

## PROCESS SIMULATIONS FOR PRODUCTION OF SYNTHETIC NATURAL GAS (SNG) FROM SYNGAS – TECHNICAL AND ECONOMICAL EVALUATION

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Fawad Akhtar Soomro<sup>1</sup>, Imran Nazir Unar<sup>2</sup>, Sikandar Mustafa Almani<sup>3</sup>,

<sup>1</sup> Research student, Department of Energy system Engineering, MUET, Jamshoro. <sup>3,4</sup>Department of Energy system Engineering, MUET, Jamshoro

**Abstract:** Pakistan is facing sever natural gas shortages and government is focusing on searching for alternatives for this crisis. Synthetic Natural Gas (SNG) is one sustainable and greener alternative which is produced from solid fuels via gasification process. In the gasification process, solid fuels like coal are heated in gasifier vessels with a small amount of oxygen or air to produce syngas. This syngas is then further processed into finished products, such as vehicle fuels like diesel, DME, and gasoline, as well as various chemicals including fertilizers, hydrogen, petrochemicals, olefins, polymers, and synthetic natural gas (SNG). In present research, a study was conducted to simulate the conversion of syngas (CO+H<sub>2</sub>) into SNG using Aspen HYSYS and Aspen PLUS simulators. The research involved two parts: firstly, a simplified model was developed in Aspen HYSYS to explore the kinetic behavior of syngas to SNG conversion based on operating parameters like feed flow, temperature, pressure, composition, and TEG feed flowrate. Subsequently, a detailed model was simulated using Aspen PLUS to economically evaluate the entire process. The study highlights the intricate relationship between syngas feed flowrate, SNG production, and its properties. While SNG production exhibited a linear increase with syngas flowrate, the HHV and CH<sub>4</sub> mole fraction demonstrated non-linear behavior. The maximum HHV of produced SNG was observed 786219.7 kJ/kgmole at 20 kg/hr syngas feed flowrate. Total capital cost including the cost of gasification and gas cleaning system was estimated 21.47 million US\$. Overall, it is concluded that the range of CO/H<sub>2</sub> ratio from 0.32 to 0.38 would be ideal to get more than 90% methane in SNG product.

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**Keywords:** Syngas, Aspen HYSYS, Natural gas, Renewable, SNG.

## **1. Introduction**

any are pursuing unconventional methods of producing natural gas due to rising natural gas demand and high natural gas costs in recent years. Synthetic natural gas or "substitute natural gas" is natural gas that can be manufactured from coal or biomass (SNG)[1]. One of the commodities that can be made from syngas extracted from coal by the methanation process is SNG. The market pricing of the coal and natural gas feedstocks to be utilized, the value of the byproducts like carbon dioxide (CO<sub>2</sub>) (which might be used for EOR), and moreover the capital cost of the gasification plant all play a significant role in the economic viability of producing SNG from coal. There is only one commercial coal-to-SNG plant operating right now in the entire world. Many suggestions for new coal-to-SNG plants in the United States were made around the middle of the previous decade when natural gas prices rose to previously unheard-of high levels. Ten were still being discussed or were at various stages of development in 2010. Many or all of these proposed SNG projects may not proceed to implementation because natural gas prices have dropped to low levels in recent years. There are numerous methods for producing natural gas, both renewable and nonrenewable. Synthetic natural gas (SNG) production processes that are more traditional rely on nonrenewable resources like coal. In contrast, a more sustainable method of producing SNG uses biomass from landfills, livestock farms, and waste treatment [<u>2</u>, <u>3</u>].

## 2. Natural Gas Scenario of Pakistan

For the past ten years, Pakistan has been at the epicentre of the global energy problem (particularly with regard to natural gas) [4]. Because of increased security concerns in the nation, both supply and demand are becoming increasingly diverse. Natural gas reserves (12 trillion cubic feet) were found in Pakistan in 1952 near Sui (Baluchistan) [5]. For home consumption, the production of power, and industrial usage, gas infrastructure was created. Sui Northern Gas Pipelines Limited (SNGPL) and Sui Southern Gas Company Limited are responsible for the country's gas transmission (SSGCL) [6]. In Pakistan, the excessive use of natural gas as a fuel had been growing over time. By 2005, Pakistan's use of natural gas reached a peak of about 50% of its total energy consumption [7]. Natural gas reserves started to run out quickly starting in 2006 as a result of overuse, poor management, and insufficient exploration of the new gas reserves. As a result, there is a natural gas deficit since natural gas output has not kept pace with demand.

