

# Simulation of a NGCC Power Generation Plant for the Production of Electricity from CO<sub>2</sub> Emissions Part I: The Methanation Reactor

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**How to cite this paper:** Daful, A.G. and Dadach, Z.E. (2019) Simulation of a NGCC Power Generation Plant for the Production of Electricity from CO<sub>2</sub> Emissions Part I: The Methanation Reactor. *Journal of Power and Energy Engineering*, 7, 1-14.  
<https://doi.org/10.4236/jpee.2019.77001>

**Received:** May 28, 2019

**Accepted:** June 30, 2019

**Published:** July 3, 2019

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## Abstract

The final goal of this applied research is to simulate a Natural Gas Combined Cycle (NGCC) power plant with a CO<sub>2</sub> capture unit. The originality of this investigation is the integration of a methanation process to produce the natural gas of the power plant from the captured CO<sub>2</sub>. The objective of this first part of the investigation is to simulate a methanation reactor for the production of methane using 1 kg/hr. of captured carbon dioxide containing 95% mol. CO<sub>2</sub> and 5% mol. H<sub>2</sub>O. To reach this goal, Aspen Plus software and the Redlich-Kwong-Soave equation of state with modified Huron-Vidal mixing rules are utilized. Three parameters are considered in order to maximize the production of CH<sub>4</sub> production: 1) temperature, varying from 250°C to 300°C, 2) pressure varying between 10 atm to 40 atm and 3) [H<sub>2</sub>/CO<sub>2</sub>] ratio which varies between 2 to 6. The maximum production of methane of 0.875 kmol/hr. was obtained for the following operating conditions: [H<sub>2</sub>/CO<sub>2</sub>] ratio of 3.5, at relatively low temperature (250°C - 270°C) and high pressures 30 and 40 atm.

## Keywords

Methanation Reactor, NGCC, CH<sub>4</sub>, CO<sub>2</sub>, Simulation, Reaction Kinetics

## 1. Introduction

Electricity production is vital for the economic growth of the UAE. However, power generation plants contribute greatly to the annual CO<sub>2</sub> emissions of the country. For example, these plants released about 33% of the 200 Million tons of the total CO<sub>2</sub> emitted in 2013 [1]. These emissions can be reduced in four main paths: 1) increasing efficiency of industrial plants; 2) carbon Capture and sto-

rage; 3) chemical conversion and utilization of CO<sub>2</sub>; 4) use of renewable energies. The actual carbon capture and storage (CCS) strategy has a safety problem due to CO<sub>2</sub> leakage from underground and has also no commercial value to attract potential investors.

The utilization of CO<sub>2</sub> emissions as carbon source for the production of chemicals and fuels is the needed path for a more sustainable use of the resources which can indeed lead to less consumption of carbon-based fossil resources. First, carbon dioxide can be converted into several value-added chemicals following stoichiometric reactions, thermochemical, electrochemical, photoelectrochemical, photocatalytic paths. However, the amount of products obtained by conversion of carbon dioxide represents only a few percentages of the total global CO<sub>2</sub> emissions. A good example is the use of CO<sub>2</sub> for the production of urea, which is used primarily as a fertilizer, by reacting ammonia with carbon dioxide [2].

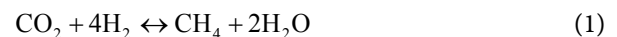
The utilization of CO<sub>2</sub> emissions as a feed for the synthesis of fuels is more sustainable than their production from conventional paths with low efficiency. In this perspective, the use of carbon dioxide for the production of methanol is investigated in order to reduce carbon dioxide emissions and decrease dependence on fossil fuels [3]. The utilization of carbon dioxide emissions is crucial and beneficial to maintain a long-term and sustainable production of electricity in the United Arab Emirates. Because natural gas (NG) is the cleanest fossil fuel for electricity production, the Natural Gas Combined Cycle (NGCC) power generation plants are the best technology in order to meet the United Arab Emirates ever growing energy needs and reduce its environmental impact. However, even with the UAE's massive total of proved natural gas reserves, the country still needs to import natural gas in order to meet the energy market [4]. Therefore, the production of synthetic natural gas (SNG) by the methanation of carbon dioxide emissions has the potential to both reduce greenhouse gas emissions and mitigate dependence on natural gas.

