International Journal of Biological, Physical and Chemical Studies
ISSN: 2709-1554
DOI: 10.32996/ijbpcs
Journal Homepage: www.al-kindipublisher.com/index.php/ijbpcs

IJBPCS

AL-KINDI CENTER FOR RESEARCH AND DEVELOPMENT

| RESEARCH ARTICLE

Determination of the Optimum Operating Conditions for Integrated Methanol and Ethanol Plant from Natural Gas Reactors

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| ABSTRACT

Methanol and ethanol can be produced from many kinds of feedstock. One of the most preferred methods to synthesize methanol is from natural gas, which is reformed to form synthesis gas (syngas) and converted by a catalyst to form methanol. Conversely, ethanol production mostly comes from biomass, which competes with human food fulfilment. Several pieces of literature conduct syngas transformation to ethanol to solve this problem. However, the experiment is conducted on a lab scale or pilot scale. Before the technology can be mass-produced on a plant scale, we must determine the most suitable operating condition for the reactor to escalate the reactor's productivity. This study is aimed to determine the optimal operating condition for the integrated methanol and ethanol plant, which is the reactors. The software used for the study is Aspen Plus V12.1. The independent variables for all the reactors in this study are the pressure (P) and the temperature (T). We add the feed molar flow ratio as the independent variable for the Steam Methane Reforming (SMR) and the ethanol synthesis reactor. The dependent variable that will be used for the determination of the optimal operating condition of the reactors is the reactant conversion and the product yield. The data validation between the experimental data conducted by other authors and the process modeling result is in good agreement with less than 6% of error for all three reactors. After performing the process simulation and sensitivity analysis to determine the optimal operating condition for the reactors, it is found that the optimal operating condition for the reactors is as follows: (1) SMR reactor: 25 bar pressure, 1,223 K temperature, feed molar flow ratio (H_2O/CH_4 ratio) of 3, (2) methanol synthesis reactor: 100 bar pressure and 503 K temperature, and (3) ethanol synthesis reactor:110 bar pressure, 583 K temperature, and feed molar flow ratio (H_2/CO ratio) of 0.75.

| KEYWORDS

Catalytic conversion, experimental data validation, natural gas reforming, process modeling, sensitivity analysis

| ARTICLE INFORMATION

ACCEPTED: 30 March 2023 **PUBLISHED:** 03 April 2023 **DOI:** 10.32996/ijbpcs.2023.5.1.2

1. Introduction

Methanol and ethanol can be used as a standalone fuel or mixed with other chemicals, such as gasoline [Khadzhiev, 2016] [Waluyo, 2021]. The example of most preferred method to synthesize methanol is from natural gas, which is done by reforming the natural gas to produce synthesis gas (syngas) and then converting the syngas with a catalyst to produce methanol [Zhang, 2016]. The methanol synthesis from the syngas process has been studied extensively in the world before [Blumberg et al. 2017]. In contrast, the most popular method to synthesize ethanol is the biomass fermentation process, which competes with the fulfilment of human sources of foods [Mussatto, 2010]. To solve the problem, several pieces of literature have been conducted on the synthesis of

ethanol from other methods, such as carbon dioxide, dimethyl ether, and syngas (carbon monoxide and hydrogen) [Tabassum, 2021].

One of the promising ways of synthesizing ethanol from natural gas is via the syngas route, which could be produced from natural gas by reforming the natural gas. By reforming the natural gas to produce syngas, we could synthesize both methanol and ethanol simultaneously. Several pieces of literature already conduct the catalytic transformation of syngas to ethanol on a bench or pilot scale. Kulawska and Skrzypek reported in their study that their Cu/ZnO catalyst could produce C_1-C_5 alcohols with CO conversion of up to 50% [Kulawska, 2001]. Yin et al. proposed the Rh-Mn-Li-Fe/SiO_2 catalyst to convert the syngas to produce ethanol and other products such as propanol, butanol, acetaldehyde, and ethyl acetate [Yin, 2002]. However, the side products that are made will require us to have a complex separation system. One of the most promising catalysts to be explored further is the K-Co-MoS_2 catalyst reported by Portillo et al., where they successfully synthesize ethanol with relatively simple side products such as methanol, propanol, methane, and carbon dioxide [Portillo, 2016].