Instead of utilizing its own alternative energy sources, Pakistan has resorted to importing liquefied natural gas (LNG) from Qatar, following the same importation pattern as it does with fossil fuels (petrol and diesel). The 175BT (Billion Tons) of coal reserves in Thar, Sindh, are one such alternative supply [8]. Through either above-ground gasification or underground coal gasification (UCG), coal is utilized to create syngas [9]. Synthetic natural gas (SNG), a

Corresponding author Email address: ssss@gmail.com

substitute for natural gas or *suigas*, can be created by further processing the synthetic gas (syngas) that results from the gasification of coal. As a result, countries like China and India that use above-ground gasification have also witnessed a trend towards increasing syngas output [10].

#### 2.1 Process chemistry

Researchers Sendersen and Sabatier developed the CO and CO2 methanation technique as a way to manufacture natural gas artificially in 1902 [11]. Gasification is the first step of a multi-phase process that produces SNG. Coal (nonrenewable) and biomass (renewable) are burned with oxygen or water vapour to begin the process.  $N_2$  is eliminated from the process to make the gasifier's interior a more  $O_2$  rich environment, which will help the combustion reaction occur.

The following equations provide the two synthetic natural gas reactions:

 $2C + O_2 \to 2CO \tag{1}$ 

$$C + H_2 0 \leftrightarrow C 0 + H_2 \tag{2}$$

The carbon in the biomass and coal molecules is denoted by C in equations 1 and 2 [12]. CO and H<sub>2</sub>, referred to as the producer gas, are produced during the gasification process. To distinguish between the usable gas product and the solid trash, the gasification process is carried out at extremely high temperatures and pressures. The useful gas/producer gas occasionally includes CO<sub>2</sub>, H<sub>2</sub>O, and CH<sub>4</sub> in addition to CO and  $H_2$  [13, 14]. Not all waste is, however, eliminated; occasionally, the usable gas also contains additional waste materials, including tar, complex hydrocarbons, NH<sub>3</sub>, SOx, and other compounds. After that, a scrubbing method is used to eliminate any leftover waste materials. What is now referred to as the synthesis gas should ideally include just H<sub>2</sub>, CO, and CO<sub>2</sub> after the gas scrubbing procedure is finished. It should be noted that while traces of undesirable substances may still be present in this mixture, they do not dominate or drive the process.

A water gas shift/methanation procedure is necessary after the cleaning procedure. The carbon water vapour reacts with the carbon dioxide during the methanation process to produce more  $H_2$  and  $CO_2$ , represented by the following response:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \tag{3}$$

then, a reaction between CO and  $H_2$  produces CH<sub>4</sub>. A catalyst can be used to speed up the chemical reaction. Frequently, these catalysts are metallic complexes like Ni-TiO<sub>2</sub>, Ni/Al<sub>2</sub>O<sub>3</sub>, and NiO-CeO<sub>2</sub>, including others [15-18]. CO and H<sub>2</sub> react chemically in the following ways:

$$CO + 3H_2 \to CH_4 + H_2O(g) + \left(-260\frac{kJ}{mol}\right)$$
 (4)

After being created, natural gas can be used as an energy source for a system by being burned during a combustion reaction. However,  $CO_2$  can also be employed as a reactant during the methanation process in place of CO. H<sub>2</sub> and CO<sub>2</sub> are reactants in the stage of gas mixing if CO<sub>2</sub> is employed in the methanation process. Following is the CO2 methanation equation:

$$CO_2 + 4H_2 \to CH_4 + 2H_2O(g) + \left(-164\frac{kJ}{mol}\right)$$
 (5)

There is currently infrastructure in place in the United States and Canada to convert coal or biomass to SNG. Canada is currently the world's fourth-largest producer of natural gas, ranking behind the United States, Russia, and Iran in terms of output, and the sixth-largest exporter of natural gas [3] through a renewable technique such as electrolysis.