The production of methane by hydrogenation of carbon dioxide, known as the Sabatier's reaction, is an important research topic in many research centers and industrial applications around the world [3]. The first commercial synthetic gas plant opened in 1984 and is the Great Plains Synfuel plant in Beulah, North Dakota, and USA [4] [5]. The CO<sub>2</sub> methanation process was initially utilized in order to remove trace carbon oxide from the feed gas for ammonia synthesis [6]. Recently, the CO<sub>2</sub> methanation has gained renewed interest due to its application in the so-called power-to-gas technology [7] as well as biogas upgrading. In power-to-gas technology, hydrogen produced from excess renewable energy is reacted with CO<sub>2</sub> (from power plants, industrial or biogenic processes) and chemically transformed to methane, which can be stored and transported through the well-developed natural gas infrastructure already in place [8]. The originality of this investigation is the integration of the methanation process with a Natural Gas Combined Cycle (NGCC) power plant and a CO<sub>2</sub> capture unit. The produced synthetic natural gas (SNG) will be utilized as a combustible

for a Natural Gas Combined Cycle (NGCC) power plant for the production of electricity. The flue gas leaving the Heat Recovery Stream Generator (HRSG) of the power plant will be treated in a CO<sub>2</sub> capture plant. The resulting concentrated carbon dioxide will be recycled and reutilized as the feed for the methanation process. The first objective of this study is to simulate a methanation reactor integrated with a NGCC power plant and a carbon capture unit. The simulated plant will then be utilized in order to investigate the amount of electricity produced using 1 kg/hr. of captured carbon dioxide containing 95% mol. CO<sub>2</sub> and 5% mol. H<sub>2</sub>O.

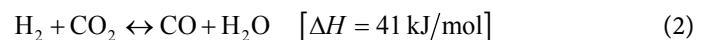
## 2. Fundamentals

The Sabatier process is a highly exothermic reaction that releases 165 kJ/mole for the reaction with carbon dioxide and 201kJ/mole for the reaction with carbon monoxide [6]. It is a thermodynamically favorable reaction ( $\Delta G = -113, 5$  kJ/mole) in a big range of temperatures and pressures [6]. On the other hand, the reduction of carbon dioxide to methane is kinetically limited [9]. Thus, a catalyst is needed to reach acceptable conversion rates and selectivity to methane. Observed by Paul Sabatier over a Nickel catalyst, the exothermic equilibrium reaction has the following equation [7]:

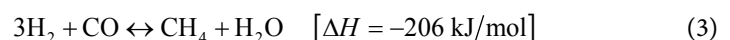


Many general paths have been proposed for the simple chemical reaction (1). In the most popular two-steps mechanism: carbon dioxide is first converted to carbon monoxide in an endothermic reverse water-gas shift (RWGS) reaction followed by the exothermic methanation of carbon monoxide for production methane [8].

Reverse Water-Gas Shift (RWGS):



Methanation:



Since the reaction is exothermic, the optimal operating window for CO<sub>2</sub> methanation is at low temperatures, where the conversion of CO<sub>2</sub> and CH<sub>4</sub> selectivity can reach close to 100% [7]. On the other hand, from the kinetic point of view, the reaction rate increases with temperature. However, increasing the temperature above 500°C is favorable for the RWGS (reverse water-gas shift) reaction [7]. In the catalytic methanation reactor, a temperature increase can also generate a thermal runaway and catalyst deactivation. To overcome this situation, isothermal reactor, adiabatic reactor with recycling and fluidized bed reactor and addition of steam are proposed in the literature [10] [11] [12].

Moreover, According to le Chatelier's principle, the CO<sub>2</sub> methanation is favored at elevated pressures. A pressure of 10 to 30 atm. is considered mild in terms of stress on the catalyst and should therefore not cause sintering for the catalyst [13]. Usually, industrial applications for the methanation of CO and CO<sub>2</sub>

take place at reactors of more than to 20 atm. of pressure in order to ensure high conversion rates of reactants and high purity of methane [14]. The most widely studied material for the hydrogenation of CO<sub>2</sub> is Nickel (Ni). The Ni catalyst is usually supported by another material that plays an important role in the reaction process. The material affects the catalytic activity and selectivity towards the final products [15]. The materials used typically as supports in Nickel catalysts are oxides. Like TiO<sub>2</sub>, SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, CeO<sub>2</sub> and ZrO<sub>2.3</sub> [16].

