CHEMICAL ENGINEERING TRANSACTIONS Volume 21, 2010
Editor J. J. Klemeš, H. L. Lam, P. S. Varbanov
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DOI: 10.3303/CET1021233

Optimal design and operation of a gas-to-liquid process

Ahmad Rafiee, Magne Hillestad*
Department of Chemical Engineering, Norwegian University of Science and Technology, Sem Sælands vei 4, 7491 Trondheim, Norway
magne.hillestad@chemeng.ntnu.no

In this study we used a commercial process simulator to model a gas to liquid (GTL) plant and evaluated different process alternatives from an economical point of view. These alternatives include different syngas unit configurations and the effect of removing CO_2 from the tail gas. The criteria used to compare different syngas configurations is payout time. Results show that the most economically attractive syngas technology for GTL applications is an ATR. A case study is conducted to investigate the effect of removing CO_2 from the tail gas. Results show that the carbon efficiency for an optimized ATR-based process with and without CO_2 removal unit is 77.3 % and 73.5 %, respectively.

1. Introduction

Part of natural gas reserves are in remote areas. Available technologies offer some options to monetize stranded gas such as compressed natural gas (CNG), liquefied natural gas (LNG) or to convert the gas chemically to stable liquids, mainly, gas to liquids (GTL) and gas to chemicals (GTC). In the last decades, the conversion of natural gas through GTL technology has shown to be an alternative for the use of natural gas to obtain liquid transportation fuels. An increasing world-wide demand for clean-burning fuels has sparked a renewed interest in the study of the Fischer-Tropsch synthesis.

The main objective of this study is to evaluate different process alternatives for the integrated GTL process. These alternatives include syngas configurations (Steynberg and Dry 2004) and removing CO_2 from the tail gas. Here we have used UNISIM DESIGN process simulator. The payout time for each syngas configuration is estimated as function of the natural gas price.

2. Process description

A GTL plant consists of three main units: 1) Syngas production, 2) Fischer-Tropsch synthesis, and 3) Product Upgrading. A schematic GTL process structure is illustrated in Figure 1.

Please cite this article as: Rafiee A. and Hillestad M. (2010), Optimal design and operation of a gas-to-liquid process, Chemical Engineering Transactions, 21, 1393-1398 DOI: 10.3303/CET1021233

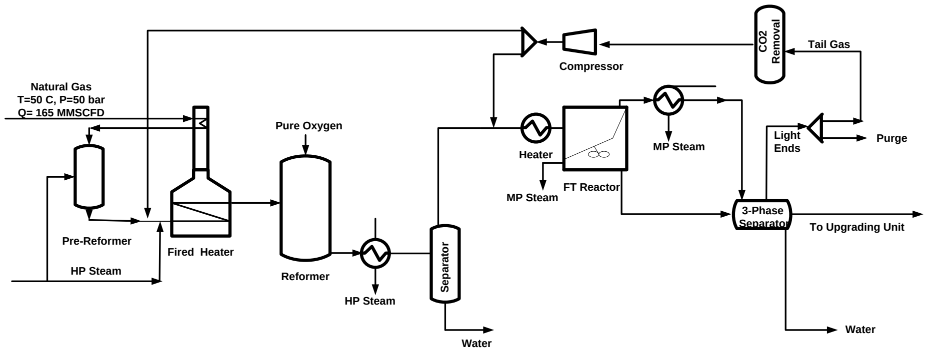

Figure 1: A schematic representation of a GTL plant in this study

2.1 Syngas production

The syngas step converts the natural gas into hydrogen and carbon monoxide by steam methane reforming, autothermal reforming, gas heated reforming, and combinations thereof.

Steam reformers are not the preferred technology for the large-scale GTL applications, but they play a role in optimised GTL plants in the form of adiabatic prereforming or heat exchange reforming.

Basically, a heat exchange reformer is a steam reformer where the heat required for the reaction is supplied predominantly by convective heat exchange. The heat can be supplied from a flue gas or a process gas - or in principle by any other available hot gas.

The cases may be divided into two main types, series and parallel arrangements.

In series arrangements, all the process feed gas passes first through a heat exchange reformer and then through a second reformer, and the product gas from the second reformer supplies heat to the heat exchange reformer. The second reformer in the series arrangement may be a fired tubular reformer. Alternatively, the second reformer may be an air or O_2-blown secondary reformer.

In parallel arrangements, the feed gas is split into two streams (Steynberg and Dry 2004). One goes directly to a conventional reformer, while the other goes to a gas heated reformer heated by the outlet gas from the conventional reformer and it is in principle possible to produce two different product gases.

In the pre-reformer, we assume that higher hydrocarbons are completely converted to syngas. For the reformer, we assume chemical equilibrium which is a reasonable assumption since the outlet temperature is quite high.

