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Research Article

# Assessment of Methanol Production Potential from Industrial By-Product Gases

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**Abstract**

As global efforts intensify to mitigate climate change, innovative strategies are being explored to convert industrial by-product gases into valuable commodities, thereby contributing to sustainable practices and reducing carbon footprints. This study focuses on the potential for methanol production from carbon monoxide (CO) and carbon dioxide ($CO_2$) present in industrial gases, reacting with hydrogen. Conversion rates calculated from the kinetic models used in ASPEN HYSYS were subsequently validated through laboratory-scale experiments. The highest conversion rates achieved were 69% for CO and 10% for $CO_2$ and the results highlighted the feasibility of converting waste gases into methanol, a key component in the circular economy.

**Keywords:** CCUS, circular economy, methanol production, $CO_2$ conversion, CO conversion

# Endüstriyel Yan Ürün Gazlarından Metanol Üretim Potansiyelinin Değerlendirilmesi

**Öz**

İklim değişikliği etkilerini azaltmak için küresel çapta yürütülen çalışmalar artarken, endüstriyel yan ürün gazlarını değerli kimyasallara dönüştürmek için yenilikçi stratejiler geliştirilerek sürdürülebilir uygulamalara katkı sağlanmakta ve karbon ayak izi azaltılmaktadır. Bu çalışma, endüstriyel gazlarda bulunan karbon monoksit (CO) ve karbondioksittin ($CO_2$) hidrojen ile reaksiyonu sonucu metanol üretim potansiyeline odaklanmaktadır. ASPEN HYSYS'e girilen kinetik modeller ile hesaplanan dönüşüm oranları daha sonra laboratuvar ölçekli deneylerle doğrulanmıştır. Elde edilen en yüksek dönüşüm oranları CO için %69 ve $CO_2$ için %10 olmuştur ve elde edilen sonuçlar atık gazların döngüsel ekonomide önemli bir ürün olan metanole dönüştürülmesi potansiyelini ortaya koymuştur.

**Anahtar Kelimeler:** CCUS, döngüsel ekonomi, metanol üretimi, $CO_2$ dönüşümü, CO dönüşümü.

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## 1. Introduction

The steel sector is a cornerstone of economic development and industrial growth, playing a critical role as a fundamental input for infrastructure, manufacturing, and construction industries across the globe. Beyond its strategic economic importance, the sector is a key focus in global efforts to achieve decarbonisation and drive the green transformation, as it contributes nearly 10% of global energy-related $CO_2$ emissions and approximately 30% of industrial carbon emissions. The sector's significant carbon footprint largely stems from its reliance on the blast furnace-basic oxygen furnace (BF-BOF) production route, which depends heavily on carbon-intensive coking coal as its primary energy source. This conventional production method results in substantial carbon intensity, with emissions ranging from 1.8 to 4.0 tons of $CO_2$ per ton of steel produced in many countries, underscoring the urgent need for cleaner and more sustainable technologies in steelmaking [1] Carbon Capture, Utilization, and Storage (CCUS) is one of the few transformative technologies capable of delivering large-scale carbon emission reductions for the iron and steel industry, which is a major contributor to global emissions and holds a critical role in the transition to a low-carbon economy. CCUS not only supports emissions abatement but also provides a pathway for industries to align with global decarbonisation goals.

Utilization of steel-making industry gases offers an innovative approach to securely embed off-gases into marketable products. The process has the potential to promote circular economy, reduce dependence on virgin raw materials, and generate economic incentives for carbon capture by creating new revenue streams. As an example, the $CO_2$ utilization market was valued at approximately USD 4.02 billion in 2022 and is projected to grow significantly, reaching USD 14.2 billion by 2032 [2]. The transformation of industrial waste gases into useful chemicals represents a crucial step towards achieving a circular economy, where resources are reused and emissions minimized. Methanol, in particular, holds promise due to its versatility as a fuel and feedstock for various industrial processes. This study aims to assess the practicality of methanol production from industrial by-product gases, specifically focusing on the conversion of CO and $CO_2$. By focusing on the conversion of industrial gases to methanol, this research contributes to the broader discourse on sustainable practices in industrial emissions management and energy production. Further investigation in this area is essential for advancing both environmental and economic objectives.

Methanol is a versatile chemical with a wide range of industrial, commercial, and energy-related applications. It is a key raw material in the production of formaldehyde, which is used in the manufacture of resins, plastics, and textiles. Methanol is also a feedstock for producing acetic acid, which has applications in the production of adhesives, coatings, and solvents. Methyl Tertiary Butyl Ether (MTBE) is used as an additive in gasoline to improve octane rating and reduce emissions. Dimethyl Ether (DME) is used as a propellant in aerosol products and as a clean-burning fuel [3].