However, to produce ethanol on a much bigger scale, we must scale up the experiment conducted that has been done before. To scale up the process, we must determine the operating condition of the essential equipment of the plants, which is the reactors. The literature discussed before has not yet determined the optimal operating condition for methanol and ethanol on a plant scale. At one time, the optimal operating condition of the reactors is needed to maximize the plant's productivity and minimize the feedstock used for the operation of the plant. We could use process simulation software to test the reactions on a larger scale to determine the reactor's optimal operating condition. Examples of operating conditions that could influence the reactor's performance are pressure, temperature, and feed molar flow ratio entering the reactor [Portillo, 2016], which is the independent variable of the reactor. We can determine the optimal operating condition by varying the independent variable, such as the pressure, the temperature, and the feed molar flow ratio, to see their effect on the dependent variable, such as the reactant's conversion or the product's yield [De, 2020]. Also, before the process simulation is conducted, we must ensure that the real-world experiment and the process simulation result agree with each other, called the process modeling data validation stage.

Therefore, in this study, we focused on determining the optimal operating condition of the reactors in an integrated methanol and ethanol production plant with process simulation software. This study evaluates the impact of several parameters, such as the pressure and the temperature, to determine the most optimum operating condition for the reactors by considering the reactant's conversion and the yield of the product. For the SMR reactor and the ethanol synthesis reactor, we add the feed molar flow ratio as one of the independent variables. Furthermore, this study will also check the data validation between the experimental data conducted on the bench or pilot scale and the process modeling data so the process modeling simulation will agree well with the application in the real world.

2. Methodology

This study involved two primary stages in general: data validation, process modelling, and sensitivity analysis. All the stages are conducted by using the Aspen Plus V12.1 software. Due to the presence of polar compounds capable of creating an azeotrope with one another, such as methanol, ethanol, and propanol, the selected thermodynamics property package is the Universal Quasichemical (UNIQUAC) – Soave-Redlich-Kwong (SRK) [De, 2020]. The natural gas used for process modeling is the South Sumatra West Java (SSWJ) transmission pipe's natural gas [Azmi, 2020].

2.1. Data Validation

The initial stage of this study involves comparing the data obtained from real-world experiments with the process modelling result. The data validation stage aims to ensure that the process modelling result outcomes accurately reflect real-world conditions. In this study, it is set that the maximum average error between the experimental result and the process modelling result is 10% for the data to be considered valid. Also, we conduct the process modeling data validation by referencing the experimental model reported by the paper.

The first reactor under consideration is the SMR reactor, which consists of these reactions: (1) steam reforming of methane (SRM), which reacts the methane with the water to form syngas, (2) water-gas shift (WGS), which react the carbon monoxide and water, and (3) reverse CO_2 methanation (RCM) reactions, which is the global reaction occurred in this reactor. These three reactions are shown in Table 1 in Equations 1-3. To model these reactions, the Langmuir-Hinshelwood-Hougen-Watson (LHHW) modeling and kinetic rate expressions were used. Specifically, this study utilized the kinetic rate expression introduced in the research conducted by Xu and Froment (1989) using Ni/$MgAl_2O_4$ catalyst, shown in Table 2 at Equations 12-15 [Xu, 1989].

The second reactor considered in this study is the methanol synthesis reactor, which involves three reactions: (1) carbon monoxide hydrogenation (CMH), which reacts the carbon monoxide with hydrogen to form methanol, (2) reverse water-gas shift (RWGS), which react the carbon dioxide and hydrogen, and (3) carbon dioxide hydrogenation (CDH), which is the global reaction occurred

in this reactor. These three reactions are shown in Table 1 in Equations 4-6. Similar to the SMR reactor, The LHHW modeling and kinetic rate expressions were utilized to simulate the reactions in the methanol synthesis reactor. This study utilized Cu/Zn/Al/Zr catalyst and kinetic rate expression introduced in the research reported by Kiss et al. (2016), shown in Table 2 at Equations 16-19 [Kiss, 2015].

The third reactor evaluated in this study is the ethanol synthesis reactor, which involves five reactions: (1) carbon monoxide hydrogenation (CMH), which produces methanol, (2) ethanol synthesis (ETS), which uses methanol to produce ethanol, (3) propanol synthesis (PRS), which used ethanol to produce ethanol, (4) methanol hydrogenation (MTH), which form methane from methanol, and (5) water-gas shift (WGS) reactions. These five reactions are shown in Table 1 in Equations 7-11. Both power law and the LHHW modeling and kinetic rate expressions were employed to simulate the reactions that occurred. In this study, the kinetic rate expression proposed by Portillo et al. (2016) over K/Co/MoS_2 catalyst was utilized and is shown in Table 2 at Equations 20-25 [Portillo, 2016].