2.2 Fischer-Tropsch synthesis

Conversion of the syngas to liquid hydrocarbon is a chain growth reaction of carbon monoxide and hydrogen on the surface of a heterogeneous catalyst. In a cobalt based FT reactor, the syngas reacts to form a mixture of liquid hydrocarbons:

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

The kinetic model applied in this study is the one given by Iglesia, et al., (1993). The chain growth probability is calculated from an empirical correlation reported by Song and Ramkrishna, (2003). The FT reactor is approximated by a continuous stirred tank reactor (CSTR). The operating temperature and pressure of the FT reactor is 210 °C and 20 bar. It is assumed that olefin to paraffin ratio (γ) is constant and equal to 0.35 (Schanke and Sogge, 2010).

3. Economical analysis

3.1 Capital costs estimation

In order to do an economical analysis, it is necessary to estimate the capital cost of the major equipments. We have applied the Module Costing Technique reported by Turton et al., (2009) to do this estimation. It is generally accepted as the best for making preliminary cost estimation. The investment needed for commercial Air separation unit (ASU) and steam methane reformer (SMR) suggested by Schanke and Sogge (2010) are given below:

- ASU: 19.1 M$ for a 325 t O_2/day, scaling factor=0.7;
- SMR: 22 M$ for a SMR with a duty of 70 MW, scaling factor=0.9;
- Energy required for ASU: 300 kW/ (t O_2/h).

3.2 Estimation of Cost of Manufacturing (COM)

There are many elements that influence the cost of manufacturing (Turton et al., 2009), e.g. Cost of raw material, Cost of utilities, Cost of waste treatment, Cost of operating labor, etc.

4. Results

4.1 Exploring the best syngas configuration for GTL applications

UNISIM OPTIMIZER is used to implement case studies. The syngas configurations were optimized to find which one(s) are more suitable for GTL applications. The objective function is defined as maximizing annual profit.

The criterion used to compare different scenarios is the Payout Time (Sinnott and Towler, 2009). This measure does not take into account time value of money.

The operational parameters optimized here are:

- Steam to carbon ratio
- Oxygen to carbon ratio (O/C) where ATR is applied
- Purge gas ratio
- Natural gas split ratio for parallel arrangements

Natural gas price and selling price of final product for all of the cases are $0.5/MMBTU and $132.25/bbl, respectively. The results are shown in Table 1. Accepting Payout time as a criterion to compare different configurations, it is obvious from Table 1 that the most economically attractive technology for GTL applications is ATR. Figure 2 shows the changes in payout time vs. natural gas price for different syngas configurations.

Table 1: Results of economical analysis for different syngas configurations

Syngas Configuration	*Methane conversion (%)*	*H_2/CO ratio*[1]	*Carbon efficiency*[2] *(%)*	*S/C*[3]	*O/C*	*Purge %*	*Payout time (y)*
ATR	93	2.1	77.3	0.44	0.51	3	4.58
Combined[4]	61 in SMR 33 ATR	3.2	64.2	0.87	0.56	21	8.81
Gas Heated Prereforming	18 in GHR 55 in SMR	3.02	36	0.825	-	93	10.17
Two-step reforming with GHR	20 in GHR 75 in ATR	2.34	79.2	0.4	0.57	1	5.18
Combined Reforming with GHR	16 in GHR 79 in ATR	2.28	73.26	0.4	0.53	1.5	5.35
ATR and GHR in parallel arrangement	11 in GHR 83.7 in ATR	4.26[5] 1.96	78.12	0.4	0.53	1	5.06