The simplest model studied is a power law (PL) solely considering the reaction orders of hydrogen and carbon dioxide [17]:

$$r = k \cdot p_{\text{H}_2}^{n_{\text{H}_2}} \cdot p_{\text{CO}_2}^{n_{\text{CO}_2}} \left( 1 - \frac{p_{\text{CH}_4} \cdot p_{\text{H}_2\text{O}}^2}{p_{\text{H}_2}^4 \cdot p_{\text{CO}_2} \cdot K_{eq}} \right) \quad (4)$$

where the equilibrium constant ( $K_{eq}$ ) could also be approximated by the empirical formula [18]:

$$K_{eq} = 137 \cdot T^{-3.998} \cdot \exp\left(\frac{158.7 \text{ kJ/mol}}{R \cdot T}\right) \quad (5)$$

However, since the methanation process is a catalytic reaction, the rate equation is usually derived from the Langmuir-Hinshelwood-Hougen-Watson (LHHW) approach, which is one of the most commonly used ways of deriving rate expressions for fluid solid catalytic reactions. In this approach, the rate equations take into account the surface coverage of the relevant adsorbed species. A rate-determining step is then assumed for the reaction mechanisms and the elementary step is considered as the slowest reaction step responsible for the overall rate. All other reaction steps are regarded to be in equilibrium or irreversible [16]. As shown in Equation (6), the resulting rate equations include the “driving force” in terms of partial pressure of the gas phase species and the “adsorption term”, which summarizes the retarding effects of the adsorbed reactants and products:

$$r = \frac{\text{kinetic term} \times \text{Driving force}}{\text{Adsorption term}} \quad (6)$$

For a typical range of temperatures (280°C -380°C) used for the study of the Sabatier’s reaction, the values of the equilibrium constant are small enough ( $K_{eq} = 55.2 - 15.1$ ) to include the reverse reaction in the rate of reaction [10]. For the sixteen models presented in the literature, the generalized rate equation for the WGS with an adsorbed H<sub>2</sub>O can be written as [16]:

$$r_{\text{WGS}} = \frac{k_2 \left( K_{\beta} \cdot p_{\text{CO}} \cdot p_{\text{H}_2\text{O}} - \frac{p_{\text{CO}_2} \cdot p_{\text{H}_2}}{K_{eq}} \right)}{\left( 1 + \sqrt{K_{\text{H}_2}} \cdot p_{\text{H}_2} + K_{\text{CO}} \cdot p_{\text{CO}} + K_{\text{H}_2\text{O}} p_{\text{H}_2\text{O}} + K_{\text{C}_y} \cdot p_{\text{CO}}^e \cdot p_{\text{H}_2}^f \right)^2} \quad (7)$$

On the other hand, the values of the equilibrium are very large of the methanation reaction are very large ( $K_{eq} > 5.6 \times 10^4 \text{ bar}^{-2}$ ) at temperatures below 380°C. The reverse reaction (methane steam reforming) can be therefore be neglected in the rate of reaction [16]. Assuming H<sub>2</sub>O as adsorbed species, the

rate can be written as

$$r_{\text{methanation}} = \frac{k_1 (K_{C,x} \cdot K_{H_2}^a \cdot p_{CO}^b \cdot p_{H_2}^c)}{\left(1 + \sqrt{K_{H_2}} \cdot p_{H_2} + K_{CO} \cdot p_{CO} + K_{H_2O} p_{H_2O} + K_{C_y} \cdot p_{CO}^e \cdot p_{H_2}^f\right)^g} \quad (8)$$

### 3. Literature Review

The effects of temperature, pressure, ratios of H<sub>2</sub>/CO and H<sub>2</sub>/CO<sub>2</sub>, and the addition of other compounds in the feed gas on the conversion of carbon monoxide and carbon dioxide, methane selectivity and yield, as well as carbon deposition were investigated in the literature [16] [18] [19] [20]. The greatest challenge involved in methanation is the temperature control of the exothermic reactions, meaning an efficient heat removal. In this perspective, the effects of temperature on the process were investigated by Jiajian Gao, *et al.* [18].

For the methanation of carbon monoxide (**Figure 1(a)**), the products mainly contain methane, water and little carbon dioxide by-product at low temperatures (200°C - 300°C) without deposition of carbon. With an increase in reaction temperature, the mole fraction of CH<sub>4</sub> decreases, whereas the unreacted carbon monoxide, hydrogen, carbon dioxide, and deposited carbon increase simultaneously [18]. Methane and water are the main products of methanation of carbon dioxide (**Figure 1(b)**) at low temperatures (200°C - 250°C). Raising the reaction temperature above 450°C, results in the increase of the carbon monoxide by-product, due to the reverse water-gas shift reaction, and meanwhile, unreacted carbon dioxide and hydrogen also increase, along with a decrease in the methane yield [18]. The effects of pressure on the CO<sub>2</sub> conversion were also investigated. The positive effects of increasing the pressure are more important at higher temperatures [17].