Table 1. Reactions occurred in the SMR, methanol synthesis, and ethanol synthesis reactors [Kiss et al. 2015**].**

Steam Methane Reforming (SMR) Reactor

$$\text{SRM: } CH_4 + H_2O \rightleftharpoons CO + 3H_2;\ \Delta H^o_{298K} = +206.0\frac{kJ}{mol} \quad (1)$$

$$\text{WGS: } CO + H_2O \rightleftharpoons CO_2 + H_2;\ \Delta H^o_{298K} = -41.0\frac{kJ}{mol} \quad (2)$$

$$\text{RCM: } CH_4 + 2H_2O \rightleftharpoons CO_2 + 4H_2;\ \Delta H^o_{298K} = +165.0\frac{kJ}{mol} \quad (3)$$

Methanol Synthesis Reactor

$$\text{CMH: } CO + 2H_2 \rightleftharpoons CH_3OH;\ \Delta H^o_{298K} = -90.8\frac{kJ}{mol} \quad (4)$$

$$\text{RWGS: } CO_2 + H_2 \rightarrow CO + H_2O;\ \Delta H^o_{298K} = +41.2\frac{kJ}{mol} \quad (5)$$

$$\text{CDH: } CO_2 + 3H_2 \rightarrow CH_3OH + H_2O;\ \Delta H^o_{298K} = -49.1\frac{kJ}{mol} \quad (6)$$

Ethanol Synthesis Reactor

$$\text{CMH: } CO + 2H_2 \rightarrow CH_3OH \quad (7)$$

$$\text{ETS: } CH_3OH + CO + 2H_2 \rightarrow C_2H_5OH + H_2O \quad (8)$$

$$\text{PRS: } C_2H_5OH + CO + 2H_2 \rightarrow C_3H_7OH + H_2O \quad (9)$$

$$\text{MTH: } CH_3OH + H_2 \rightarrow CH_4 + H_2O \quad (10)$$

$$\text{WGS: } CO + H_2O \rightleftharpoons CO_2 + H_2 \quad (11)$$

Table 2. Kinetic rate expression for the reactions occurred in the SMR, methanol, and ethanol synthesis reactors [Kiss et al. 2015**].**

Steam Methane Reforming (SMR) Reactor

$$\text{SRM: } r_{CO} = \frac{k_1}{p_{H_2}^{2,5}}\left[p_{CH_4}p_{H_2O} - \frac{p_{H_2}^3 p_{CO}}{K_{eq,1}}\right]\left(\frac{1}{\kappa}\right)^2 \quad (12)$$

$$\text{WGS: } r_{CO_2} = \frac{k_2}{p_{H_2}}\left[p_{CO}p_{H_2O} - \frac{p_{H_2}p_{CO}}{K_{eq,2}}\right]\left(\frac{1}{\kappa}\right)^2 \quad (13)$$

$$\text{RCM: } r_{CO_2} = \frac{k_3}{p_{H_2}^{3,5}}\left[p_{CH_4}p_{H_2O}^2 - \frac{p_{H_2}^4 p_{CO_2}}{K_{eq,3}}\right]\left(\frac{1}{\kappa}\right)^2 \quad (14)$$

$$\kappa = 1 + K_{CO,SMR}p_{CO} + K_{H_2,SMR}p_{H_2} + K_{CH_4,SMR}p_{CH_4} + K_{H_2O,SMR}\frac{p_{H_2O}}{p_{H_2}} \quad (15)$$

Methanol Synthesis Reactor

$$\text{CMH: } r_{CH_3OH} = k_4\left[\frac{K_{CO,MeOH}\left[p_{CO}p_{H_2}^{\frac{3}{2}} - \left(\frac{1}{K_{eq,4}}\right)\left(\frac{p_{CH_3OH}}{p_{H_2}}\right)\right]}{\phi}\right] \quad (16)$$

$$\text{RWGS: } r_{CO} = k_5\left[\frac{K_{CO,MeOH}\left[p_{CO}p_{H_2}^{\frac{3}{2}} - \left(\frac{1}{K_{eq,5}}\right)\left(\frac{p_{CH_3OH}}{p_{H_2}}\right)\right]}{\phi}\right] \quad (17)$$

$$\text{CDH: } r_{CH_3OH} = k_6\left[\frac{K_{CO,MeOH}\left[p_{CO}p_{H_2}^{\frac{3}{2}} - \left(\frac{1}{K_{eq,6}}\right)\left(\frac{p_{CH_3OH}}{p_{H_2}}\right)\right]}{\phi}\right] \quad (18)$$

$$\phi = \left(1 + K_{CO,MeOH}p_{CO} + K_{CO_2,MeOH}p_{CO_2}\right)\left(p_{H_2}^{0,5} + \frac{K_{H_2O,MeOH}}{K_{H_2,MeOH}^{0,5}}p_{H_2O}\right) \quad (19)$$