Methanol serves as a versatile solvent across numerous industries, including producing paints, coatings, varnishes, and cleaning products. It is commonly blended with gasoline as a fuel additive, enhancing combustion efficiency and reducing the emission of pollutants. Methanol is used in direct methanol fuel cells (DMFCs) as a hydrogen carrier and fuel source for generating electricity. In certain markets, particularly those with renewable methanol production or stringent emissions regulations, methanol is utilized as a standalone vehicle fuel. Furthermore, methanol plays a crucial role in automotive antifreeze formulations and is used to denature ethanol, rendering it undrinkable for industrial applications and thereby avoiding alcohol taxes. Methanol is widely used in laboratories as a solvent and reagent in chemical reactions [4]. Methanol production from captured carbon dioxide ($CO_2$) is being explored as a means of reducing greenhouse gas emissions and utilizing waste carbon. Methanol can be part of integrated biorefinery processes where biomass and waste materials are converted into multiple products, including fuels and chemicals.

Commercial catalysts employed in methanol production are specifically engineered for optimal performance within the methanol synthesis loop of a production facility. Typically, copper-based catalysts supported on alumina ($Cu/ZnO/Al_2O_3$) are utilized for these processes.

The chemical reactions involved in methanol synthesis, which typically includes the conversion of carbon monoxide (CO) /carbon dioxide ($CO_2$) and hydrogen ($H_2$) into methanol ($CH_3OH$). These reactions are represented by the chemical equation 1 and 2:

$$CO + 2H_2 \leftrightarrow CH_3OH \qquad (1)$$

$$\Delta H^o_{298K} = -90{,}6\ kj/mol$$
$$\Delta G^o_{298K} = -29{,}1\ kj/mol$$

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \qquad (2)$$

$$\Delta H^o_{298K} = -49{,}5\ kj/mol$$
$$\Delta G^o_{298K} = -9{,}04\ kj/mol$$

Catalyst is used in fixed-bed reactors within methanol plants where the syngas is processed over the catalyst to produce methanol. The catalyst's performance is crucial for achieving high methanol yield, selectivity, and stability over prolonged operation periods. Factors such as catalyst activity, surface area, and resistance to deactivation (e.g., by coke formation) are important considerations [5].

The yield of methanol production from carbon dioxide ($CO_2$) and hydrogen ($H_2$) can vary depending on several factors, including the catalyst, reaction conditions, and process efficiency.

The effectiveness of the catalyst in converting $CO_2$ and $H_2$ to methanol is crucial. High selectivity towards methanol minimizes the formation of by-products, thereby improving overall yield.

Temperature, pressure and $H_2/CO$ ratio are important Reaction Conditions:

- Temperature: Typically operated at temperatures around 200°C to 300°C.

-Pressure: Higher pressures, often between 20 to 100 bar (2 to 10 MPa), favour the equilibrium towards methanol formation.

- The stoichiometric ratio of $H_2$ to $CO_2$ influences the reaction kinetics and methanol yield.

Efficient use of energy and effective removal of methanol from the reactor can enhance yield. Minimizing side reactions and catalyst deactivation (e.g., by carbon deposition) is crucial for maintaining high yield over time.

The conversion efficiency of $CO_2$ into methanol can range from 10% to 30% under optimal conditions. Selectivity towards methanol can vary significantly depending on the catalyst and reaction conditions. High selectivity (>90%) is desirable to maximize methanol yield. Taking into account both conversion and selectivity, typical methanol yield can be around 3% to 10% based on the initial moles of $CO_2$ fed into the reactor [6].

There are some challenges of the reaction such as energy intensity, catalyst stability and economic viability. $CO_2$ hydrogenation requires substantial energy input compared to methanol production from CO and $H_2$. Catalyst deactivation due to carbon deposition or sintering can reduce yield over time. The overall cost-effectiveness of methanol production from $CO_2$ and $H_2$ is influenced by factors such as energy costs, catalyst longevity, and market demand for methanol. In conclusion, while methanol production from $CO_2$ and $H_2$ shows promise as a pathway for carbon dioxide utilization and renewable methanol production, achieving high yields requires optimizing catalyst performance, reaction conditions, and process efficiency. Ongoing research and development efforts aim to improve these factors to make $CO_2$ hydrogenation economically viable and environmentally sustainable. The cost of producing 1 kg of methanol from carbon dioxide ($CO_2$) can vary widely depending on several factors, including the specific technology used, the scale of production, energy costs, catalyst costs, and other operational expenses. Currently, direct methanol production from $CO_2$ is an emerging technology with ongoing research and development efforts to improve efficiency and reduce costs [7].

