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Process Simulation, Economic and Environmental Sustainability Assessment of a Gas-To-Liquids Process

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Abstract

Natural gas is recognized as one of the cleanest and most abundant fossil fuels. In the past decades, the price ratio of crude oil to natural gas has continuously fluctuated. The gas-to-liquid industry has received continuous interest due to the abundant supply of conventional and unconventional natural gas (shale gas, etc.), as well as the environmental advantages of FT technology. The GTL process chemically converts natural gas to long chain hydrocarbons (naphtha, diesel, wax, etc.) through three main steps, i.e., natural gas reforming, Fischer-Tropsch synthesis (FTS), and products upgrading. In this work, a rigorous simulation model including gas sweetening, syngas production, FTS, and product fractionation is provided. Among different routes for natural gas reforming and different reactors for FTS in a GTL process, autothermal reforming (ATR) and slurry bubble column reactor (SBCR) were chosen respectively, due to their advantages over other solutions. Meanwhile, the economic and environmental analyses were also conducted for the sustainability assessment of provided GTL process using Aspen Icarus and WAR software.

Keywords: Natural gas; GTL process; FT technology; Sustainability; Process simulation

Introduction

Natural gas is recognized as one of the cleanest and most abundant fossil fuels. The price ratio of crude oil to natural gas has continuously [1,2] fluctuated in the past decade as shown in Figure 1. Due to the abundant supply of conventional and unconventional natural gas (shale gas etc.), the gas-to-liquid industry has received continuous interest. Furthermore, the continuous development of shale gas has made the flare problem an increasingly serious, worldwide issue. GTL processes will open up new resources, such as capturing gases and making profit, while minimizing flare problems. The GTL process converts natural gas to longer-chain hydrocarbons (naphtha, diesel, wax, etc.). These conversions take place through reforming of natural gas to syngas and Fischer-Tropsch (FT) synthesis of syngas to higher hydrocarbon products, i.e., long-chain hydrocarbon molecules.

GTL provides a good method of utilizing many "stranded gas resources", which are located too far from potential markets for economically feasible transportation. There are also environmental advantages for using FT-based GTL technology. Compared to conventional fuels derived from crude oil, FT fuels contain low concentrations of sulfur compounds, NO_x, and aromatics. These properties, along with a high cetane number (approximately 70) result in superior combustion characteristics for the FT diesel fuel. As the market normally requires a cetane number of at least 45, the FT diesel can be used in both areas where there are very tight constraints on diesel quality and as a blending stock to upgrade lower quality diesel fuels [3]. Additionally, GTL technology can also help suitable countries achieve a more secure energy supply.

Several GTL plants are operated or under construction in places like South Africa, Nigeria, Qatar, United States, etc. In addition to the 14,500 bbl/day GTL plants in Malaysia, which began operation in 1993, Shell has also built a world scale GTL plant (Pearl GTL plant) with a capacity of 140,000 bbl/day in Qatar, which started production in 2011. In addition to its plants in South Africa, Nigeria, and Qatar, Sasol announced a new GTL plant in the United Sates with a capacity of 96,000 bbl/day and began construction in 2013. Furthermore, several GTL plants have been under construction since 2015 worldwide. In addition to the large-scale plants in South Africa and Uzbekistan, multiple companies have been investing in small scale GTL plants in Russia and US to convert natural gas resources instead of flaring [4].

Another hotspot of GTL process is modular design of small-scale GTL plant. Much of the remaining natural gas resource is in the form of associated or stranded gas which is hard to monetize due to its low volume and lack of supporting infrastructure. Modular GTL plant provides a way to take advantage of this potentially abundant energy resource economically and in an environmentally responsible way. Essentially, these technologies involve pre-manufacturing unit which is compact and can be shipped to site of interest and easy to assemble and dis-assemble. These technologies are currently in the early stages of commercialization by several companies, such as Compact GTL, Verdis Fuels and Velocys [5].

A GTL process mainly comprises of three steps, as shown in Figure 2, which are the reforming of natural gas to syngas, Fischer-Tropsch reaction of syngas to hydrocarbons (also called syncrude), and upgrading of syncrude by fractionation, hydro-treating, hydro-cracking, and hydroisomerization to yield products that meet the petroleum product market's specifications.

Acid Gas Removal and Syngas Production Modeling

If the sour gas content is high, the first step of a GTL process will be an acid gas removal unit, where CO_2 and H_2S are removed, as

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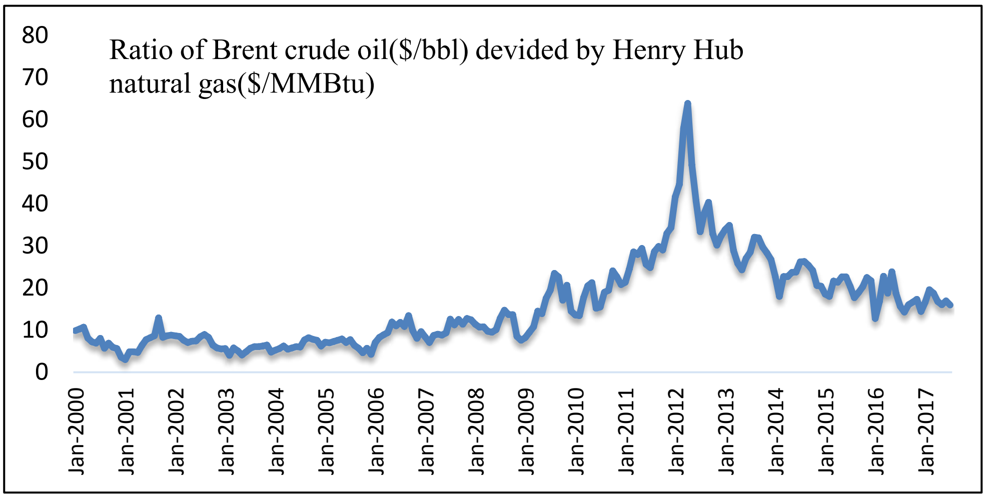

Figure 1: Price ratio of crude oil to natural gas during Jan 2000-Jul 2018.