Ethanol Synthesis Reactor

$$\text{CMH: } r_{CH_3OH} = k_{0,7}\exp\left(-\frac{E_7}{RT}\right)P_{CO}^{A}P_{H_2}^{B} \quad (20)$$

$$\text{ETS: } r_{C_2H_5OH} = k_{0,8}\exp\left(-\frac{E_8}{RT}\right)P_{CO}^{E}P_{H_2}^{F}P_{CH_3OH}^{G} \quad (21)$$

$$\text{PRS: } r_{C_3H_7OH} = k_{0,9}\exp\left(-\frac{E_9}{RT}\right)P_{CO}^{H}P_{H_2}^{I}P_{C_2H_5OH}^{J} \quad (22)$$

$$\text{MTH: } r_{CH_4} = k_{0,10}\exp\left(-\frac{E_{10}}{RT}\right)P_{H_2}^{C}P_{CH_3OH}^{D} \quad (23)$$

$$\text{WGS: } r_{CO_2} = k_{0,11}\exp\left(-\frac{E_{11}}{RT}\right)[P_{CO}P_{H_2} - \frac{k_x}{k_{WS}}P_{CO_2}P_{H_2}] \quad (24)$$

$$k_x = 0.85;\ k_{WS} = \exp\left(-\frac{\Delta G_{WS}}{RT}\right);\ \Delta G_{WS}\ [\text{cal/mol}] = -8514 + 7.17\ T(K) \quad (25)$$

2.2. Process Modeling and Sensitivity Analysis

After the experiment data and the process modeling data are validated, the next step of the study is to do the process modeling. Figures 1-3 illustrate the process flow diagram used in the process. In the Aspen Plus configuration, we used the fixed bed reactor with the isothermal configuration (reactor with constant specified temperature) to better simulate the real-world experiment with the process modelling simulation. The data inputted for the process modeling configurations are available from the same references as the process modeling data validation step [Xu et al. 1989]. Note that the configuration of the reactors in this plant is as follows: the first reactor is the SMR reactor, which then the syngas is separated into two reactors, the methanol synthesis reactor and the ethanol synthesis reactor. The reactor's configuration is also necessary because we are also minorly considering the other effect, such as the selected operating condition's implication to the overall process.