Methanol synthesis from $CO_2$ contributes to carbon capture and utilization strategies, mitigating greenhouse gas emissions by converting $CO_2$ into a useful chemical. Methanol can be produced from renewable sources, such as biomass or captured $CO_2$ from industrial processes, enhancing its role in sustainable energy systems [8].

Ongoing research focuses on improving catalyst efficiency, reducing energy consumption, and exploring alternative feedstocks for methanol production. Advances in catalyst design, reactor engineering, and process optimization are crucial for enhancing the economic viability and environmental sustainability of methanol synthesis processes [9].

Methanol synthesis is a pivotal industrial process with significant applications across various sectors, offering pathways for reducing carbon emissions and promoting sustainable development. Continued advancements in technology and research are essential for further optimizing methanol production processes and expanding its role in a low-carbon economy [10].

Lee (1993) studied the methanol production from $CO_2/H_2$ and $CO/H_2$ gas streams on $Cu/ZnO/Al_2O_3$ catalyst. They found the rate of methanol synthesis from $CO_2/H_2$ is much faster than the rate from $CO/H_2$ gas stream [11].

Sun (1997) investigated the effect of catalyst structure and reaction condition on methanol yield from $CO_2/H_2$ gas stream. They concluded that as the copper content in the catalyst increases, the catalytic activity increases and methanol is directly produced from $CO_2$ hydrogenation, the role of reverse water gas shift reaction and CO hydrogenation is not significant [12].

Lee (2000) studied the effect of space velocity on methanol production from $CO/CO_2/H_2$ gas mixture. They stated that while higher space velocity causes an increase in $CO_2$ hydrogenation, it causes a decrease in CO hydrogenation. Besides, they gave the optimum $CO_2$ content in the gas stream as 5-10% for maximum methanol yield [13].

Yin (2005) investigated the effect of operating parameters on a commercial $Cu/ZnO/Al_2O_3$ catalyst using gas stream of biomass gasification. They stated 245°C as optimum temperature and as space velocity increase causes the methanol yield increase [14].

Xin (2009) studied the $CO_2$ hydrogenation to methanol at various operating conditions (temperature, pressure, space velocity). They found the highest methanol production rate at 523K, 5 MPa and 6 L/gcat.hr [15].

Samiee (2021) studied the effect of operating parameters by using $CO/CO_2/H_2$ gas stream on $Cu/ZnO/Al_2O_3$ catalyst and the kinetic models given in the literature. They gave the optimum temperature between 200-220°C for maximum methanol yield and for better kinetic model, both CO and CO2 hydrogenation rate terms must be included in kinetic model [16].

Adil (2024) investigated the effect of operating parameters (temperature, pressure and space velocity) on methanol production rate from two gas streams coming from methane reforming and biomass gasification. They concluded that lower temperature, higher pressure and higher space velocity gave the maximum methanol yield [17].

The aim of this study is to analyse the operating parameters (temperature, pressure and space velocity) effect on $CO/CO_2$ conversion to methanol from a steel industry by-product gas stream by using a commercial catalyst and determine the optimum conditions in these operating parameters based on conversion. Besides, CO and $CO_2$ conversion obtained from the experiments are compared with the ASPEN kinetic model simulation using a kinetic model taken from the literature.

## 2. Experimental Methodology

### 2.1 Comparison of Simulation with Experimental Data

Validating the accuracy of ASPEN HYSYS simulations is crucial through comparison with experimental data. Key parameters for methanol production comparison typically include methanol yield, purity, conversion efficiency, energy consumption, and temperature/pressure profiles. Comparing ASPEN HYSYS simulation results with experimental data is a crucial step in validating the accuracy of your process model [18].

### 2.2 Experiment

In this study, experimental studies were conducted to investigate methanol production using a commercially available catalyst, with a focus on optimizing process conditions for each specific gas composition. The studies involved conducting systematic experiments with predefined gas compositions, using parameters established through simulations to identify the optimal operating conditions.

Effects of varying pressures (75, 85, 90 bar), temperatures (225, 250, 275 °C), and space velocities (5, 6, 7 NL/h/g-cat) on catalyst performance were investigated. The matrices established for methanol synthesis, as presented in Table 1, detail the operating pressure, temperature, and space velocity (SV).