In order to investigate the thermodynamic of the methanation reaction, G. Granitsiotis [21] constructed a Gibbs reactor based using the software Aspen Plus. The reactor was designed based on the experimental conditions. The pressure of the reactor was set at 1 bar and the composition of the inlet stream was 76.19% N<sub>2</sub>, 19.05% H<sub>2</sub> and 4.76% CO<sub>2</sub>. The effects of temperature on the conversion of carbon dioxide were studied. The simulation results indicate that the conversion starts decreasing from 120°C and the value of conversion at 400°C is 77.08%. The outputs of the simulation also indicate that, above the temperature of 200°C, the pressure influences immensely the performance of reaction.

For example, Kopyscinski [16] presented a LHHW kinetic model of the methanation reaction in a fixed bed reactor using a commercial catalyst Ni/Al<sub>2</sub>O<sub>3</sub> (50 wt% Ni/Al<sub>2</sub>O<sub>3</sub>, with a BET (Brunauer-Emmett-Teller) surface area equal to 183 m<sup>2</sup>/g. Using the same properties of the catalyst, Hanaâ Er-rbib and Chakib Bouallou modified the equations representing the model in order to adjust the kinetic model to meet Aspen plus™ requirements. The simulation of the methanation process consisted of three adiabatic reactors with intermediate cooling at

280 °C and 1.5 MPa and a recycle ratio of three [19]. The rate for the Water-Gas Shift reaction was described by [19]:

$$R_{\text{WGS}} \text{ (mol/kg} \cdot \text{catalyst} \cdot \text{s)} = \frac{k_2 \cdot 10^{-3} \cdot (K_3 p_{\text{CO}} \cdot p_{\text{H}_2\text{O}} \cdot p_{\text{H}_2}^{-0.5} - K_4 \cdot p_{\text{CO}_2} \cdot p_{\text{H}_2}^{0.5})}{1 + K_1 p_{\text{CO}}^{0.5} + K_2 p_{\text{H}_2\text{O}}^1 p_{\text{H}_2}^{-0.5}} \quad (9)$$

where

$$k_2 \text{ (mol/bar}^{1.5}\text{)} = 9.62 \times 10^{14} \times \exp\left(\frac{-161740}{RT}\right) \quad (10)$$

The rate of the carbon monoxide methanation process was represented by the equation [19]:

$$R_{\text{Methanation}} \text{ (mol/kg} \cdot \text{catalyst} \cdot \text{s)} = \frac{k_1 \cdot 10^{-3} K_1 p_{\text{H}_2}^{0.5} p_{\text{CO}}^{0.5}}{1 + K_1 p_{\text{CO}}^{0.5} + K_2 p_{\text{H}_2\text{O}}^1 p_{\text{H}_2}^{-0.5}} \quad (11)$$

where

$$k_1 \text{ (mol/kg} \cdot \text{catalyst} \cdot \text{s)} = 3.34 \times 10^6 \times \exp\left(\frac{-74000}{RT}\right) \quad (12)$$

In Equations (6) to (9), the pressure is expressed in Pa and the temperature in K. The equilibrium constants were presented by [19]:

$$\ln(K_i) = A_i + \frac{B_i}{T} \quad (13)$$

The values of  $A_i$  and  $B_i$  are given in **Table 1**:

This kinetic model operates in a temperature range of [473 - 673] K and high pressure [19]. The methanation of carbon monoxide was simulated by Hanaâ Er-rbib and Chakib Bouallou using Aspen plus software. The process consisted of three adiabatic reactors with intermediate cooling at 280 °C and 1.5 MPa. and a recycle ratio of three [15]. It is found that for storing 10 MW of renewable electricity, methanation unit is composed of three adiabatic reactors with recycle loop and intermediate cooling at 553 K and 1.5 MPa. The methanation unit generates 3778.6 kg/h of steam at 523.2 K and 1 MPa (13.67 MW). The model was validated by comparing the simulated results of gas composition ( $\text{CH}_4$ , CO,  $\text{CO}_2$  and  $\text{H}_2$ ) with industrial data.

