CBGTL (coal, biomass and natural gas to liquid) plants have to be studied more.

5. *Detailed life cycle assessment (LCA) analysis:* To calculate the cost of CO_2 mitigation and investigate the GHG emission of the CTL and GTL plant, a complete life cycle assessment analysis must be done and the results should be compared with cost of mitigation of conventional and unconventional fuels. Future studies should consider how the environmental loads can be reduced through energy saving technology such as heat integration and CCS. As a developed-conversion process, the installation of CCS unit will reduce the overall GHG emissions.

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