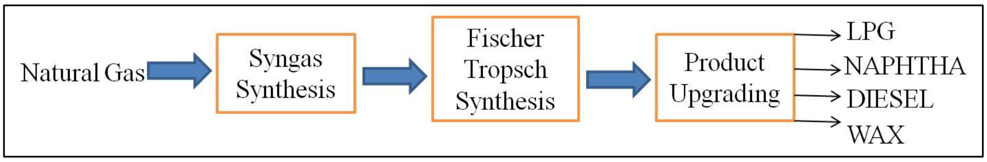

Figure 2: Schematic Diagram for a General GTL Process.

sulfur compounds will poison the active sites of catalyst used in the subsequent process. They must be removed before the feedstock is sent to the subsequent process steps. Moreover, acid gas removal is necessary to meet the pipeline requirements and for the protection of equipment from corrosion. Many processes have been developed and are commercially available to remove acid impurities. Amine gas treating refers to a group of processes that utilize aqueous solutions of various amines to remove hydrogen sulfide and carbon dioxide from gases.

This work reports an Aspen Plus rate-based model using DEA (Diethanolamine) to remove acid gas from a natural gas mixture of 92.4 mol% CH_4, 3.6 mol% C_2H_6, 1.6 mol% C_3H_8, 1 mol% N_2, 1.3 mol% CO_2 and 0.1 mol% H_2S. The flowsheet for syngas production including acid gas removal is shown in Figure 3. Natural gas feedstock enters at the bottom of the absorber, at a temperature of 22°C and pressure of 63 bar. The lean solvent amine solution with 30 wt% DEA flows from the top of absorber at 39°C and 63 bar. CH_4, C_2H_6, C_3H_8, N_2, CO_2, and H_2S are treated as Henry-components.

The Electrolyte NRTL method and RK equation of state are used to compute the liquid and vapor properties in the amine gas treating section respectively [5]. This rigorous simulation includes electrolyte thermodynamics, solution chemistry, and reaction kinetics for the liquid phase reactions and rate-based multi-stage distillation. The key simulation results are presented in Table 1. Sweetened natural gas leaves from the top of the absorber to the reforming section to produce syngas, and the removed acid gas leaves the top of the stripper for further treatment before emission, which is not included in this study.

There are many different reforming routes to produce syngas from natural gas, such as catalytic steam methane reforming (SMR), autothermal reforming (ATR), non-catalytic partial oxidation (POX), catalytic partial oxidation (CPOX), and heat exchange reforming (HER). The manner in which syngas is produced can be influenced by, and in turn can profoundly impact many factors of the overall GTL process design, factors such as the plant size and location, syngas composition and its associated effects on FT synthesis, yields, etc.

Among the different syngas production technologies for natural gas feedstock, much of the forward-looking considerations have focused on ATR, one of the most attractive and economical technologies to date. This is, in part, due to the desired H_2/CO ratio (approximately 2) obtained from ATR for FT synthesis. However, this also reflects other attributes of ATR, such as relative compactness, lower capital cost, and greater potential for economies of scale, which significantly contribute to the economic viability of GTL plants [6]. There are several commercial and demonstration applications of ATR technologies in Qatar, South Africa, and Nigeria, which have been developed by Sasol, Exxon, Haldor Topsøe, etc. The Oryx plant in Qatar, with a production capacity of 34000 bbl/day liquid fuels, uses ATR technology for syngas production and a cobalt-based slurry bubble column reactor for low temperature FT synthesis [7].

The Peng Robinson equation of state with the Boston-Mathias modification was used as the property method for the physical property calculations in the syngas production section. To avoid the potential problem of ATR working as a steam cracker, which produces olefins from higher hydrocarbons in the feed, a pre-reformer is introduced. The removal of higher hydrocarbons also allows a higher preheat temperature to the ATR, which results in reduced oxygen consumption [8].