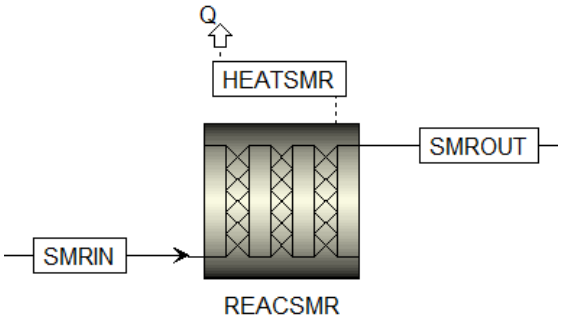

Figure 1. SMR reactor illustration for sensitivity analysis

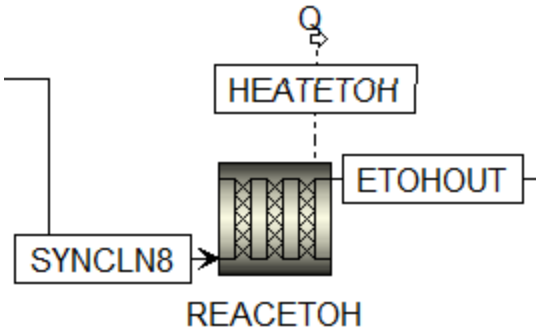

Figure 2. Ethanol synthesis reactor illustration for sensitivity analysis

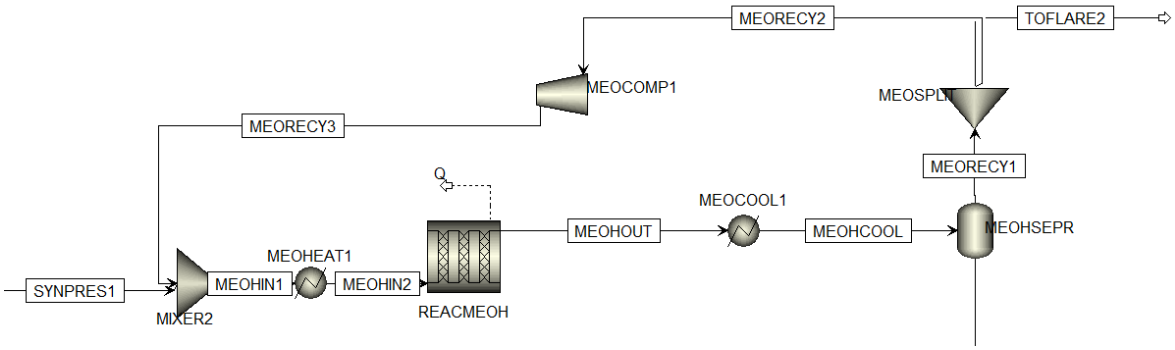

Figure 3. Methanol synthesis reactor illustration for sensitivity analysis

Sensitivity analysis is done at the reactors' configuration to determine the optimal operating condition. The sensitivity analysis range is conducted within the range with the usual range of operating conditions based on real-world applications, except for the ethanol synthesis reactor, which used the same literature as the data validation step, as the ethanol synthesis reactor is not commercially available in the world yet. The independent variable (the operating condition varied) included in this study is the pressure, the temperature, and the feed molar flow ratio (only for SMR and ethanol synthesis reactor). The three variables varied to see their effect on the dependent variable: the reactant's conversion and the product yield.

3. Results and Discussion

3.1. Process Modeling Data Validation

This study's process modeling data validation is conducted on all three reactors. This data validation is conducted by comparing the reactant's conversion of each reactor in the experimental result and the process modeling result. Table 3 below displays the conversion error of CH_4, CO_2, and CO between the process modeling and the experimental result.

The first reactor is the SMR reactor. Its kinetic rate expressions and data model are based on the experimental result from Xu and Froment [1989]. According to the data validation, it is shown that the average error between the experimental result and the process modeling result is 1.48% at a constant temperature of 848 K. The second reactor is the methanol synthesis reactor. The data model and kinetic rate expressions are derived from the experimental result by An et al. [2009]. It is shown that the average error between the experimental and process modeling data is 4.50% at a constant temperature of 523 K. The third reactor is the ethanol synthesis reactor, and the kinetic rate expression and data model is derived from the experimental result by Portillo et al. [2016]. The data validation shows that the average error between the experimental and process modeling data is 5.64% at a constant temperature of 583 K. The conversion errors of each reactor are less than 6%. Therefore, it can be concluded that the kinetic rate expression and data model is reliable and suitable for design purposes.

Table 3. Experimental and process modeling result data comparison for the three reactors.

Steam Methane Reforming (SMR) Reactor		
W/F_{CH4} (gcat.h/mol)	CH_4 Conversion (Experiment)	CH_4 Conversion (Simulation)
0,1	8.49%	8.84%
0,2	12.21%	12.34%
0,3	13.75%	13.73%
0,4	14.36%	14.28%
Methanol Synthesis Reactor		
GHSV (mL/gcat.h)	CO_2 Conversion (Experiment)	CO_2 Conversion (Simulation)
1000	26.20%	24.29%
2000	26.00%	24.29%
4000	25.60%	24.23%
6000	25.00%	23.99%
8000	24.30%	23.62%
100000	23.00%	23.21%
Ethanol Synthesis Reactor		
W/F_{CO} (kgcat.s/kmol)	CO Conversion (Experiment)	CO Conversion (Simulation)
46670	18.07%	19.09%
57930	25.37%	24.21%
74670	32.69%	31.71%
93330	39.76%	39.69%
115820	55.22%	48.15%
152730	62.75%	59.31%

3.2. Process Modeling and Sensitivity Analysis

In this study, process modeling and sensitivity analysis are employed to identify the optimal operating conditions for the three reactors: the SMR, the methanol synthesis, and the ethanol synthesis reactors. The main operating conditions studied in this study are pressure (P) and temperature (T). Note that for the SMR and ethanol synthesis reactor, the feed molar flow ratio is also included as a variable. The sensitivity analysis range is obtained from other literature sources [Zhang et al. 2021]. The main operating conditions of the process are varied to determine their impact on the dependent variable, such as the reactant conversion and the product yield of the reactors. The process modeling and sensitivity analysis results are presented in Figures 3-10.