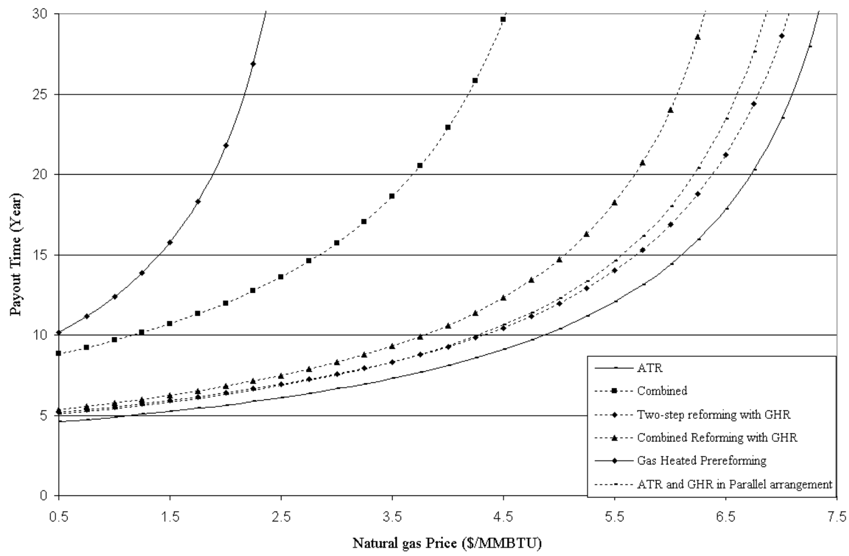

Figure 2: Payout time vs. natural gas price for different syngas configurations

1 At the outlet of syngas unit.

2 It is assumed that 10% of carbon is lost in product upgrading unit.

3 S/C ratio after Pre-Reformer. Water is also produced in Pre-Reformer due to water gas shift reaction. This low steam to carbon ratios to a SMR or Gas Heated Reformer (GHR) will lead to coke formation but here the ratio is optimized without regard to coke formation

4 Conversion of methane in SMR is fixed.

5 In this configuration, two product gases can be produced. The hydrogen rich stream can be used in upgrading unit. Here, these two streams are mixed.

4.2 Effect of removing CO_2 from the tail gas

In the case that there is no CO_2 removal unit, the H_2/CO ratio at the outlet of ATR decreases. The reason is due to accumulating large amount of CO_2 (68,500 kmol/h) in process. It is possible to adjust the H_2/CO ratio to the desired value of 2.0 by adding more steam and changing amount of purge (Table 2). From this table, it can be seen that the carbon efficiencies are quite close.

Table 2: Optimal design of an ATR-based GTL plant with or without CO_2 Removal Unit

	With CO_2 Removal	*Without CO_2 Removal*
S/C	0.44	1.29
O/C	0.51	0.525
Purge (%)	3	6
Carbon Efficiency	77.3	73.5
Payout Time (year)	4.58	5

4.3 Relationship between natural gas price and product selling price

One of the important factors which affect profitability of a GTL plant is the natural gas price. The relationship between natural gas price and product selling price in an ATR-based GTL plant is shown in Figure 3. From this figure, the average selling price of final products should be 87.5 $/bbl to have a payout time of 10 y.

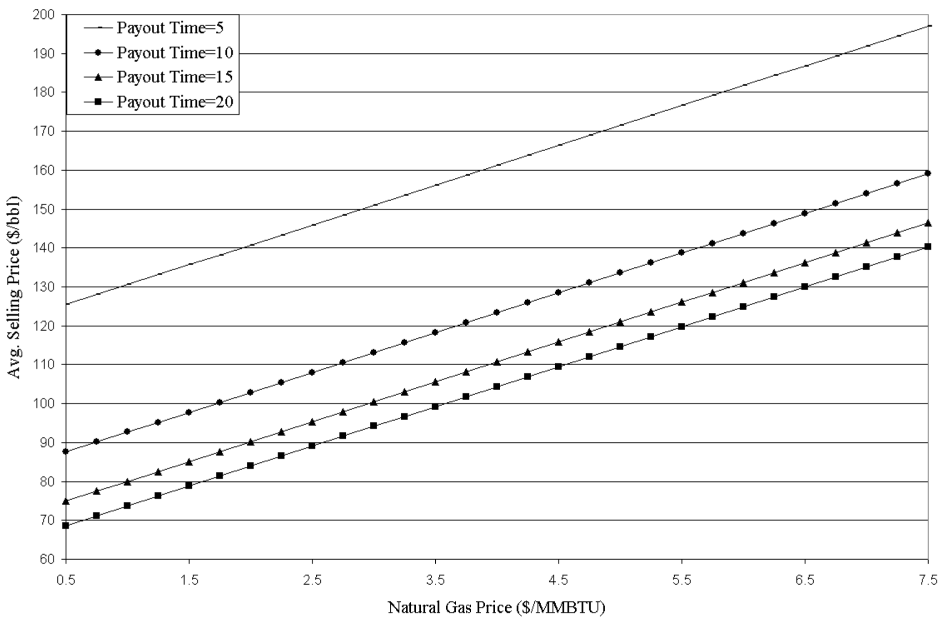

Figure 3: Relationship between natural gas price and product selling price (Fixed Capital Investment= $1.54 billion)

5. Conclusions

In this study we modeled a cobalt based GTL plant using UNISIM DESIGN process simulator and studied different configurations of syngas production unit from an economical point of view. The results show that the most attractive and economical syngas technology for GTL applications is an ATR. A case study, conducted to study the effect of removing CO_2 from tail gas shows that the carbon efficiencies for an optimized ATR-based process are 73.5 % and 77.3 % with and without CO_2 removal. Fixed capital investment required for an ATR-based GTL plant is estimated to $1.54 billon. The average selling price of final products should be above 87.5 $/bbl to have a payout time of 10 years.

Acknowledgments

The authors gratefully acknowledge financial support from the Research Council of Norway.

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