As shown in Figure 3, the sweet gas leaves the top of absorber

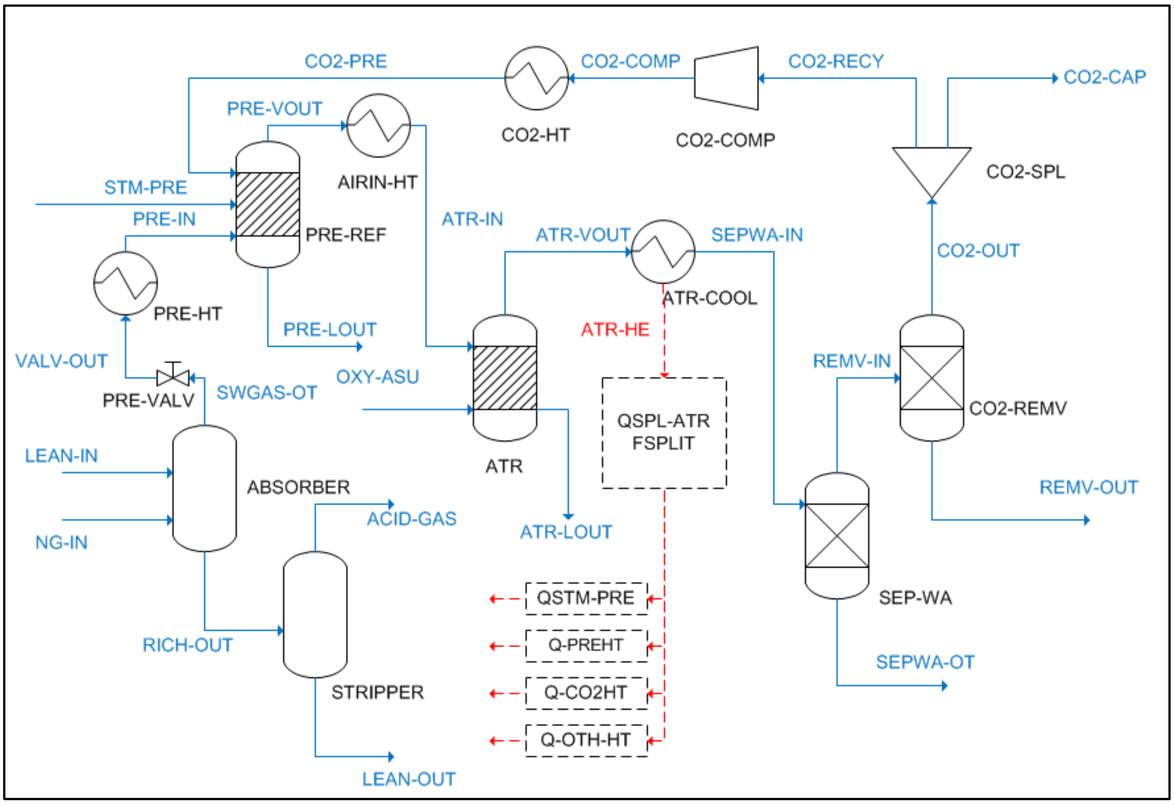

Figure 3: Simulation Flowsheet for Syngas Production.

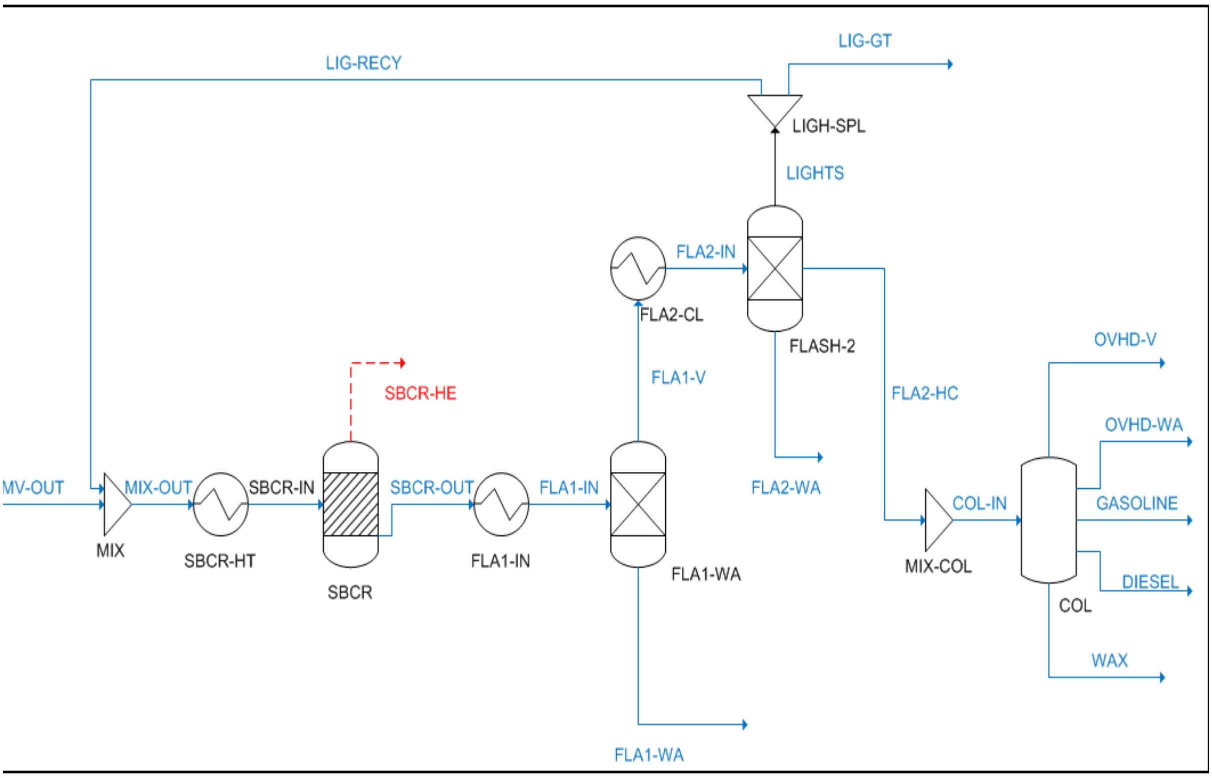

Figure 4: Simulation Flowsheet for Low Temperature FT Synthesis.

column at a temperature of 45°C and pressure of 63 bar. After reducing the pressure to 30 bar through a valve and preheating the temperature to 455°C by a heat exchanger, the sweet gas enters the pre-reformer with the steam and recycled CO_2 streams (both at 455°C and 30 bar). The pre-reformer is an adiabatic, fixed-bed reactor loaded with highly active nickel catalysts. It is assumed that all the hydrocarbons heavier than methane are converted to CO and H_2. In addition, the Steam Methane Reforming (SMR) and Water Gas Shift (WGS) reactions are also present and assumed to be in equilibrium [9]. Based on the feed composition in this study, all of the reactions occur in the pre-reformer are listed below.

Complete conversion (endothermic):

$$C_2H_6+2H_2O\rightarrow 2CO+5H_2 \quad \Delta H°=350 \text{ kJ/mol} \qquad (1)$$

$$C_3H_8+3H_2O\rightarrow 3CO+7H_2 \quad \Delta H°=500 \text{ kJ/mol} \qquad (2)$$

Equilibrium reactions (exothermic):

$$CO+3H_2\leftrightarrow CH_4+H_2O \quad \Delta H°=-210 \text{ kJ/mol} \qquad (3)$$

$$CO+H_2O\leftrightarrow CO_2+H_2 \quad \Delta H°=-41.2 \text{ kJ/mol} \qquad (4)$$

The pre-reformer is modeled as an adiabatic reactor. Despite the exothermic equilibrium reactions, the overall reactions are endothermic. In this simulation, all the feed streams enter at 455°C and the outlet stream leaves at approximately 430°C. A heater is used to increase the outlet stream temperature to 655°C in this work. The oxygen stream from cryogenic air separation unit (ASU) section is blown to the burner of the ATR reactor at a temperature of 200°C.

The key part of the syngas unit is the autothermal reformer which converts the methane into syngas by reacting with steam and oxygen. The ATR is modeled as an adiabatic equilibrium reactor according to the following reactions [9].