#### 1.3 Some latest Work on SNG Production

Gomez et al, (2023) [19] demonstrated the methanation process under quasi commercial conditions for a syngas generated from biomass gasification. The influence of process variables like pressure, steam/CO ratio and syngas composition (i.e. content of CO<sub>2</sub>, CH<sub>4</sub> and light hydrocarbons) were analyzed to evaluate the maximum CH4 purity achieved in a commonly used two-step methanation process. Katla et al., (2023) [20] presented the results of tests conducted on the methanation reactor installation at the Silesian University of Technology. The reactor was a fixedbed type and it consisted of one tube filled up with the nickel powder and Ru/(Al<sub>2</sub>O<sub>3</sub>) used as a catalyst.

Chen and Abdel-Mageed (2023) [21] conducted a review to focus on the recent advancements of the methanation of CO and CO<sub>2</sub> on oxide supported Ni and Ru catalysts in the frame of their use in the abovementioned applications. They concentrated on the structure-reactivity relationships of CO and CO<sub>2</sub> methanation in different applications, highlighting limitations and advantages of different catalytic systems. Krammer and Lehner (2023)[22] presented the requirements for the successful methanation of co-solid oxide electrolysis cell syngas at the catalyst, reactor, and plant levels. Reaction kinetics and thermodynamics define the baseline for wellbalanced reaction conditions. The catalytically active materials, carrier materials, and catalyst forms used for chemical methanation need to be considered to maximize performance.

Bartik et al., (2022) [23] investigated the catalytic methanation of syngas from dual fluidized bed steam gasification of biomass in an innovative bubbling fluidized bed methanation reactor with an optimized catalyst. Syngas from conventional gasification and a novel combination with

syngas from sorption enhanced reforming were investigated. Zhang et al., (2022)[24] investigated and analyzed a series of coal-based SNG processes with different coal ranks and gasification technologies based on rigorous process modeling and simulation.

All the literature cited above were the efforts to study the production of efficient SNG from syngas using some advanced technologies. However, scant literature was available to emphasize the optimized CO/H2 ratio in terms of maximum conversion and optimized economics. Moreover, there is no study available in the perspective of Pakistan as the country has huge coal reserves.

The natural gas resources of Pakistan are limited and currently country is facing lots of issues regarding shortage of natural gas in the domestic and commercial network. On the other side, Pakistan has huge low-grade coal reserves at Thar coal field. The coal excavation activities are started since couple of years, but the coal-to-power is not feasible solution as Pakistan's has already enough power generation capacity.

Therefore, the extracted low-grade coal could be utilized in other means like for the synthesis of important chemicals like ethanol, fuels, or synthetic natural gas (SNG). The production of SNG is possible via coal gasification process. Already several studies were conducted to design an indigenous coal gasifier. The syngas produced from those gasification process could be utilized to produce SNG which could fulfil the countries shortcomings of natural gas. The process of conversion of syngas to SNG is a complicated process and needs to be investigated on the basis of local coal characteristics.

In this cutting-edge research, we delve into the fascinating realm of generating SNG from the dynamic synergy of syngas (CO+H<sub>2</sub>), employing the renowned Aspen HYSYS and Aspen PLUS simulators. Our investigation unfolds in a two-fold manner: firstly, an elegantly simplified model takes shape within Aspen HYSYS. This model serves as a window into the intricate kinetics governing the metamorphosis of syngas into SNG. The impact of a symphony of operational parameters-feed flow, temperature, pressure, composition, and TEG feed flowrate-gracefully dance into view through this model. A natural progression leads us to the grandeur of an Aspen PLUS detailed simulation. Here, coal size reduction, screening, gasification, shift conversion reactions, and the mystical art of methanation intertwine. Within this intricate tapestry, we navigate the entire process, culminating in a thorough economic evaluation that promises to illuminate the path forward.