**Table 1** Experimental Matrix of Methanol Production

| **Pressure (bar)** | **Temperature(°C)** | **SV (**NL/h/g-cat**)** |
|---|---|---|
| 75 | 225 | 5-6-7 |
| | 250 | 5-6-7 |
| 85 | 225 | 5-6-7 |
| | 250 | 5-6-7 |
| | 275 | 5-6-7 |
| 95 | 225 | 5-6-7 |
| | 250 | 5-6-7 |
| | 275 | 5-6-7 |

The experimental studies carried out in a high throughput catalyst screening system (Amtech RS8 Parallel Fixed Bed Reactor System) utilizing a commercial catalyst to simulate real-world industrial conditions. This system (Figure 1) contains 8 fixed-bed reactors, enabling the simultaneous testing of one catalyst under 8 different conditions or testing 8 different catalysts under the same or different conditions. While temperature, pressure, and gas feed rate can be adjusted to different values in each reactor, the only fixed operating condition in the system is the composition of the feed gas. The feed gas composition given in Table 2, which is simulating the gas compositions in steelmaking processes, were prepared using calibrated gas cylinders.

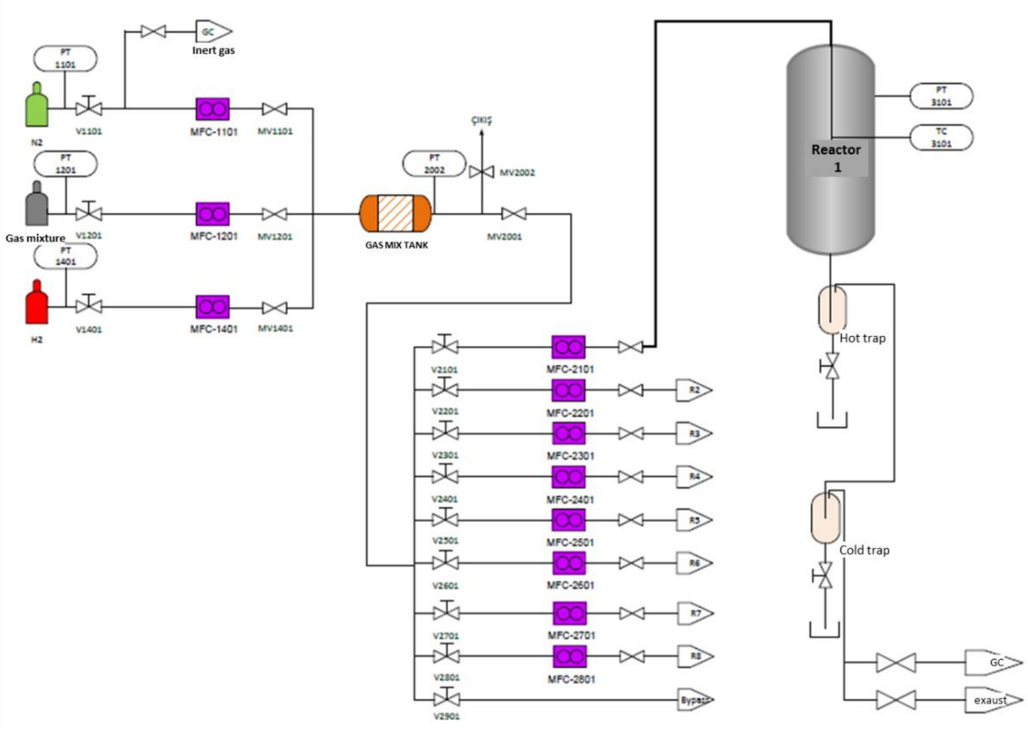

**Figure 1** Experimental setup flow diagram

**Table 2** Gas Composition of Steel Making Process

| Component | Percentage |
|---|---|
| CO | 7.6 |
| $CO_2$ | 5.7 |
| $H_2$ | 33.6 |
| $N_2$ | 20.6 |
| $CH_4$ | 32.5 |

Methanol production from syngas is based on three reactions; Methanol production from $CO_2$ (equation 3), Reverse water gas shift reaction (equation 4), and Methanol Production from CO (equation 5).