Partial oxidation of Methane (exothermic)

$$CH_4+3/2O_2\leftrightarrow CO+2H_2O \quad \Delta H°=-520 \text{ kJ/mol} \qquad (5)$$

Steam methane reforming (endothermic)

$$CH_4+H_2O\leftrightarrow CO+3H_2 \quad \Delta H°=210 \text{ kJ/mol} \qquad (6)$$

Water gas shift reaction (exothermic)

$$CO+H_2O\leftrightarrow CO_2+H_2 \quad \Delta H°=-41.2 \text{ kJ/mol} \qquad (7)$$

The low steam-to-carbon (H_2O/C) ratio is desired for ATR. In this work, a low steam-to-carbon (H_2O/C) ratio of 0.6 and oxygen-to-carbon (O_2/C) ratio of 0.53 is adopted for the base case ATR simulation [9]. Due to the large amount of heat released by the partial oxidation reaction, the overall reaction of ATR is exothermic and the hot syngas leaves the reactor at 1013°C in this simulation. The hot syngas is cooled to ambient temperature for the removal of water and CO_2. Since the subsequent FT synthesis also produces a huge amount of water, there is no strict limitation on the water composition in the cooled syngas. The removal of water can reduce the flow and water partial pressure to the FT reaction.

Due to the water gas shift (WGS) reaction in the natural gas reforming step, a significant amount of CO_2 is also produced and present in the exit gas leaving the reformers. CO_2 removal is required by the downstream FT synthesis. The membrane for CO_2 removal is modeled as a component separator. Part of the removed CO_2-rich stream is recycled back to the pre-reformer to achieve the desired H_2/CO ratio of 2 for FT synthesis. The recycle of CO_2 can suppress the WGS reaction and increase the carbon efficiency of the entire process. This also reduces CO_2 emission. By careful adjustment of the amount of CO_2 recycle, a syngas with a H_2/CO ratio of 2.077 is achieved in this simulation. Table 2 shows the key simulation result of the produced syngas stream.

From Figure 3, it can be seen that there are huge amounts of heat released for cooling the hot syngas from ATR. In addition to the heat needed to preheat the natural gas stream, oxygen stream, recycled CO_2 stream, and to generate the required steam stream for ATR, shown in Table 3, there is still roughly 40% percent of extra heat, which can be used elsewhere, such as in medium pressure (MP) stream generation, compressor usage, etc.

Fischer Tropsch Synthesis Process Modeling

The Fischer-Tropsch reaction is highly exothermic. Thus, reactor design and process development has focused heavily on heat removal and temperature control. The main reaction can be expressed by the following equation [10]:

$$nCO+2n\ H_2\leftrightarrow -(CH_2)n-+nH_2O \quad \Delta H°=-167 \text{ kJ/mol/CO} \qquad (8)$$

Where n is an integer. The FT process conditions are usually chosen to maximize the formation of longer chain hydrocarbon liquid fuels, which are higher value products. Depending on the types and quantities of FT products desired, either low temperature (200-240°C) or high temperature (300-350°C) synthesis can be used with either an iron or cobalt catalyst [3]. Low temperature FTS favors the yield of high molecular weight waxes with long linear carbon chains. While high temperature FTS favors the production of gasoline and low molecular weight olefins.

Anderson-Schulz-Flory (ASF) product distribution is often used to describe the product distribution of the Fischer-Tropsch Synthesis, as shown in the following equation,

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

Where n is carbon number and W_n is the mass fraction of the

Process Stream	CO_2 mole fraction	H_2S mole fraction
NG-IN	0.013	0.001
SWGAS-OT	234 PPM	413 PPB
ACID-GAS	0.894	0.07

Table 1: Key simulation results of acid gas removal.

Temperature (°C)	40	
Pressure (bar)	20	
	Mole Flow (kmol/hr)	Mole Fraction
H_2	5665	0.648
CO	2731	0.312
CH_4	181	0.021
CO_2	104	0.012
H_2O	33	0.004

Table 2: Key simulation results of the produced syngas stream.

Total Heat Generation (Gcal/hr)	104
Natural Gas Preheat (Gcal/hr)	15.2
Reformer Steam Generation (Gcal/hr)	26
Oxygen Preheat (Gcal/hr)	20
Recycle CO_2 Preheat (Gcal/hr)	1.3
Available Heat for Other Use (Gcal/hr)	41.5

Table 3: Heat Load Calculation for ATR Process.

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species with carbon number *n*. *α* is the chain growth probability, a parameter independent from hydrocarbon chain length. In this work, a slurry bubble column reactor (SBCR) with cobalt catalyst is simulated for the low temperature Fischer-Tropsch Synthesis with a chain growth probability α of 0.85. The liquid slurry bed in SBCR has a high heat removal efficiency and offers better temperature control [11].

The kinetic expression derived by Yates and Satter field [11] for the SBCR, using $Co/MgO/SiO_2$ catalyst under the condition of 220-240°C, 0.5-1.5 Mpa, and H_2/CO feed ratio of 1.5-3.5, is adopted. The derived Langmuir-Hinshelwood-Hougen-Watson (LHHW) type kinetic equation is written in Eq. (10):

$$-R_{co} = \frac{aP_{co}P_{H_2}}{(1+bP_{co})^2}\,Kmol/(\text{kg}_{\text{catalyst}}.\text{s}) \tag{10}$$

Where *a* and *b* are assumed to be temperature dependent constants, *a* being the kinetic parameter and *b* the adsorption coefficient.

$$a = 8.037\times10^{-12}\,e^{-37369/8.31/T}\ Kmol/(\text{kg}_{\text{catalyst}}.\text{s}.\text{Pa}^2) \tag{11}$$

$$b = 1.243\times10^{-12}\,e^{-68478/8.31/T}\ 1/Pa \tag{12}$$

The constants in Eq. (11) and (12) are estimated using data from Yates and Satterfield [12]. Temperature in the equations are in units of Kelvin.