### 3. Methodology

In the present research the process of conversion of syngasto-SNG was simulated using standard process simulation software, Aspen HYSYS V11. The work was divided into two broad sections. In the first section, the fundamental and simple process was designed using Aspen HYSYS V11.0 to check the conversion reaction mechanism. In this simple simulated process, the syngas was assumed to be only composed of CO and  $H_2$ . After the development and successful convergence of basic simple model, detailed parametric investigations were conducted on simple model.

#### 3.1 Development of Simplified model

The material and energy balances for the syngas-to-SNG conversion process were estimated using the ASPEN HYSSY V11 simulation software, which was used to create the first model (the simplified model). In order to enhance the design of the base cases, it was also used to address whatif analyses and do sensitivity assessments. Since it was the suggested thermodynamic property package for hydrocarbon systems, the Peng-Robinson equation of state (Eq. (6))[25] was employed.

$$P = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}(\hat{v} + b) + b(\hat{v} - b)}$$
(6)

where

Р	=	Pressure
Т	=	Temperature
R	=	General gas constant
	=	Specific volume
Z	=	Compressibility factor of real gas

The converged process flow diagram (PFD) of the syngas to SNG conversion process is shown in Fig. 1:



Fig. 1: Converged PFD for the SNG production process from syngas

#### **3.2** Characteristics of feed steams

In this model, there are two feed streams utilized in the process model. One is the syngas feed stream whereas the other is the TEG feed stream used to remove  $H_2O$  from the product stream of SNG. It was assumed that the feed stream containing syngas is composed of only CO and  $H_2$  which are the primary components of syngas. The operating parameters with compositions are given in the Table 1.

Table 1: Parameters of feed streams				
Parameter	Syngas Feed Stream	TEG stream		
Name of stream	FEED	TEG_Feed		
Temperature (°C)	30	60		
Pressure (kPa)	210	210		
Mass flowrate (kg/hr)	20	7000		
Composition	CO=20%,	Triethyl glycol=99%		
	H <sub>2</sub> =80%	H <sub>2</sub> O=1%		

not suitable for the absorption process. Hence the temperature of this raw product stream needs to be reduced as per need. Hence a cooler (E-101) is installed. The outlet temperature from this cooler is fixed at 120° C for stream "Raw\_Cold\_Prod". No pressure drop for the cooler was assumed. The detailed parameters for Absorption column (T-100) which was installed to recover the water by showering Triethylene glycol (TEG), are tabulated in Table 3.

## Table 3: Design parameters for Absorption Column (T-100)

#### 3.3 Modeling of Reactor (PFR-100)

Synthetic natural gas was produced from syngas using the plug flow reactor (SNG). The reaction as per Eq. (4) was modeled with heterogeneous kinetic parameters. The reaction parameters were taken from earlier research work [16]. The catalyst was Ni-TiO<sub>2</sub> as per pervious research [3]. As the reaction is reversible reaction, hence it has forward as well backward reaction kinetics. The whole reaction rate can be expressed as in Eq. (7).

$$Rate = \frac{k_f [CO] [H_2]^{-2.5} - k_b [CH_4] [H_2 O]}{(1 + k_{CH_4} [CH_4] + k_{CO} [CO] + k_{H_2} [H_2] + k_{H_2 O} [H_2 O])^2}$$
(7)

Where  $k_f$  and  $k_b$  are the rate constants for forward and backward reactions. The  $k_{CH4}$ ,  $k_{CO}$ ,  $k_{H2}$  and  $k_{H2O}$  are the rate constnats for individal species CH<sub>4</sub>, CO, H<sub>2</sub> and H<sub>2</sub>O respectively. All the rate constants are temperature dependent quantities and following the Arrhenius relation as described in Eq. (8).

$$k = A e^{-E/RT} \tag{8}$$

where, respectively, A and E stand for pre-exponential factor and activation energy. The kinetic parameters and different constants used in Eq. (7) and Eq. (8) are tabulated in Table 2.