J. Porubova *et al.* [20] studied three process models of the methanation of carbon dioxide using the Aspen Plus<sup>®</sup> program: 1) adiabatic methanation; 2) adiabatic methanation scheme of the  $\text{CO}_2$  extraction and 3) Isothermal methanation. For the two adiabatic processes, a heat exchanger was added upstream of

**Table 1.** Parameter values for the equilibrium constants.

$K_1$	$A_1 = -23.24$	$B_1 = 7355.77$
$K_2$	$A_2 = -20.49$	$B_2 = 8731.97$
$K_3$	$A_3 = -19.64$	$B_3 = 781.25$
$K_4$	$A_4 = -13.208$	$B_4 = -4400$

each of the three reactors. In order to control the temperature, it was also necessary to have a partial gas recirculation downstream of the first methanation reactor. For the adiabatic reaction, CO<sub>2</sub> concentration had a significant impact on the methanation reaction. On the other hand, In the case of isothermal methanation, an increase of CO<sub>2</sub> concentration only affected the flow of carbon monoxide, and other parameters, such as yield of methane and hydrogen, remained unchanged [20]. It was concluded that at constant temperature, CO<sub>2</sub> concentration does not affect the efficiency of the methanation process.

The aim of this first part of this study is to simulate the methanation process in an adiabatic Plug flow (PF) reactor. The model incorporates the catalytic reaction kinetics for the methanation reaction. The effects of temperature, pressure and H<sub>2</sub>/CO<sub>2</sub> ratio on the yield of methane will be investigated. In the second part of this investigation, the produced synthetic natural gas (SNG), based on the optimum operating conditions, will be utilized as combustible for a Natural Gas Combined Cycle (NGCC) power plant for the production of electricity. The flue gas leaving the Heat Recovery Stream Generator (HRSG) of the power plant will be treated in a CO<sub>2</sub> capture plant. The resulting concentrated carbon dioxide will be recycled and reutilized as the feed for the methanation process. It will be assumed, in this investigation, that the hydrogen gas needed for the methanation reaction is provided by a Reforming Catalytic Reactor followed by a sweetening process to remove the acid gases.

#### 4. Simulation Tool and Selection of Operating Conditions

Aspen Plus<sup>®</sup> model of the methanation process is developed and simulated in this work. The thermodynamic and transport properties of the following Compounds, Water (H<sub>2</sub>O), carbon dioxide (CO<sub>2</sub>), methane (CH<sub>4</sub>), hydrogen (H<sub>2</sub>) and carbon monoxide (CO) are calculated using a property method of RKSMHV2 along with their all needed binary interaction parameter values. The RKSMHV2 property method is based on the Redlich-Kwong-Soave equation of state with modified Huron-Vidal mixing rules. This model is used for mixtures of non-polar and polar compounds, in combination with light gases. The kinetic rate equations for the methanation and water gas shift reaction are considered as shown in Equations (2)-(10). An adiabatic fixed bed reactor is modeled on a Plug Flow Reactor (PFR), as shown in **Figure 1**.

Three parameters are considered to study for the effect of CH<sub>4</sub> production: 1) temperature, 2) pressure and 3) [H<sub>2</sub>/CO<sub>2</sub>] ratio. The following range of values was selected for each parameter based on operating conditions reported in literature [5] [17] [22].

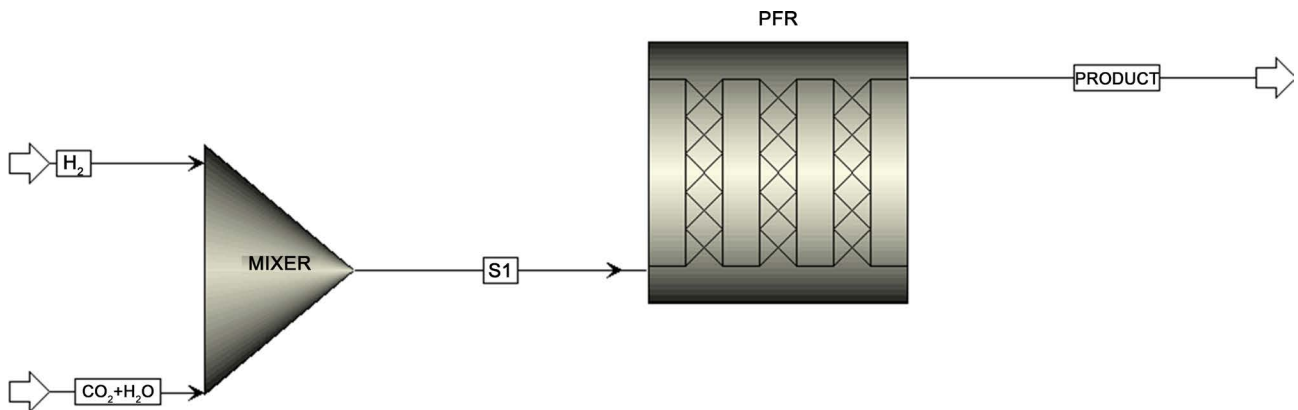
- 1) The pressure of the methanation reaction varies from 10 atm to 40 atm.
- 2) The temperature of the methanation reaction varies from 250°C to 300°C.
- 3) The amount of H<sub>2</sub> fed for the methanation reaction with respect to the CO<sub>2</sub> feed is measured as H<sub>2</sub> to CO<sub>2</sub> ratio (H<sub>2</sub>:CO<sub>2</sub> ratio) varies from 2 to 6.