The selectivity factor, *γ*, which is the olefin to paraffin ratio of hydrocarbons [13] with the same carbon atom number *n*, is predicted by the following Eq. (13).

$$\gamma = \frac{O_n}{P_n}\alpha\,e^{-0.25\times n}\,,for\ n>4 \tag{13}$$

Where, O_n and P_n are the molar fractions of olefin and paraffin hydrocarbons with *n* carbon atoms respectively.

For carbon numbers from 2 to 4, the C_2H_4/C_2H_6, C_3H_6/C_3H_8, C_4H_8/C_4H_{10} ratios are set to 0.05, 2, and 2 respectively based on literature [13,14].

All the other very small quantities of byproducts, like aldehydes, acids, are not considered in this simulation. Based on Ahon's work, the following equations can be derived [15]:

$$R_{CH4}=-(1-\alpha)^2R_{CO} \tag{14}$$

$$R_{CnH2n+2}=R_{CH4}\,\alpha^{(n-1)}/(1+\gamma) \tag{15}$$

$$R_{CnH2n}=R_{CH4}\,\alpha^{(n-1)})\,\gamma/(1+\gamma) \tag{16}$$

For olefin products, all olefin hydrocarbons from C_2 to C_{12} are simulated. For carbon atoms larger than 12, the olefin to paraffin ratio is less than 0.05 (mole ratio) and the olefin products can be omitted. For paraffin products, C_1 to C_{39} synthesis reactions are modeled, where hydrocarbons above $C_{30}H_{62}$ are modeled as hydrocarbon groups represented by a single component as follows: C_{31} - C_{33} as $C_{32}H_{66}$ and C_{34}-C_{39} as $C_{36}H_{74}$.

Figure 4 illustrates the process flow diagram for the simulated low temperature FT synthesis. The Peng Robinson equation of state with the Boston-Mathias modification was used as the main property method for the physical property calculations, with the exception of the rigorous distillation column calculations, in which the Grayson method was used. The syngas from the ATR section has a H_2/CO ratio of 2.077, mixed with the tail gas (containing unreacted CO, H_2 and several light hydrocarbons) has an overall H_2/CO ratio of 2.01. After preheating the feed temperature to 227°C at 20 bars, the feed stream feeds into the SBCR, which was modeled as a CSTR. A catalyst load of 245 kg catalysts/(m^3 reactor volume) was used for the simulation [12]. The FT is a highly exothermic reaction process and it was assumed that heat is removed quickly and efficiently. The two sequential three-phase separators are used to separate the huge amount of water generated together with the tail gas. A portion of the tail gas is recycled back to the SBCR to increase the conversion of FTS, while the remaining tail gas can be sent to gas turbine or furnace for the generation of electricity, or used as fuel feedstock. In this simulation, 65% of the tail gas is recycled back to the SBCR.

The raw hydrocarbon products are sent to an atmospheric distillation column for the fractionation of different hydrocarbon products. A three-phase condenser is used to separate water from the overhead vapor (LPG) and gasoline streams (C_5-C_{11}) at the top of the tower. A diesel product stream (C_{12}-C_{18}) is also drawn from the column with an initial boiling point of around 270°C. The wax product (C_{19}^{+}) at a temperature of 383°C is obtained at the bottom. The upgrading section is not included in this study. This study simulates a GTL plant with a capacity of 4,000 bbl/day (about 571 tonnes/day) liquid fuels. The wax product can be shipped to refineries for further cracking treatments to produce more diesel products.

Table 4 lists the mass fractions of the FT products exiting the SBCR. The SBCR has a volume of 2000 m^3, which is set to achieve a single pass CO conversion of 80%. By recycling 65% of the tail gas, the overall CO conversion can be increased to 85%, as shown in Table 4. Also, it can be observed that a large amount of water, around 30 wt%, is produced and thus must be removed by flash separation before the products go to the distillation column. Approximately 486 PPM of $C_{12}H_{24}$ is produced, indicating that olefins with carbon atoms larger than 13 can be omitted. Figure 5 compares the product distribution between the simulation results and ASF prediction. Aside from hydrocarbons of methane, ethane, and ethylene, the simulation results fit the ASF prediction very well for larger hydrocarbons.

The distillation column was designed with 30 sieve trays with a diameter of 2.36 meters. The column is operated at 1.5 bar for the top stage with no pressure drop. Table 5 shows the mass fraction of different hydrocarbon products obtained from the distillation column.

Economic Analysis

The economic analysis for a GTL plant with a 20 year lifetime was conducted. Table 6 shows the equipment cost estimated by Aspen Icarus software.

To make this economic analysis more precise and realistic, cost information of Shell's new GTL plant in Qatar, was considered. Based on Shell's data, the total capital cost of the plant was $18-19 billion with a product capacity of 260,000 bbl/day [16], the quivalent of $69,231~73,077 per daily barrel produced. In this work, a smaller plant with a capacity of 4,424 bbl/day products was studied. Therefore, a scaling factor was used to estimate the $74,910 per daily barrel products for the smaller GTL plant studied in this work. The total capital investment including the piping, instrumentation, labor, etc., was scaled to $331,403,100.

Tables 7 and 8 provide the price information of the utility and material respectively, mostly from the U.S. EIA (Energy Information Administration) and ICIS websites. All of the hydrocarbon products prices (LPG, gasoline, diesel, wax) in Table 8 were discounted based on the EIA information, since upgrading may be needed for sale to the market. A GTL plant consisting of ATR and FT processes is energy-intensive and releases a huge amount of heat, which can be integrated for the generation of MP (medium pressure) and HP (high pressure)