#### Table 2: Reaction parameters

Sr. No.	Parameter	Pre-Exponential Factor	Activation Energy (J/Kmol)
1	$k_{f}$	$A = 1.17 \times 10^{15}$	$E = 1.0322 \times 10^5$
2	$K_b$	$A = 1.25 \times 10^{8}$	$E = 3.2 \times 10^{6}$
3	$k_{CH_4}$	$A = 6.65 \times 10^4$	E = -16457
4	k <sub>co</sub>	$A = 8.23 \times 10^{5}$	E = -30374
5	$k_{H_2}$	$A = 6.12 \times 10^9$	E = -35641
6	$k_{H_2O}$	$A=1.77{\times}10^5$	E = 38126

# 3.4 Modeling of Cooler (E-101) and Absorption Column (T-100)

The product stream coming out from PFR-100 reactor named as "Raw Product" is at elevated temperature which is

Sr. No	Parameter	Value	
1	No. of stages	10	
2	Pressure at Top stage	180 kPa	
3	Pressure of Bottom stage	210 kPa	
4	Internal Type	Sieve Plates	
5	Diameter of column	1.5 m	
6	Tray spacing	0.5 m	
7	Tra volume	0.8836 m <sup>3</sup>	

### 3.5 Development of detailed Model In Aspen Plus

After the convergence and parametric investigations on simplified model, a detailed model of SNG production was developed in Aspen Plus V11 software. in this model all steps like coal crushing and sizing, coal gasification and syngas cleaning, shift conversion reaction, and methanation reaction for producing sng are involved. Fig.2 displays the full converged process flow diagram.



Fig. 2: Process Flow Diagram of Detailed Model for SNG Production

#### 3.6 SIMULATION PARAMETERS

After the convergence of model as per Fig. 1, the converged model was used to investigate the performance of whole process at varying different operating conditions. After the careful literature review, it was finalized that the most important operating parameters which could affect the overall performance of process are Flow of syngas feed stream, pressure of feed stream, temperature of feed stream, composition of syngas feed stream and flowrate of TEG stream. The detailed values of mentioned parameters are tabulated in Table 4.

#### **Table 4: Varying Operating Parameters**

Sr. No	Doromotor	Unite	Value	
		UIIIts	Minimum	Maxim
1	Feed Flowrate	Kg/hr	20	100
2	Feed Pressure	kPa	200	300
3	Feed Temp	° C	30	80
4	TEG FEED	Kg/hr	7000	20000
5	Composition	Mass fraction of CO	0.2	0.32

#### 3.7 Economic Evaluation

The economic evaluation of any process is necessary to check the financial viability of the process. For the purpose the detailed process (Fig. 2) was evaluated economically using in built capability of the Aspen Plus software through Aspen Icarus [26]. The program is built on the Icarus assessment engine, which makes use of industry standards, design guidelines, and comprehensive real-world engineering and construction data. The database and analytical tools have been upgraded in the most recent release to guarantee that investment decisions are based on exceptionally precise estimations that take into account contemporary international design and construction methods. The economics of the process was assessed in the current study in terms of capital costs, operational costs, equipment costs, and utility costs.

#### 4 RESULTS AND DISCUSSION

In present research, the process for producing synthetic natural gas (SNG) from syngas  $(CO+H_2)$  was simulated using standard Aspen HYSYS and Aspen PLUS simulators. The work was divided into two portions, in first section a simplified model was developed in Aspen HYSYS for investigating the kinetic behavior for conversion of syngas in to SNG. The simplified model was used to investigate the effects of various operating parameters like feed flow, feed temperature, feed pressure, feed composition and TEG feed flow rate.

After that a detailed model was simulated using Aspen PLUS in which coal size reduction and screening, coal gasification, shift conversion reaction and methanation reactions were simulated. The detailed model was used to investigate whole the process for economic evaluation. The results are discussed in the following sub-sections.

### 4.2 Performance Variables

The overall performance of the process can be seen by investigating the impacts of different output parameters. In current research, four variables were selected to check the overall performance of SNG production process using simplified model. The selected four variables and their concerned material/energy streams are given are as under: • The mass flowrate of product stream (SNG\_Product in Fig. 1).