As discussed in the introduction section of this paper, the simulated plant will

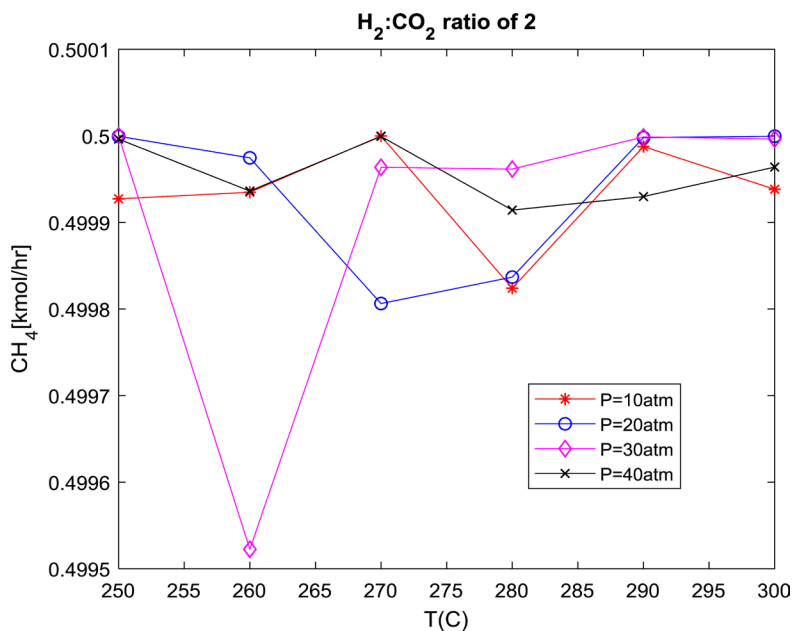
be utilizing a captured carbon dioxide containing 95% mol.  $\text{CO}_2$  and 5% mol.  $\text{H}_2\text{O}$ , where 1 kmol/hr. of the mixture is used as a base for the simulation.

## 5. Analysis of Simulation Results

The performance of the methanation reactor is measured by the production rate of  $\text{CH}_4$  in kmol/hr. Variation of the three cited operating conditions are utilized in order to obtain the maximum production of methane. As the methanation reaction is strongly exothermic, the control of the heat of reaction is a key task when designing methanation. 1) The temperature of the reaction is considered to vary  $250^\circ\text{C}$  to  $300^\circ\text{C}$  with an increment of  $10^\circ\text{C}$ . 2) The reaction pressure is considered to be 10 atm, 20 atm, 30 atm, 40 atm. 3). The third parameter (ratio of moles of  $\text{H}_2$  fed relative to the  $\text{CO}_2$  present), varies from 2 to 6. The simulation results of the present work are shown in from **Figure 2** to **Figure 7**. The resulted