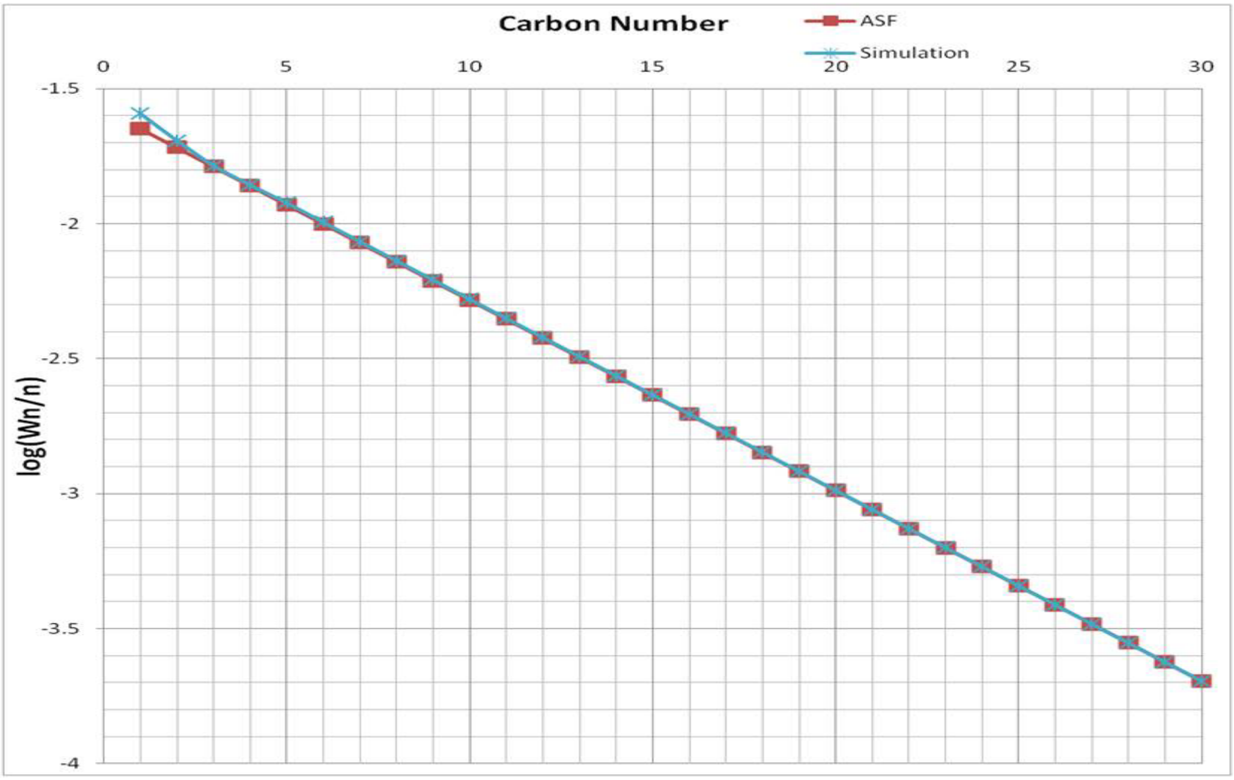

Figure 5: Comparison of Product Distribution.

Temp. (°C)	227	Pres. (bar)	20	Mass Flow (kg/hr)		145879	
Reactor Volume. (cu.m)		2000		CO conversion		85%	
Mass Fraction							
CO	0.22	C5	0.017	C11	0.011	C22	0.004
H_2	0.028	C6=	0.003	C12=	486 PPM	C23	0.003
CO_2	0.087	C6	0.014	C12	0.01	C24	0.003
H_2O	0.292	C7=	0.002	C13	0.01	C25	0.003
C1	0.073	C7	0.012	C14	0.009	C26	0.002
C2=	0.001	C8=	0.002	C15	0.008	C27	0.002
C2	0.024	C8	0.012	C16	0.007	C28	0.002
C3=	0.019	C9=	0.001	C17	0.006	C29	0.002
C3	0.01	C9	0.012	C18	0.006	C30	0.001
C4=	0.018	C10=	0.001	C19	0.005	C32	0.003
C4	0.009	C10	0.011	C20	0.005	C36	0.004
C5=	0.005	C11=	664 PPM	C21	0.004		

Table 4: Product Mass Fraction Out of the SBCR.

Product	Mass Flow (kg/hr)	Mass Percentage (%)
OVHD Vapor (LPG)	1599	5.7
Gasoline (C5-C11)	11891	42.6
Diesel (C12-C18)	9180	32.9
Wax (C19+)	5264	18.8

Table 5: Mass Fraction of Distillation Column Products.

Component Name	Component Type	Equipment Cost ($)
ABSORBER-tower	DTW TRAYED	381,400
ATR	DAT REACTOR	3,568,200
ATR-COOL	DHE FLOAT HEAD	101,400
CO_2-COMP	DGC CENTRIF	766,000
CO_2-HT	DHE FLOAT HEAD	16,900
CO_2-REMV	DVT CYLINDER	53,400
COL-tower	DTW TRAYED	301,500
COL-cond	DHE FIXED T S	26,300
COL-cond acc	DHT HORIZ DRUM	15,500
COL-reflux pump	DCP CENTRIF	5,400
COL-reb	DRB U TUBE	19,000
FLA1-CL	DHE FLOAT HEAD	49,600
FLA2-CL	DHE FLOAT HEAD	62,400
FLASH-1-flash vessel	DVT CYLINDER	41,800
FLASH-2-flash vessel	DVT CYLINDER	34,400
PRE-HT	DHE FLOAT HEAD	16,900
PRE-REF	DAT REACTOR	6,276,600
SBCR	DAT REACTOR	6,227,400
SBCR-HT	DHE FLOAT HEAD	66,500
SEP-WA-flash vessel	DVT CYLINDER	41,800
STRIPPER-tower	DTW TRAYED	299,400
STRIPPER-cond	DHE FIXED T S	20,400
STRIPPER-cond acc	DHT HORIZ DRUM	13,700
STRIPPER-reflux pump	DCP CENTRIF	4,200
STRIPPER-reb	DRB U TUBE	38,700
ATRIN-HT	EFU HEATER	1,045,500
Sum		19,494,300

Table 6: Equipment Costs Estimation for a GTL Plant.

Utility	Unit Price	Heating/Cooling Value
Water	$0.1/GJ	4.184 kJ/kg
Electricity	$0.067/kWh [1]	-

Table 7: Utility Price Information.

steams. The utility cost calculation is presented in Table 9, which shows that although the purchase of electricity and fuel was needed, in general, the plant could gain around $7 million/year by the generation of steams, which could be used in an industry complex.