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \qquad \Delta H^o_{298K} = -49{,}5\ kj/mol \tag{3}$$

$$CO_2 + H_2 \leftrightarrow CO + H_2O \qquad \Delta H^o_{298K} = +41{,}2\ kj/mol \tag{4}$$

$$CO + 2H_2 \leftrightarrow CH_3OH \qquad \Delta H^o_{298K} = -90{,}6\ kj/mol \tag{5}$$

The kinetic model and model constants used in this study are given below and in Table 3 [19].

$$r'_{CH_3OH,A3} = \frac{k'_{ps,A3} K_{CO} K_{H_2} \left[ f_{CO} f_{H_2}^{3/2} - f_{CH_3OH} / (f_{H_2}^{1/2} K_{P_1}^0) \right]}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}) \left[ f_{H_2}^{1/2} + (K_{H_2O} / K_{H_2}^{1/2}) f_{H_2O} \right]} \tag{6}$$

$$r'_{H_2O,B2} = \frac{k'_{ps,B2} K_{CO_2} K_{H_2} \left( f_{CO_2} f_{H_2} - {f_{H_2O} f_{CO}} \big/ {K_{P_2}^0} \right)}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}) \left[ f_{H_2}^{1/2} + (K_{H_2O} / K_{H_2}^{1/2}) f_{H_2O} \right]} \tag{7}$$

$$r'_{CH_3OH,C2} = \frac{k'_{ps,C2} K_{CO_2} K_{H_2} \left[ f_{CO_2} f_{H_2} - f_{CH_3OH} f_{H_2O} / (f_{H_2}^2 K_{P_3}^0) \right]}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}) \left[ f_{H_2}^{1/2} + (K_{H_2O} / K_{H_2}^{1/2}) f_{H_2O} \right]} \tag{8}$$

**Table 3** Model Constants of the Equations 6-7-8

| **Parameters** | **A** | **B** |
|---|---|---|
| $\boldsymbol{K_{P_1}^0}$ **[1/bar$^2$]** | 2,391E-13 | 98388 |
| $\boldsymbol{K_{P_2}^0}$ **(-)** | 1,068E+02 | -39683 |
| $\boldsymbol{K_{P3_1}^0}$ **[1/bar$^2$]** | 2,55E-11 | 58705 |
| $\boldsymbol{k'_{ps,A3}}$ **[mol/(s.kg.bar)]** | 4,89E+07 | -113000 |
| $\boldsymbol{k'_{ps,B2}}$ **[mol/(s.kg.bar^0,5]** | 9,64E+11 | -152900 |
| $\boldsymbol{k'_{ps,C2}}$ **[mol/(s.kg.bar)]** | 1,09E+05 | -87500 |
| $\boldsymbol{K_{CO}}$ **[1/bar]** | 2,16E-05 | 46800 |
| $\boldsymbol{K_{CO_2}}$ **[1/bar]** | 7,05E-07 | 61700 |
| $\boldsymbol{K_{H_2O}/K_{H_2}^{1/2}}$ **[1/bar$^{0,5}$]** | 6,37E-09 | 84000 |

## 2.3 Optimum Conditions

The optimum reaction conditions for methanol production using catalysts depend on achieving a balance between high conversion efficiency, selectivity towards methanol, and operational feasibility. The key parameters that influence the optimum reaction conditions are temperature, pressure, feedstock composition, catalyst activity, space velocity, catalyst bed design and heat management [20].

Methanol synthesis typically occurs at temperatures ranging from 200°C to 300°C. The exact temperature depends on the catalyst used, with higher temperatures generally favouring higher reaction rates but potentially reducing selectivity due to increased side reactions. Methanol synthesis is typically conducted at pressures ranging from 50 to 100 bar (5 to 10 MPa). Higher pressures can enhance reaction rates and favour higher methanol yields by shifting the equilibrium towards methanol formation. The composition of the feedstock, which is usually a mixture of carbon monoxide (CO), hydrogen ($H_2$), and possibly carbon dioxide ($CO_2$), plays a crucial role. The optimal ratio of CO to $H_2$ is often around 1:2 to 1:3 for methanol synthesis.

## 3. Results

The effectiveness of the catalyst in promoting the methanol synthesis reaction is vital. Catalyst activity can be influenced by factors such as its surface area, metal dispersion, and resistance to deactivation by impurities or coke formation. The space velocity, which refers to the rate at which the feed gases pass through the catalyst bed per unit time and volume of catalyst, affects the conversion efficiency and selectivity. Higher space velocities can increase throughput but may reduce contact time and thus affect conversion efficiency. The design of the catalyst bed, including its size, shape, and distribution of catalyst particles, influences the efficiency of heat and mass transfer within the reactor, thereby impacting reaction kinetics. Effective control of temperature gradients and heat transfer mechanisms within the reactor is crucial to maintain stable reaction conditions and optimize the yield of methanol.