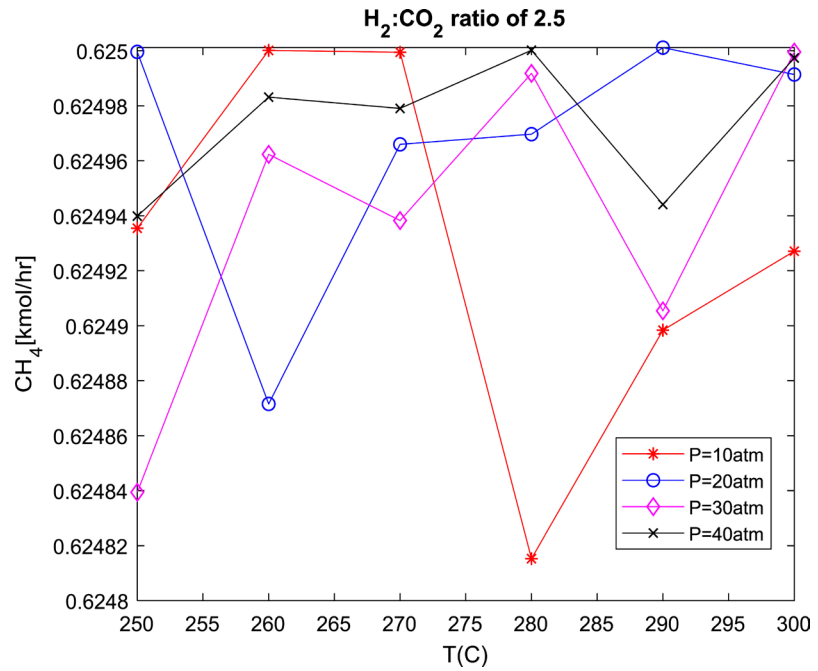


**Figure 1.** Flowsheet of a plug flow reactor for methanation reaction.

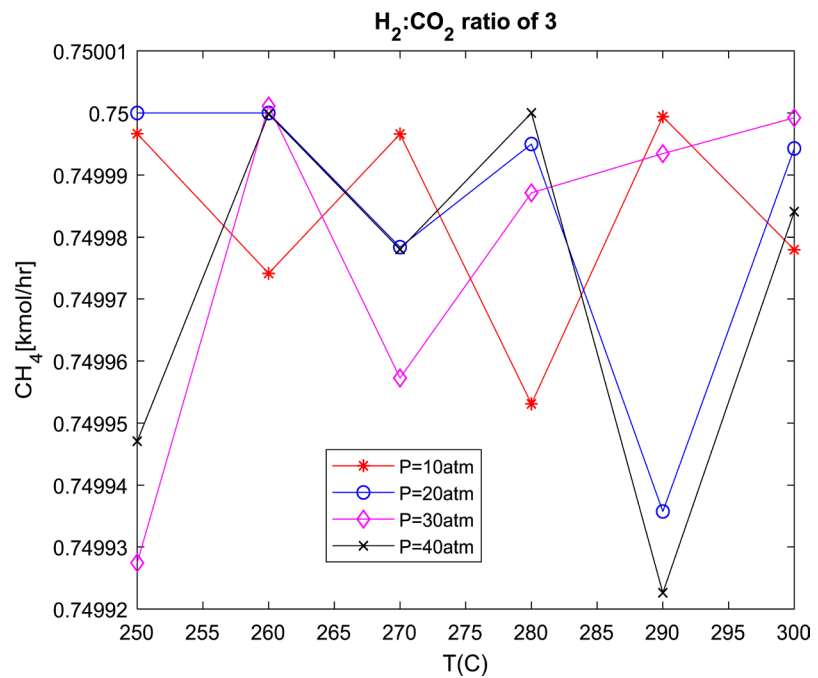


**Figure 2.** Molar flow of  $\text{CH}_4$  produced at different temperature and pressure for the  $[\text{H}_2/\text{CO}_2] = 2$ .





**Figure 3.** Molar flow of CH<sub>4</sub> produced at different temperature and pressure for [H<sub>2</sub>/CO<sub>2</sub>] = 2.5.

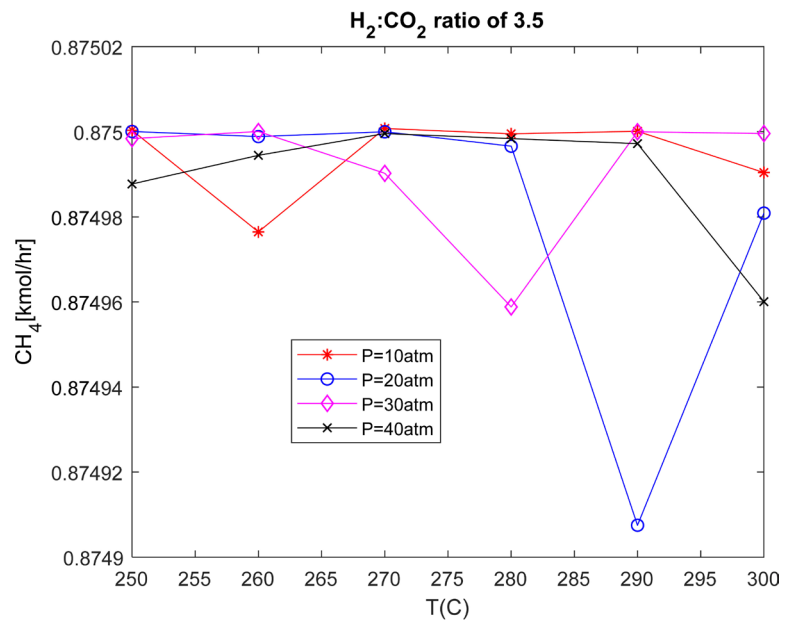


**Figure 4.** Molar flow of CH<sub>4</sub> produced at different temperature and pressure for [H<sub>2</sub>/CO<sub>2</sub>] = 3.