NPV (Net Present Value) and IRR (Internal Rate of Return) were adopted for the economic analysis. NPV calculates the current worth of all the net earnings through future period. If the NPV value is negative in a particular period, then the proposed investment is not profitable. A positive NPV indicates a profitable investment. A zero value NPV, demonstrates a project without any loss or gain in profit. IRR is related to NPV in that IRR is the interest rate which results a zero NPV value. In this case study, the following parameters were adopted: 20 years plant life, 10% interest rate, 30% tax and 20% of total investment as salvation value.

Further work was conducted to assess the economics of GTL plant at different oil price to natural gas ratio. The range from 7.27(crude oil price at dollar per barrel/natural gas price at dollar per MMBTU) to 42.43 was studied in this research. Table 10 and Figure 6 show the detailed results of the investment analysis of NPV versus price ratio. The figure showed that a ratio of 15 was the threshold for profitability. The project would become profitable if the price ratio was higher than 15.

The relationship of NPV along a 12 year period of time was shown in Figure 7. The figure showed that the NPV value has fluctuated sharply in the past decades. In the recent 3 years, NPV value has stabilized around zero, which means a balance of income and expenditure for the project.

Environmental Analysis

WAR software introduced by Yong and Cabezas (US EPA) [17] was used to assess the environmental impacts of the GTL plant. A database of relative environmental impact scores had been created and embedded into the WAR software to provide the basic information of potential environmental impact for each chemical component. It uses a basic PEI index (potential environmental impact) to represent the relative environmental friendliness or unfriendliness of a specific chemical process. The PEI index was based on the traditional mass and energy balance, which affected the environmental impact across the process boundaries. A lower PEI index stands for more environmental friendliness. Table 11 also shows the eight different categories used by the WAR algorithm to quantify the environmental index.

The simulation results file generated from Aspen Plus was imported into WAR software for evaluation. Table 12 shows the analysis results. The index "total output rate of PEI", with a unit of PEI/hour, assesses a process in terms of the potential impact on the environment external to the process. This index is influenced by the plant size. The index "total PEI leaving the system per mass of products", with a unit of PEI/kg product, allows one to assess the process regardless of manufacturing plant size. The results of these two indexes are illustrated in Figures 8 and 9 respectively. Further analysis of these indexes shows that all the toxicity related indexes, HTPI, HTPE, TTP, and ATP, has relatively high values. This is due to the toxic DEA solute adopted for the gas sweetening process. The PCOP (photochemical oxidation potential) index was also relatively high due to the sulfur compounds. All of these indices were related to acid gas removal process, which is universal for each natural gas processing industry. Several research works have been performed to compare the conventional oil industry to GTL plant. A full product life cycle assessment (LCA) was conducted for Shell, ConocoPhillips, and Sasol Chevron [18]. The results showed that, compared to conventional refinery system, the GTL process generates significantly less amount of solid waste and air pollutants emission (SO_x and NO_x for acidifying emission, volatile organic compounds emission, and particulate emission).

Conclusion

This study provides a base case simulation for a gas-to-liquid plant, using autothermal reforming technology for the syngas production and slurry bubble column reactor for the low temperature Fischer-Tropsch Synthesis. Further study about the economic and environmental analysis of the GTL plant was also conducted.

The analysis showed that the GTL plant had environment benefits, but the profit was not significant in the recent 3 years. The sensitivity analysis showed that GTL plant is able to make a profit when the crude oil to natural gas price ratio is higher than 15. Today, the price ratio fluctuates around 15 with a balance of income and expenditure under currently market price. However, due to the abundant supply of conventional and unconventional natural gas (shale gas, etc.), as well as the environmental advantages of FT technology, it appears that the gas-to-liquid industry will receive continuous interest.

Date	Crude oil Europe Brent Spot Price FOB (Dollars per Barrel)	Henry Hub Natural Gas Spot Price (Dollars per Million Btu)	New York Harbor Gasoline Regular Spot Price (Dollars per Gallon)	New York Harbor Ultra-Low Sulfur No 2 Diesel Spot Price (Dollars per Gallon)	Mont Belvieu, TX Propane Spot Price FOB (Dollars per Gallon)
Jan-2005	44.71	6.15	0.41	-	0.45
Jul-2005	56.1	7.63	0.55	-	0.52
Jan-2006	62.32	8.69	0.60	-	0.60
Jul-2006	73.14	6.17	0.73	0.66	0.71
Jan-2007	52.11	6.55	0.48	0.50	0.54
Jul-2007	77.44	6.22	0.72	0.69	0.72
Jan-2008	92.8	7.99	0.80	0.81	0.92
Jul-2008	143.68	11.09	1.15	1.29	1.19
Jan-2009	42.34	5.24	0.37	0.48	0.45
Jul-2009	58.43	3.38	0.55	0.50	0.42
Jan-2010	80.14	5.83	0.73	0.68	0.82
Jul-2010	75.2	4.63	0.69	0.65	0.60
Jan-2011	95.05	4.49	0.85	0.82	0.83
Jul-2011	117.35	4.42	1.03	1.00	0.94
Jan-2012	113.3	2.67	0.96	0.99	0.77
Jul-2012	99.23	2.95	0.94	0.90	0.50
Jan-2013	112.97	3.33	0.96	0.97	0.51
Jul-2013	108.43	3.62	1.01	0.94	0.57
Jan-2014	106.44	4.71	0.92	0.94	0.79
Jul-2014	106.2	4.05	0.97	0.91	0.64
Jan-2015	47.64	2.99	0.46	0.53	0.28
Jul-2015	57.72	2.84	0.68	0.54	0.26
Jan-2016	30.14	2.28	0.38	0.31	0.20
Jul-2016	44.04	2.82	0.46	0.43	0.30
Jan-2018	53.2	3.3	0.54	0.50	0.43
Jul-2018	46.57	2.98	0.52	0.46	0.37

Table 8: Raw Material Cost and Sales of Products [1,2].