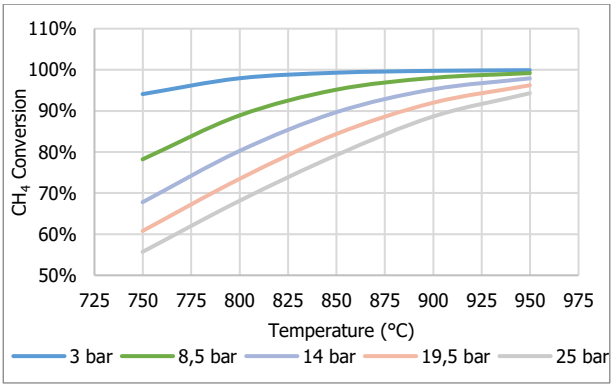

Figure 3. Impact of the SMR reactor temperature on the CH_4 conversion at various pressure values

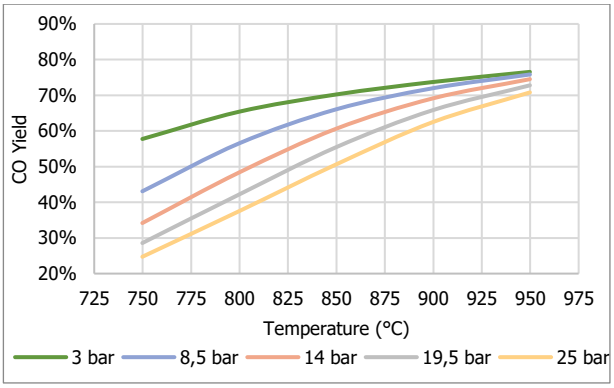

Figure 4. Impact of the SMR reactor temperature on the CO yield at various pressure values

Figures 3 and 4 above show the effect of pressure and temperature on CH_4 conversion and CO yield of the SMR reactor. The SMR reactor's pressure is varied within the ranges of 3 bar-25 bar, the temperature is varied within the ranges of 750°C-950°C, and the feed molar flow rate ratio (H_2O/CH_4) is varied within ranges of 0.5-5 [Mohanty et al. 2021]. Within the same residence time at the reactor, as pressure and temperature increase, the CH_4 conversion and CO yield in the reactor also increase. This outcome is expected based on Equations 1-3, which state the reaction occurring in the SMR reactor. According to Le-Chatelier's principle, the increased pressure causes the reaction equilibrium to favor the side with fewer molecules, i.e., the reactant side, resulting in decreased CH_4 conversion in the reactor.

Conversely, an increase in temperature leads to a shift in the reaction equilibrium towards the side with an endothermic reaction, i.e., the product side, leading to an increase in CO yield in the reactor. Therefore, choosing the lowest pressure and the highest temperature within the sensitivity analysis range is suggested. However, since the methanol synthesis reactor operates at a higher pressure, selecting the lowest pressure for the SMR reactor operating condition would require additional compressors, increasing the process's capital cost with little benefit. As a result, it would be best to operate the SMR reactor at a pressure of 25 bar.

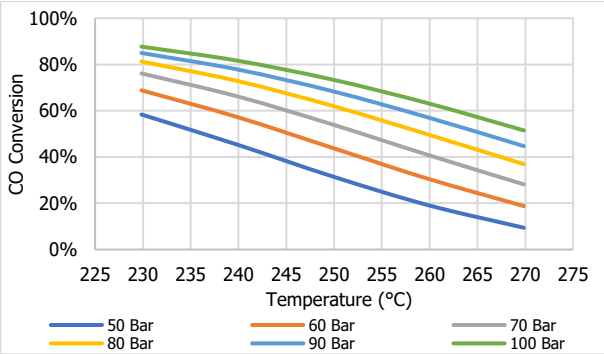

Figure 5. Impact of the methanol synthesis reactor temperature on the CO conversion at various pressure values

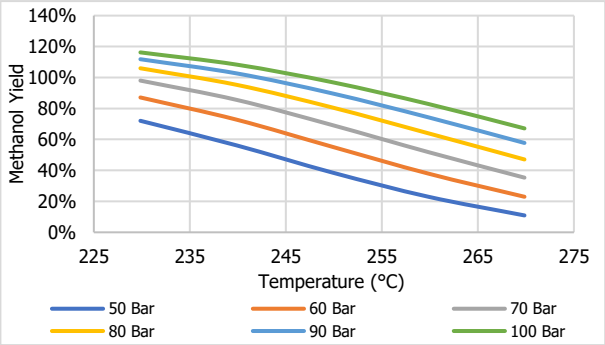

Figure 6. Impact of the methanol synthesis reactor temperature on the methanol yield at various pressure values