Determining the optimum reaction conditions typically involves a combination of experimental investigation and process simulation using tools like ASPEN HYSYS. Engineers and researchers aim to maximize methanol yield while considering factors such as catalyst stability, operational costs, and environmental impact. Optimization efforts often focus on achieving high conversion rates of CO and $H_2$ into methanol with minimal energy consumption and by-product formation. To determine how much carbon monoxide (CO) and hydrogen ($H_2$) are needed to produce 1 gram of methanol ($CH_3OH$) experimentally, we need to consider the stoichiometry of the methanol synthesis reaction and the molar masses of the reactants and products involved. Therefore, experimentally, to produce 1 gram of methanol ($CH_3OH$), you would need approximately 0.875 grams of CO and 0.125 grams of $H_2$ under stoichiometric conditions. These values are theoretical and may vary slightly in practical applications due to factors such as reaction efficiency, catalyst activity, and process conditions.

CO and $CO_2$ conversion obtained from the laboratory experiments for three different pressure, three different temperature and three different space velocity are given in Table 4. The conversion rates for CO and $CO_2$ obtained from both the experimental and ASPEN kinetic model simulation studies are given in Figure 2 and Figure 3.

**Table 4** CO and $CO_2$ conversion values for various operating parameters

| Pressure (bara) | Space Velocity (NL/h/g-cat) | Conversion (%) | Temperature | | |
|---|---|---|---|---|---|
| | | | **225°C** | **250°C** | **275°C** |
| **75** | SV: 5.0 | CO | %59.40 | %46.90 | |
| | | $CO_2$ | %8.30 | %7.00 | |
| | SV: 6.0 | CO | %58.40 | %46.90 | |
| | | $CO_2$ | %8.50 | %7.20 | |
| | SV: 7.0 | CO | %57.60 | %46.70 | |
| | | $CO_2$ | %8.20 | %7.56 | |
| **85** | SV: 5.0 | CO | %68.50 | %51.70 | %32.80 |
| | | $CO_2$ | %8.70 | %8.40 | %6.10 |
| | SV: 6.0 | CO | %66.40 | %51.40 | %32.50 |
| | | $CO_2$ | %9.00 | %8.40 | %6.50 |
| | SV: 7.0 | CO | %64.0 | %50.90 | %32.0 |
| | | $CO_2$ | %9.10 | %8.60 | %6.90 |
| **95** | SV: 5.0 | CO | %68.90 | %56.60 | %36.30 |
| | | $CO_2$ | %10.00 | %6.70 | %6.80 |
| | SV: 6.0 | CO | %66.80 | %56.30 | %36.20 |
| | | $CO_2$ | %10.20 | %7.00 | %7.00 |
| | SV: 7.0 | CO | %63.30 | %55.50 | %34.60 |
| | | $CO_2$ | %9.90 | %7.70 | %7.70 |