Component Name	Heat Duty	Utility Type	Cost ($/hr)
Stripper Condenser	-7 GJ/hr	water/elctricity	64
Stripper Reboiler	20.6 GJ/hr	fuel (Natural Gas)	59
Pre-HT	63.5 GJ/hr	By integration	0
Steam for Pre-reformer	108.8 GJ/hr	By integration	0
Oxygen for Reformer	83.7 GJ/hr	By integration	0
CO_2-HT	5.36 GJ/hr	By integration	0
ATRIN-HT	70 GJ/hr	fuel (Natural Gas)	199
ATR-COOL	-438 GJ/hr	Left for integration	-502
CO_2-COMP	115.2 kW	electricity	7
SBCR-HT	71.8 GJ/hr	By integration	0
FLA1-CL	-105.8 GJ/hr	water	3
FLA2-CL	-45.2 GJ/hr	water/elctricity	352
COL-Condenser	-9.2 GJ/hr	water	1
COL-Reboiler	17.3 GJ/hr	fuel (Natural Gas)	49
SBCR-HE	-376 GJ/hr	Left for integration	-1,070
Total Annual Cost ($/year)			-7,033,760

Table 9: Utility Cost/Gain Calculation.

Crude oil to natural gas price Ratio ($bbl/$MMBTU)	NPV (Million $)	IRR
7.96	-467	-
8.08	-365	-
11.61	-288	-0.115
11.85	-178	-0.015
12.45	-170	-0.008
12.96	-284	-0.111
13.22	-37	0.078
13.75	-108	0.034
15.62	-69	0.058
15.63	24	0.114
15.93	13	0.107
16.12	32	0.118
16.24	20	0.112
17.29	11	0.106
20.32	173	0.196
21.17	212	0.218
22.60	279	0.254
26.22	388	0.315
26.55	437	0.342
29.95	473	0.362
33.64	486	0.369
33.92	478	0.365
42.43	613	0.442

Table 10: Investment Sensitivity Analysis of crude oil to natural gas price ratio.

General impact category	Impact category
Human toxicity	Ingestion (HTPI)
	Inhalation/Dermal Exposure (HTPE)
Ecological toxicity	Aquatic toxicity potential (ATP)
	Terrestrial toxicity potential (TTP)
Global atmospheric impacts	Global warming potential (GWP)
	Ozone depletion potential (ODP)
Regional atmospheric impacts	Acidification potential (AP)
	Photochemical oxidation potential (PCOP)

Table 11: Impact Categories in WAR Algorithm.

HTPI	HTPE	TTP	ATP	GWP	ODP	PCOP	AP	Total
Total output rate of PEI (PEI/hr)								
8230	1310	8230	20900	23.9	0	23300	194	62300
Total PEI leaving the system per mass of product streams (PEI/kg product)								
0.295	0.Fif0471	0.295	0.749	0.000855	0	0.835	0.00696	2.23

Table 12: Results for Environmental Analysis.

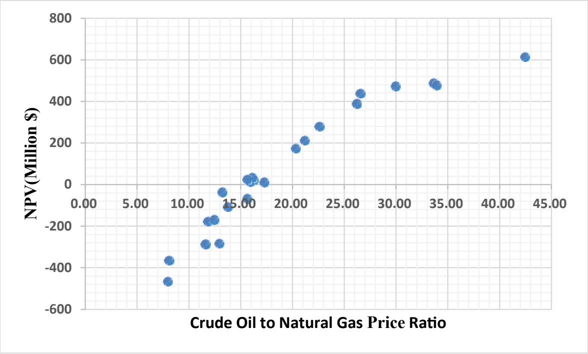

Figure 6: Investment analysis of Crude Oil versus Natural Gas Price Ratio.

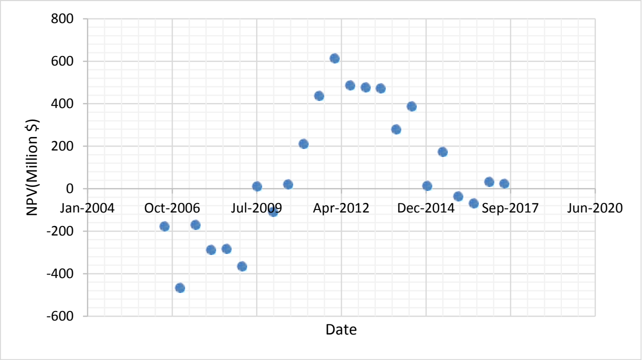

Figure 7: NPV fluctuation along time.

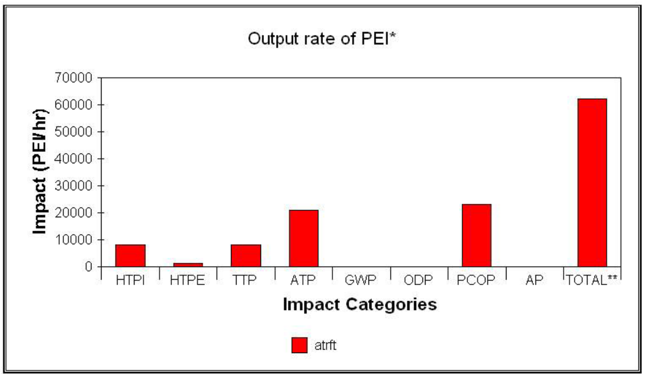

Figure 8: Output Rate of PEI for a GTL Plant.

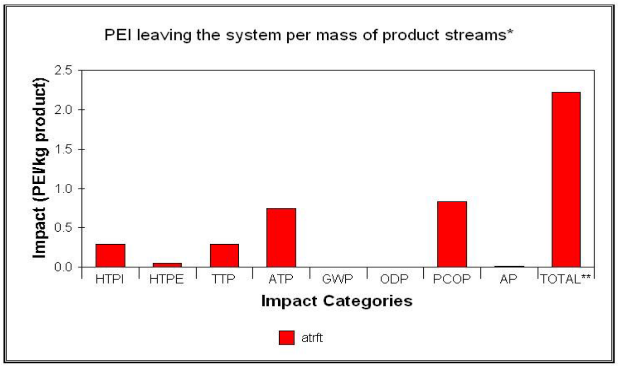

Figure 9: PEI Leaving the System per Unit Product.

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