Next, Figures 5 and 6 above show the effect of pressure and temperature on the methanol synthesis reactor's CO conversion and methanol yield. The methanol synthesis reactor's pressure is varied between 50 bar-100 bar, and the temperature is varied between 230°C-270°C [Bozzano, 2016]. As the pressure increases, the CO conversion and methanol yield also increases. According to Equations 4-6, which show the reactions occurring in the methanol synthesis reactor, and Le-Chatelier's principle, the equilibrium of the reaction favors the product side, which has fewer molecules, as pressure increases. Similarly, increasing the temperature favors the endothermic reaction on the reactant side. Therefore, selecting the maximum pressure (100 bar) and minimum temperature (230°C) is recommended to increase both the CO conversion and methanol yield in the methanol synthesis reactor.

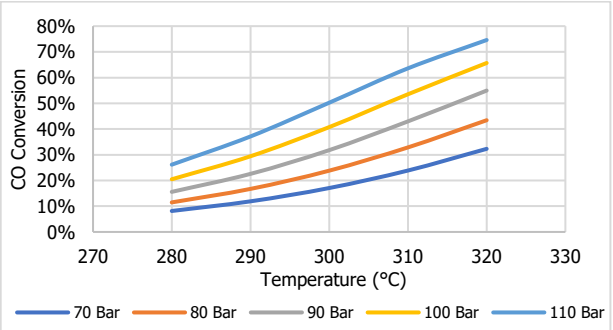

Figure 7. Impact of the ethanol synthesis reactor temperature on the CO conversion at various pressure values

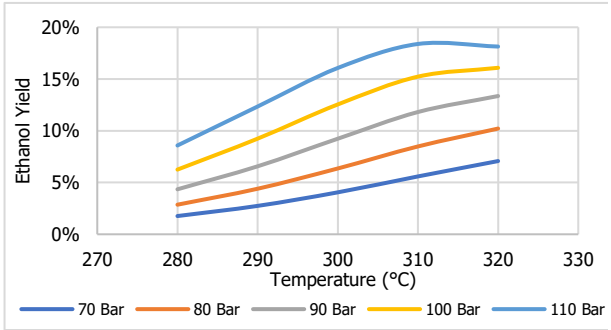

Figure 8. Impact of ethanol synthesis reactor temperature on the ethanol yield at various pressure values

Subsequently, Figures 7 and 8 above show the effect of pressure and temperature on the ethanol synthesis reactor's CO conversion and ethanol yield. The ethanol synthesis reactor's pressure is varied between 70 bar-110 bar, the temperature is varied between 280°C-320°C, and the feed molar flow ratio (H_2/CO ratio) is varied within the 0.5-2 range [Portillo, 2016]. As the pressure and

temperature increase, the CO conversion increases. Similarly, but not identically, the ethanol yield increases and then decreases at a temperature higher than 310°C. This trend may be caused by the reaction mechanism in the ethanol synthesis reactor, which differs from the previous reactors as it comprises five distinct, sequential, and parallel reactions. At temperatures above 310°C (Pressure = 110 bar), the propanol synthesis reaction is likely to occur more quickly than the ethanol synthesis reaction, leading to a decrease in the ethanol yield and an increase in CO conversion. Thus, we select the ethanol synthesis reactor's operating condition at 310°C temperature and 110 bar pressure.

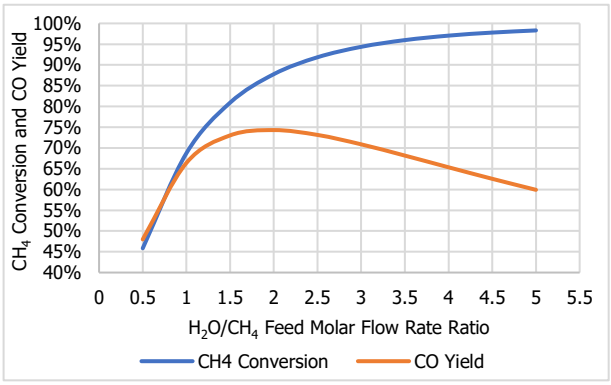

Figure 9. Impact of the H_2O/CH_4 molar flow ratio inlet into the SMR reactor on the CH_4 conversion and CO yield