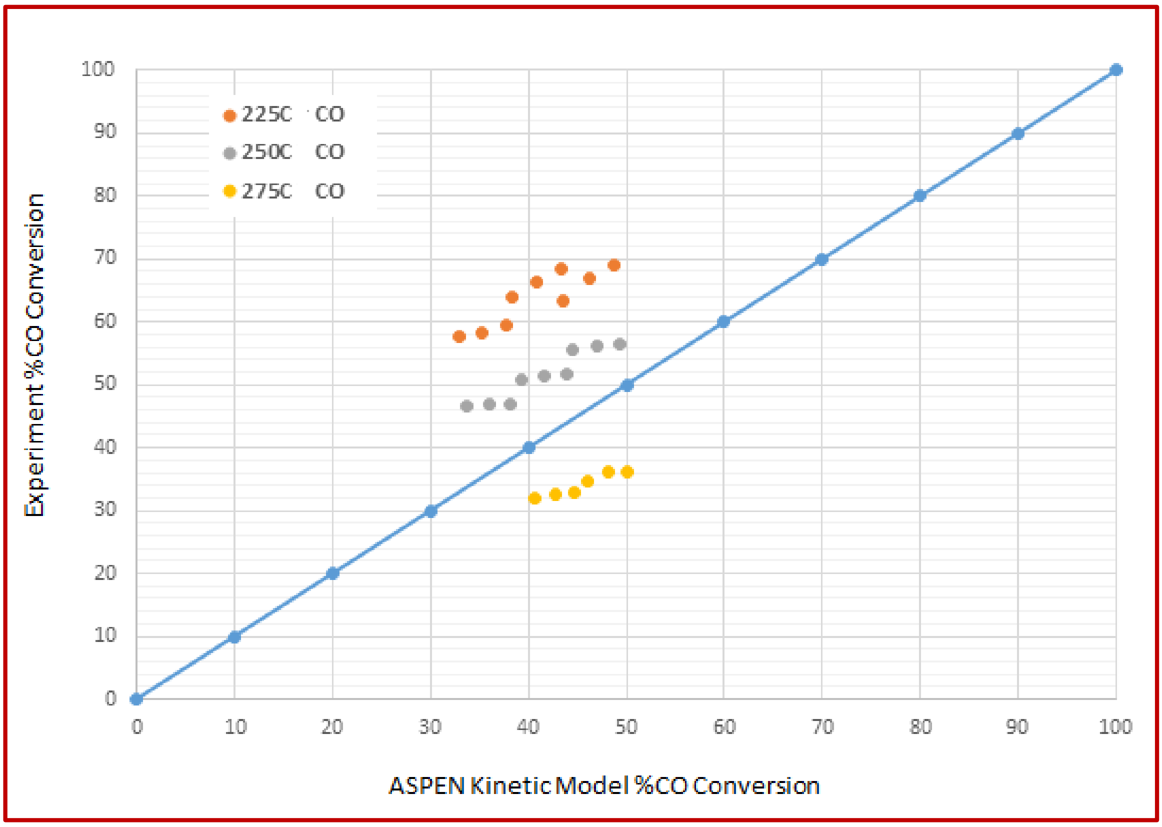

**Figure 2** Comparison of the experiment and kinetic model % CO conversion

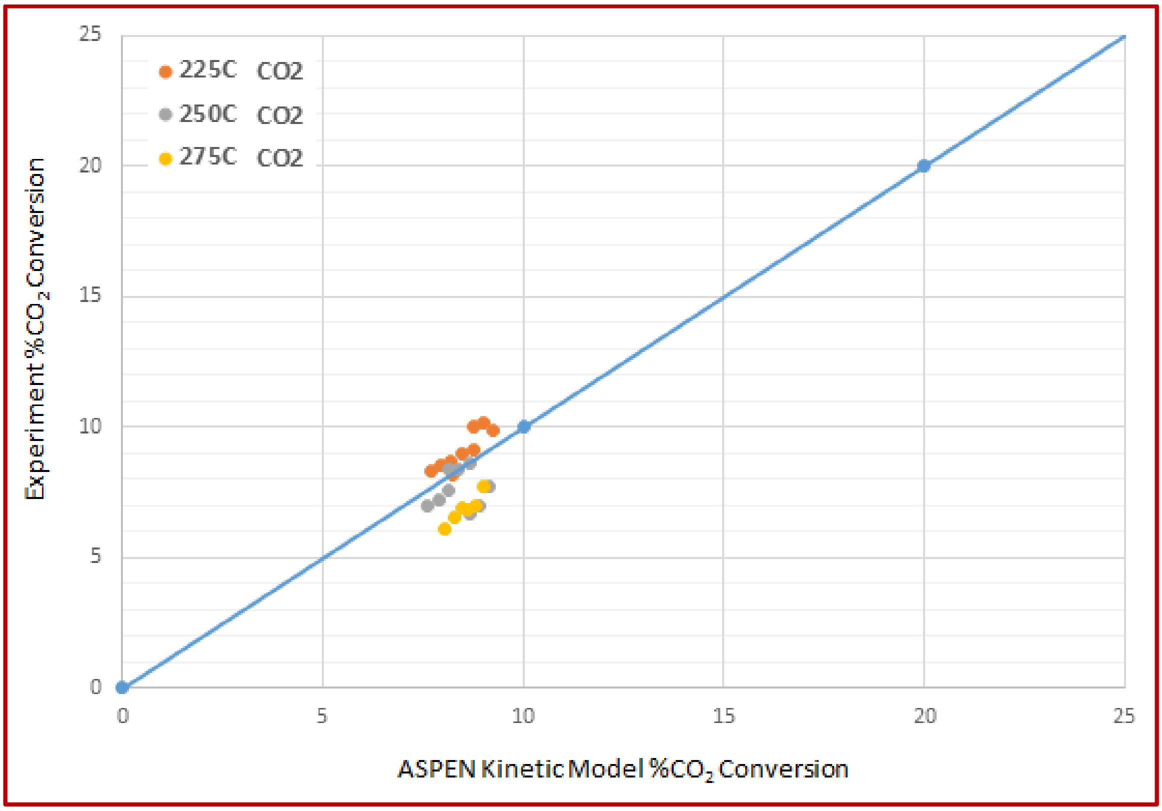

**Figure 3** Comparison of the experiment and kinetic model %$CO_2$ conversion

## 4. Discussion

While these alternative technologies show promise in reducing carbon emissions and diversifying feedstocks for methanol production, many are still in the research and development phase or early stages of commercialization. Challenges include technological readiness, scale-up feasibility, economic competitiveness compared to conventional methods, and regulatory support for low-carbon technologies.