• Methane (CH4) percentage in the product stream (SNG\_Product in Fig. 1).

• The higher heating value (HHV) of the product stream (SNG\_Product in Fig. 1).

• The energy required via energy stream (E\_Cold) used by cooler (E101) to cool the raw product stream (Raw\_Cold\_Prod) as per Fig. 1.

#### 4.3 Effect of Syngas Feed Flowrate

The effect of syngas feed flowrate was investigated by varying mass flowrate of syngas feed stream (named as FEED) from 20 to 100 kg/hr. The effect of syngas feed flowrate ware on SNG production is shown in Fig. 3. According to Fig. 3, there is a linear increase observed in SNG production while on increasing syngas feed flowrate. The slope of the curve was observed 0.57 which means more than 50% of the total entered feed is converted into SNG.

Higher heating value (HHV) is another important aspect for any gaseous fuel. The effect of syngas feed flowrate on HHV of produced SNG is shown in Fig. 3. According to Fig. 3, there is a nonlinear decrease was observed in the HHV of produced SNG on increasing the syngas feed flowrate. The maximum HHV of produced SNG was observed 786219.7 kJ/kgmole at 20 kg/hr syngas feed flowrate. The minimum HHV of produced SNG was observed 757185.2 kJ/kgmole at 100 kg/hr syngas feed flowrate. This is about 3.7% decrease in HHV of produced SNG. The possible reason of this decrease is the over capacity of reactor as the reactor is optimized for certain conversion of feed species like CO and H<sub>2</sub> in the syngas.



## Fig. 3: Effect of syngas feed flowrate on SNG production rate and its heating value (HHV)

The decreasing trend of HHV of SNG is due to the decreasing trend of the main fuel gas component in the SNG which is the methane. The effect of syngas feed flowrate on methane (CH<sub>4</sub>) mole fraction in produced SNG is shown in Fig. 4. A nonlinear decreasing trend for the mole fraction of CH<sub>4</sub> was observed on increasing the feed flowrate of syngas. It was observed from figure that the CH<sub>4</sub> mole fraction is decreased from 0.836 to 0.7878 by increasing syngas feed flowrate from 20 to 100 kg/hr. The reason of this decrease is

the limitation of reactor capacity which was originally designed from 20 kg/hr. However, increasing the feed flowrate of syngas increases the overall yields of the SNG.

The product of reactor is a raw SNG contains moisture as main unwanted component. Prior to purifying it in gas absorption column via showering ethylene glycol, there is need to reduce the temperature of SNG for getting maximum efficiency of absorption column. Hence a cooler is used to cool raw SNG. The energy for cooling is plotted against the syngas feed flow rate in Fig. 4. A liner increasing trend was observed in the cooling energy requirement v/s syngas feed flowrate. It is an obvious trend as more energy is required to heat or cool to a higher amount of that substance.



Fig. 4: Effect of syngas feed flowrate on methane composition in produced SNG and energy required for cooling operation

#### 3.4 Effect of Syngas Feed Temperature

The effect of syngas feed temperature is discussed in this section. The temperature of feed stream is a critical parameter for any process particularly where reaction is involved. The impact of temperature is highly dependent on the sensitivity of temperature with respect to selected operations. The effects of syngas feed temperature on SNG production and higher heating value (HHV) of produced SNG are shown in

Fig. 5 whereas mole fraction of  $CH_4$  in produced SNG and cooling energy of raw SNG are shown in 6. It was observed that feed temperature which was varied from 30 to 80° C remained insensitive for SNG Production rate (Fig. 6), HHV of SNG (Fig. 7) and  $CH_4$  mole fraction in SNG (Fig. 8). However, a linear increase was observed in the cooling energy requirement for raw SNG material stream as increasing the temperature of syngas feed stream. This increase in energy is due to an increase in the thermal content by increasing the temperature of that stream which is to be cooled. So, this increase is obvious and considered as a natural effect.