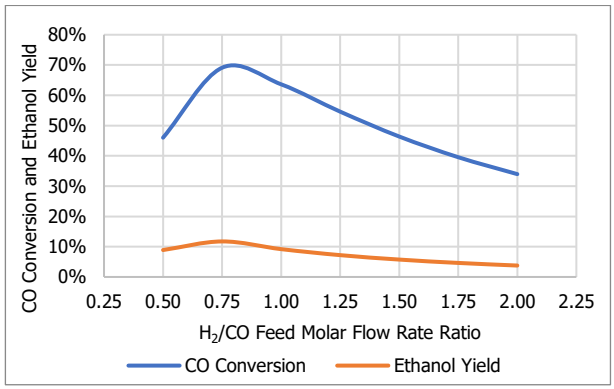

Figure 10. Impact of the H_2/CO molar flow ratio inlet into the ethanol synthesis rector on the CO conversion and ethanol yield

In addition to the effect of pressure and temperature, we also studied the impact of the feed molar flow rate ratio of the SMR reactor and ethanol synthesis reactor, shown in Figures 9 and 10. For the SMR reactor, the CH_4 conversion increases as the feed molar flow rate ratio (H_2O/CH_4 ratio) increases. This phenomenon could be expected because as the number of H_2O increases, the number of reacting CH_4 molecules also increases, in accordance with the reaction in the SMR reactor. However, the CO yield initially rises and reaches its maximum at a feed molar flow rate ratio of 2 but then declines as the feed molar flow rate increases. This phenomenon occurs due to the reaction mechanism that occurs in the SMR reactor, where the WGS reaction uses up CO to generate CO_2, thereby reducing the overall yield of CO. As a result, an H_2O/CH_4 feed molar flow rate ratio of 3 for the SMR reactor is chosen.

Lastly, for the ethanol synthesis reactor, the CO conversion and ethanol yield first increase and then start to decrease with an increasing H_2/CO feed molar flow rate ratio. The reaction mechanism in the ethanol synthesis reactor, which involves both sequential and parallel reactions, may explain this phenomenon. Increasing the H_2 molar flow rate leads to more CO reacting in the reactor. However, based on Equation 11, which describes the water-gas shift reaction, where CO and H_2O are in equilibrium with CO2 and H2 under constant temperature and pressure conditions, we can expect an increase in CO concentration with an increase in H_2, as there are no temperature and pressure variations. We should choose the H_2/CO feed molar flow ratio with the highest CO conversion and ethanol yield to maximize CO conversion and ethanol yield. Hence, this reactor's selected feed molar flow rate ratio is 0.75.

4. Conclusion

In this study, the operating conditions of Steam Methane Reforming (SMR), methanol synthesis, and ethanol synthesis reactors are determined using process simulation and sensitivity analysis. The SMR reactor is used to convert the natural gas to synthesis gas (syngas), which later would be converted by the catalyst in the reactor to produce both methanol and ethanol. The study also validated the experimental data performed in the real world and the process modelling simulation to confirm that the result produced in the process modelling simulation agree with each other.

This study shows that the reactant conversion average error for the SMR reactor is 1.48% (T = 848 K), for the methanol synthesis reactor is 4.50% (T = 523 K), and for the ethanol, synthesis reactor is 5.64% (T = 583 K). The average errors for all the reactors are lower than the maximum error required, which is 10%, so the process simulation is considered valid. Moreover, it is determined that the optimal operating conditions for the SMR reactor are at a pressure of 25 bar, a temperature of 950°C, and a feed molar flow ratio of 3. The optimal operating condition for the methanol synthesis reactor is at a pressure of 100 bar and a temperature of 230°C. Lastly, the optimal operating condition for the ethanol synthesis reactor is at a pressure of 110 bar, a temperature of 310°C, and a feed molar flow ratio of 0.75.

Highlights

1. Natural gas reformation to produce syngas and then reacted with a catalyst to form methanol and ethanol, which consists of three reactors: (1) the Steam Methane Reforming (SMR), (2) the methanol synthesis reactors, and (3) the ethanol synthesis reactors.
2. Data validation between the reactor's experimental result and the reactor's process modelling result on Aspen Plus V12.1 software.
3. Impact investigation of the pressure and temperature for all reactors and the feed molar flow ratio of the SMR and ethanol synthesis reactor on the reactants' conversion and products' yield.

Declaration of Competing Interest: The authors of this paper state that they have no financial interests or personal relationships that could influence the findings or conclusions reported in this paper

Acknowledgement: We acknowledge the scholarship called "Ganesha Talent Assistantship" that was granted to Dimas Laksana Yudharaputra by Institut Teknologi Bandung, Indonesia.

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