Techno-Economic Assessment of Conceptual Design for Methanol Production Using Coal and Natural Gas Based Parallel Process Configuration

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Abstract

Methanol production has gained a lot of attention due to its wide application in both the process and product industries. This study aims to investigate the coal/methane based process for simultaneous methanol and power generation. Two process models were developed in Aspen Plus and techno-economically compared. Case 1 is taken as a base case model that represents the coal to methanol (CTM) technology. Case 2 represents the sequential integration between the coal gasification and methane reforming technologies to enhance both the synthesis gas and methanol production capacity. It has been seen from results that case 2 design has a potential to boost up the methanol production compared to the case 1 design. In terms of process performance, the overall process efficiencies for the case 1 and case 2 is calculated as 63.2\% and 70.0\%, respectively. Moreover, the carbon conversion efficiency for case 2 design is nearly 6\% higher than the case 1 design. In terms of methanol production cost, case 1 and case 2 offered 0.25€/kg and 0.23€/kg, respectively. While evaluating other process performance and environmental quality control indicators, it has been analysed from results that case 2 offers higher process feasibility compared to the case 1 design.

Keywords: Gasification, Reforming, Methanol Synthesis, Synthesis Gas.

1. Introduction

During the last many decades, fossil fuels remained the main source of energy and power generation that not only increased the greenhouse gas emissions to unsafe levels but also caused global warming. The damaged caused by fossil fuels to environment especially by the coal based systems can be minimized using an alternative energy conversion technologies. The conventional routes of producing the methanol from fossil fuel includes two stages. In the first stage, the synthesis gas is generated from fuel which is then cleaned prior to its conversion into methanol. Natural gas to methanol (NGTM) technology has been extensive utilized around the world to meet the methanol production and supply demand. The synthesis gas can be efficiently converted to methanol if the HCR (hydrogen to carbon) ratio in the synthesis gas is between 2-2.05. Usually, steam methane reforming (SMR) technology is used to generate synthesis gas from natural gas which offers higher HCR in the synthesis gas. On the other hand, coal to methanol (CTM) converts the coal into synthesis gas by the gasification technologies. The synthesis gas generated from the coal has a lower value HCR and contains more CO\textsubscript{2} and CO. The synthesis gas from the coal gasification process is usually integrated with the water gas shift (WGS) reactors to
convert the CO in the synthesis gas to H\textsubscript{2} on reaction with the H\textsubscript{2}O. Yi et al. (2015) reported that CTM technologies produces 2.6 ton of CO\textsubscript{2} for each ton of methanol (MeOH) production, whereas, SMR technologies offers higher HCR ratio in the synthesis gas and shows very less CO\textsubscript{2} emissions. Comparing the current prices and reserves of natural gas and coal, the opportunities to develop the dual fuel conversion technologies have gained a lot of attention. The SMR and coal derived synthesis gas can be mixed to regulate the higher HCR ratio at the inlet of methanol synthesis reactor. Recently, Blumberg et al. (2019) integrated the different methane reforming technologies for enhancing the H\textsubscript{2} production, which offers higher exergetic efficiency for methanol synthesis. Ahmed et al. (2017, 2019) also showed an improvement in the power and H\textsubscript{2} production by integrating the gasification and reforming technologies in the series design configuration. Similarly, Kler et al. (2018) proposed a model for simultaneous production of methanol and electricity from coal. Chen et al. (2019) developed a model using multiple feed-stocks for MeOH synthesis while reducing the CO\textsubscript{2} emissions. In this study, coal and natural gas feed-stocks are used for the MeOH synthesis and electricity production by using the parallel design integrations between the gasification and reforming technologies. The key idea of this research is to utilize the heat energy from the gasification unit into the reforming unit to sustain the high enthalpy SMR reactions. This integration not only reduces the overall process energy requirements but also enhances the syngas production with the higher HCR ratio. The focus of this research article is to perform the techno-economic analysis of the proposed design and its comparison with the conventional processes.