Overall, the diversity of alternative production technologies reflects ongoing efforts to innovate and transition towards more sustainable and efficient methods of methanol production, aligned with global energy and environmental goals.

Table 4 shows the CO and $CO_2$ conversions at varying pressures and temperatures with a flow rate of 5 NL/h/g-cat. It was observed that an increase in temperature led to a decrease in CO and $CO_2$ conversions, whereas an increase in pressure resulted in enhanced conversions. Although the reaction rate increases by increasing the temperature, the equilibrium constant decreases by a temperature increase in exothermic reactions. This decrease in equilibrium constant leads to a decrease in CO and $CO_2$ conversions. Since the rate becomes equilibrium limited rather than kinetic limited. The operating temperature for methanol production is between 493K and 573 K [21]. Xin (2009) gave 523 K as maximum $CO_2$ conversion temperature [13] while Zhang (1997) stated 499 K as optimum reaction temperature for CO/ $CO_2$ hydrogenation to methanol [22].

Conversion trends were consistent across flow rates of 6 and 7 NL/h/g-cat, where increasing temperatures corresponded with decreasing conversion rates, and increasing pressures were associated with higher conversion rates. The maximum CO conversion of 68.9% was recorded at a pressure of 95 bar, space velocity of 5 NL/h/g-cat, and temperature of 225°C. Similarly, the highest $CO_2$ conversion of 10.2% was achieved under the same pressure conditions, with a space velocity of 6 NL/h/g-cat, and a temperature of 225°C. While CO conversion are decreasing by increasing the space velocity, $CO_2$ conversion are increasing by an increase in space velocity. Lee (1993) studied both CO and $CO_2$ conversions to methanol and stated that both conversions are decreasing by an increase in space velocity but the decrease in CO conversion is more remarkable than the decrease in $CO_2$ conversion [11]. Yin (2005) noticed that as SV increases, CO desorption accelerated and this acceleration causes a decrease in CO conversion [14]. Since CO and $CO_2$ adsorption on catalyst surface are competitive, the decrease in CO adsorption leads to an increase in CO2 adsorption, which causes an increase in $CO_2$ conversion. Sizgek (1994) also gave an increase in $CO_2$ conversion after a certain SV point [23].

As the pressure increases, both CO and $CO_2$ conversion increases which is consisted with the studies of Adil (2024) and Samiee (2021) [16, 17]. Higher pressure favours the reaction 3 and reaction 5 by Le Chatelier’s principle because of decrease in molar volume.

The CO and $CO_2$ conversion rates obtained from both experimental and simulation results for the methanol catalyst are given in Figure 2 and Figure 3. As illustrated in Figure 2, the experimental data exhibit a positive deviation from the simulation results at 225°C and 250°C for CO conversion, whereas a negative deviation is observed at 275°C. Specifically, at 225°C, the deviation in CO conversion is approximately 20%, which decreases to below 10% at 250°C.

In the case of $CO_2$ conversion, the experimental results indicate a deviation ranging from 0.5% to 1.5% compared to the simulation outcomes at 225°C and 250°C. This deviation increases to between 1% and 2% at 275°C, as shown in Figure 3.

## 5. Conclusions

According to the methanol synthesis experiment results, the highest CO and $CO_2$ conversion values were observed at 95 bar pressure, 225°C temperature, and a feed rate of 5 NL/h/g-cat, with conversion rates of 68.90% for CO and 10% for $CO_2$, respectively. In general, it was observed that CO and $CO_2$ conversions decreased with increasing operating temperature and increased with increasing pressure. The gas feed rates studied were found to have no significant effect on the conversions. The lowest conversion values were observed at 275°C.

Methanol synthesis experimental results are compared with the simulation results and following results are observed:

- %$CO_2$ Conversion: A deviation of 0.5-1.5% was observed between the experimental and simulation results at 225°C and 250°C, while this deviation increased to 1-2% at 275°C.
- %CO Conversion: A deviation of 20% was observed between the simulation and experimental CO conversions at 225°C, while this deviation dropped below 10% at 250°C.

## 6. Ethics in Publishing

There are no ethical issues regarding the publication of this study.

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