Fig. 5: Effect of syngas feed temperature on SNG production rate and its heating value (HHV)



Fig. 6: Effect of syngas feed temperature on methane composition in produced SNG

and energy required for cooling operation

#### 3.5 Effect of Syngas Feed Pressure

Like temperature pressure is another thermodynamic state variable. The pressure of any feed stream could lead to a drastic impact on the overall outputs of the chemical process. The effects of syngas feed pressure on SNG production and, higher heating value (HHV) of produced SNG and shown in Fig. 7, whereas mole fraction of CH<sub>4</sub> in produced SNG and cooling energy of raw SNG are shown in Fig. 8. From the figures it was observed that for the current process, syngas feed pressure has no significant impact on either of the investigated dependent variables. Almost all the variables i.e., SNG production, HHV of produced SNG, mole fraction of CH<sub>4</sub> in SNG and cooling energy required for raw SNG were remained constant during the varying syngas feed pressure. Major reason of this behavior of the process with respect to pressure variation is that the reaction is independent of pressure and no significant impact on the overall conversion of reacting species has reported. Hence there is no further impact observed in the rest of the process.



Fig. 7: Effect of syngas feed pressure on SNG production rate and its heating value (HHV)



Fig. 8: Effect of syngas feed pressure on methane composition in produced SNG and energy required for cooling operation

#### 4.6 EFFECT OF SYNGAS FEED COMPOSITION

Syngas feed stream is a primary feed stream in current process. It contains two species i.e., CO and H<sub>2</sub>. For investigating the effects of previous important operating conditions i.e., syngas feed flow, feed temperature, feed pressure, the composition of syngas was maintained at constant values of CO=20% and H<sub>2</sub>=80%. For investigating the variation in the fraction of these two species, a new parameter was introduced which is the ratio of CO and H<sub>2</sub> (CO/H<sub>2</sub>). Hence the increase in CO/H<sub>2</sub> ratio means there is an increase in CO and decrease in H<sub>2</sub> as a composition of feed stream.

The effect of variation in ratio of CO/H<sub>2</sub> on SNG production is shown in Fig. 9. CO/H<sub>2</sub> varies from 0.270 to 0.504 (CO=0.212 to 0.33 and H<sub>2</sub>=0.787 to 0.664). In this variation, the SNG production first decreases from 9.12 kg/hr to minimum value of 8.427 kg/hr (at CO/H<sub>2</sub>=0.328). After this the production of SNG linear increases and reaches maximum 9.59 kg/hr at maximum CO/H<sub>2</sub> = 0.504. The reason for this trend is that the reaction conversion is highly dependent on the availability of most active specie of reaction. From the analysis it was seen that CO is more important and its value above 33% is highly favorable for conversion of syngas into methane gas. The effect of variation in ratio of  $CO/H_2$  on higher heating value (HHV) of produced SNG production is shown in Fig. 9. The trend for HHV of SNG is entirely inverse as compared to SNG production with respect to variation in  $CO/H_2$  ratio. The maximum HHV was observed 858598 kJ/kgmole at the 0.328 CO/H<sub>2</sub> ratio where the minimum value of SNG produced. In terms of HHV it has been concluded that ideal  $CO/H_2$  ratio would be 0.328 where maximum HHV of produced SNG achieved.



Fig. 9: Effect of syngas feed composition on SNG production rate and its higher heating value (HHV)

The effect of variation in ratio of CO/H<sub>2</sub> on methane mole fraction in the produced SNG product is shown in Fig. 10. As expected from the HHV analysis, the trend of CH<sub>4</sub> mole fraction is almost similar to the HHV trend. This is because it is CH<sub>4</sub> which is responsible for the HHV in the SNG. The maximum mole fraction of CH<sub>4</sub> in SNG is 0.956 has achieved at 0.328 CO/H<sub>2</sub> ratio. Beyond this CO/H<sub>2</sub> ratio, the methane composition is continuously decreasing and reaches 0.73 mole fraction at highest CO/H<sub>2</sub> ratio (0.504). Hence it has concluded that the 0.328 is ideal CO/H<sub>2</sub> ratio at which maximum methane mole fraction is expected. On the safe side, the range of CO/H<sub>2</sub> ratio from 0.32 to 0.38 was observed ideal to get more than 90% methane in SNG product.