2. Process Simulation and Methodology

The process models were developed in Aspen Plus v10 where Peng Robinson with Boston Mathias equation of state is selected as an effective thermodynamic package. Coal is usually considered as an unconventional component and its composition is defined in terms of key components through Proximate, ultimate and sulfanal analysis. RGibbs reactor model is selected for the modelling of gasification, water gas shift, reforming and methanol synthesis reactor which generates the reaction products on the principle of Gibbs free energy minimization. Table 1 highlights some of the design assumptions for the design of major unit processes.

<table>
<thead>
<tr>
<th>Unit/Component/System</th>
<th>Modelling Unit</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gasification Reactor</td>
<td>RGibbs (Reactor)</td>
<td>Coal flow rate= 62.01kg/s \n Temp/Press: 1350-1370°C/56 bar</td>
</tr>
<tr>
<td>Reformer</td>
<td>RGibbs (Reactor)</td>
<td>NG flow rate: 5.5 kg/sec \n H\textsubscript{2}O:CH\textsubscript{4} = 3:1 \n Temp/Press: 900°C/32 bar</td>
</tr>
<tr>
<td>Air Separation Unit (ASU)</td>
<td>HeatX, Compr</td>
<td>Oxygen Purity 95% (vol)</td>
</tr>
<tr>
<td>Methanol Reactor</td>
<td>RGibbs (Reactor)</td>
<td>Cu based catalyst \n Pressure/Temp: 55bar/200°C</td>
</tr>
</tbody>
</table>

2.1. Case 1- Conventional Coal to Methanol (CTM) Process

Case 1 is considered as a conventional CTM where coal water slurry is fed to the coal gasification unit at 56bar, which is partially oxidized to generate synthesis gas at the
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The synthesis gas is then cooled in the radiant and convective heat exchangers followed by H₂S removal. The sulphur free synthesis gas is then passed over the Cu based catalyst in the methanol reactor at the standard temperature and pressure of 200°C and 55 bar. Figure 1 represents the conventional methanol production process from coal. Finally, series of flash drums and distillation columns are sequentially used in the downstream process chain to enhance the purity of methanol in the product stream to 99%.

2.2. Case 2- Coal and Natural Gas based Process for Methanol Production (CNPM)

Case 2 is considered as a conceptual design where coal and natural gas feed-stocks are used for methanol synthesis as represented in Figure 2. The coal gasifier derived synthesis gas usually contains high amounts of sulphur which must be removed in the H₂S removal section prior to its mixing with the reformed natural gas. The temperature and pressure of the syngas at the inlet of the methanol reactor is also maintained at 200°C and 55 bar, respectively, as done in the case 1 design. This parallel design configuration of integrating the gasification unit with the reforming unit not only reduces the process energy requirements but also helps in increasing the overall methanol production.

3. Results and Discussion

Case 1 was modelled as the conventional CTM process where cold gas efficiency (CGE) of the syngas is based on the gasifier operational conditions, type of feed and the heat
integration network. The case 1 design is then retrofitted with the SMR technology to generate the case 2 design to utilize the key technical benefits of both the gasification and reforming technologies. This retrofitting of SMR unit in the parallel design configuration not only allowed to utilize the high enthalpy heat from the gasifier derived synthesis gas but also helps in increasing the HCR ratio at the inlet of the methanol reactor. In both the cases, 62.19kg/s of the bituminous coal has been used as a feedstock for the gasification unit. Unlike case 1, the case 2 design consumes an additional natural gas at the rate of 5.5kg/s in the reforming unit. The coal to natural gas ratio of 5.5:1 is maintained in the case 2 design to utilize maximum heat from the gasification unit for the reforming of natural gas without any additional heat supply. The results showed that there is a significant increase in syngas production capacity in the case 2 design compared to the case 1. The HCR (hydrogen to carbon ratio) obtained in the case 2 design is also higher than case 1 design. Figure 3 shows the synthesis gas composition at the inlet of methanol reactor for case 1 and case 2 designs.

![Synthesis gas composition at the inlet of Methanol Reactor](Figure 3: Synthesis gas composition at the inlet of Methanol Reactor)

To ensure the unbiased analysis, the process performance indicator for calculating the overall process efficiency has been used as given in the equation 1. The overall energy efficiency is a function of heat input rates in the form of thermal energy and the heating value of the produced methanol along with the power generation potential for each case.

\[
\text{Energy Efficiency} = \frac{\text{Produced electricity} + \text{Heat of Produced MeOH}}{\text{Feed stock heating value} + \text{Energy Consumed}} \times 100 \% \tag{1}
\]

The results showed that the process efficiency calculated for case 1 and case 2 is 63% and 70%, respectively. The heat generated from both the cases has been utilized for electricity generation using steam turbine cycle. The results showed that the electricity generation potential from the case 1 and case 2 is calculated as 11.26MWc and 16.70MWc, respectively. Methanol production capacity and energy requirement from a specific fuel is also an important criterion to analyze the process technical and economic feasibility. The difference in the process configuration and the heat exchanger network highly affects the overall production capacity. The simulation results showed that the methanol production capacity from case 1 and case 2 is calculated as 171 MT/hr and 212 MT/hr, respectively, where the case 2 design shows 24% higher methanol production capacity compared to case 1. Figure 4 also represents the comparison between two cases in terms of process efficiency (%), methanol production energy (kg/kWc) and methanol production...
capacity (ton/hr). The results showed that the specific methanol production for case 1 and case 2 is calculated as 0.7 kg/watt and 0.8 kg/watt, respectively.

The estimation of capital (CAPEX) and operational (OPEX) expenditures are important factors to analyze the sustainability of any chemical process. The fixed CAPEX includes the cost of equipment, cost of land, installation costs etc. The OPEX involve the cost of feedstocks, catalysts and the utilities. The CAPEX for both the cases is calculated using the power law of capacity as shown in the equation 2, where, $x$ represents the capacity factor which is taken as 0.6 in this research.

$$\text{Cost}_{\text{New}} = \text{Cost}_{\text{Old}} \times \left(\frac{\text{Capacity}_{\text{New}}}{\text{Capacity}_{\text{Old}}}\right)^x \times \frac{\text{CEPCI}_{\text{New}}}{\text{CEPCI}_{\text{Old}}}$$  \hspace{1cm} (2)

The results showed that the CAPEX required for case 1 and case 2 is 2594.89M€ and 2895.06M€, respectively. Similarly, the OPEX calculated on the yearly basis for case 1 and case 2 is calculated as 190M€ and 225M€, respectively. Despite the higher value of the overall OEPX and CAPEX for case 2 design, the per unit cost for methanol production is lower than the case 1 due to its higher methanol production capacity. In terms of specific cost for methanol production, case 1 and case 2 offers nearly 275.2 €/ton and 258.4 €/ton, respectively. In terms of cash flow analysis throughout the lifetime of the project, the minimum payback time of the project and the expected profit has been also calculated.

![Figure 4: Comparison of Methanol Production Rates and Energy for Case 1 and Case 2](image)

![Figure 5: Cumulative cash flow for Case 1 and Case 2](image)
Figure 5 represents the cumulative cash flow analysis for both case 1 and case 2 design where the life time of the project is assumed to be 33 years. It has been analyzed from the results that the payback time for both the case 1 and case 2 is calculated as 11 years, where the case 2 design showed a higher profit potential of 2600-2700M€ as compared to the case 1 design throughout the life time of the project.

4. Conclusion

This paper represents the techno-economic analysis of two processes for methanol production. Case 1 is taken as a conventional coal to methanol (CTM) processes, whereas, case 2 represent the conceptual design of integrating of the reforming unit with the gasification unit to utilize the maximum heat to sustain the reforming reactions. It has been analyzed from the results that the case 2 design offers higher process performance and economics compared to the case 1 design in terms of methanol production. Case 2 design not only represents higher methanol production rates but also showed a reduction in the per unit production energy requirements. Moreover, case 2 design offers higher rate of return on the investments, which makes its design more sustainable compared to the conventional process.

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References