The effect of variation in ratio of CO/H<sub>2</sub> on energy required to cool raw SNG product from reactor is shown in Fig. 10. It was observed that initially the cooling energy demand is increasing with increase in CO/H<sub>2</sub> at slower slope after the optimized CO/H<sub>2</sub> ratio (i.e., 0.328) the energy is decreasing at much higher slope. The reason for this trend can be explained by observing the other gases in raw product stream which are unreacted CO and  $H_2$  which is shown in Fig. 11. It was observed that initially  $H_2$  is higher and decreases by increasing  $CO/H_2$  ratio up to its optimized value i.e., 0.328. At this optimized value of CO/H<sub>2</sub> ratio, the CO starts increasing. Now the heat capacity of H<sub>2</sub> is 14.31 kJ/kg. K. Whereas the heat capacities of CO and CH<sub>4</sub> at ambient temperature are 1.045 kJ/kg and 2.2 kJ/kg. K respectively. Both these gases are lower in their heat capacities and hence have less impact to heat or cool the gas where these are in higher fraction in the product gas. The maximum energy for cooling the raw SNG achieved is 118340 kJ/hr.



Fig. 10: Effect of syngas feed composition on methane composition in produced SNG and energy required for cooling operation



Fig. 11: Composition of CO and H<sub>2</sub> in product gases at varying CO/H<sub>2</sub> ratio in feed stream

A comparison of current study with the findings of other researchers [4, 20, 27, 28] is summarized in Fig. 12. The comparison is made on the basis of CH<sub>4</sub> composition in SNG. It was observed that current study showed maximum CH<sub>4</sub> in the produced SNG i.e., 97% as compared to other researchers. It is due to the assumption that in current study the feed was assumed to have only CO and H<sub>2</sub> instead of other usual components like CO<sub>2</sub>, H<sub>2</sub>O etc.



Fig. 12: The comparison of maximum mole fraction of CH4 in SNG between current research and literature

# 4.8 ECONOMIC EVALUATION OF THE PROCESS

The economic evaluation of the whole process was also conducted on detailed process developed in Aspen Plus software. The Aspen Economic Evaluator tool was used to conduct economical evaluation of the process. The various costs like total capital cost, total equipment and installation costs, operating costs and cost of utilities are estimated and shown in Fig. 12 (a & b)

From the figures it was observed that the total capital cost including the cost of gasification and gas cleaning system would be 21.47 million US\$. The cost of equipment was estimated 9.18 million US\$ whereas cost of installation of whole plant was estimated 14.18 million US\$. On the other side, the total operating and cost of utilizes were estimated 27.0883 million US\$ and 23.4 million US\$. The estimated cost was calculated on the basis of 20 years payback period.



Fig. 12: Economic evaluation of the developed process. (a) Total Capital Cost, Equipment Cost and Total Cost of Installation (b) Total Operating Cost and Cost of Utilities

### 5. CONCLUSION

This study employs Aspen HYSYS and Aspen PLUS to simulate converting syngas into synthetic natural gas (SNG), evaluating the impact of key operational factors like syngas flow, temperature, pressure, composition, and TEG rate on process performance and economics. SNG production linearly increased with syngas flow, at a rate of 0.57 kg/hr SNG per kg/hr syngas. HHV of produced SNG non-linearly decreased with increasing syngas flow, with a maximum of 786219.7 kJ/kgmole at 20 kg/hr and a minimum of 757185.2 kJ/kgmole at 100 kg/hr. CH4 mole fraction in SNG also decreased non-linearly with syngas flow. Cooling energy requirement for raw SNG increased linearly with syngas flow. SNG production rate, HHV, and CH4 content were insensitive to syngas feed temperature, while cooling energy increased linearly with temperature. All metrics were unaffected by varying syngas feed pressure. CO/H2 ratio impacted syngas performance, with optimal CO/H2 range of 0.32 to 0.38 for over 90% methane. Peak cooling energy was 118340 kJ/hr. Total capital cost was around 21.47 million US\$, including 9.18 million US\$ for equipment and 14.18 million US\$ for plant installation.

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