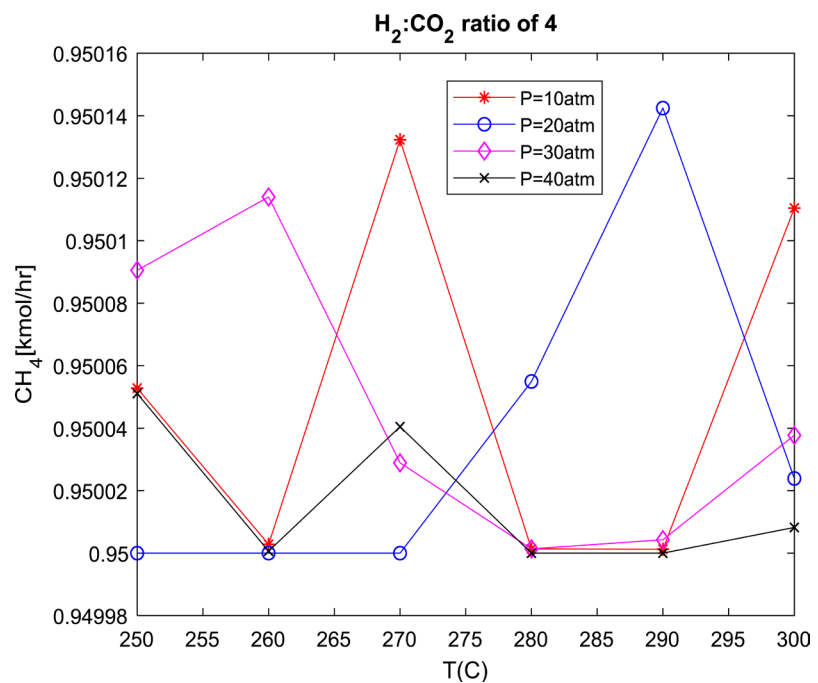
molar flowrates of CH<sub>4</sub> for different ratios of H<sub>2</sub>:CO<sub>2</sub> are obtained for a feed flowrate 1 kmol/hr of carbon dioxide containing 95% mol. CO<sub>2</sub> and 5% mol. H<sub>2</sub>O, which is used as a base for the simulation.

The CH<sub>4</sub> molar flow in kmol/hr produced if the H<sub>2</sub> feed to CO<sub>2</sub> ratio is 2.0 shown in **Figure 4**. The amount of CH<sub>4</sub> produced per kmol/hr of CO<sub>2</sub> fed is ap-

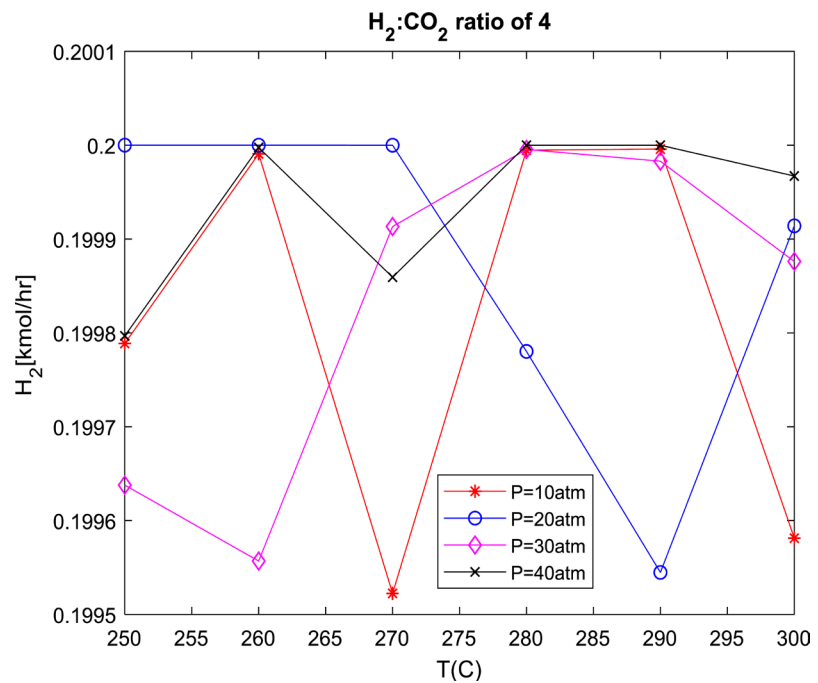
proximately equal to 0.5 kmol/hr. Similarly, the CH<sub>4</sub> molar flowrates in kmol/hr produced per kmol/hr of CO<sub>2</sub> for H<sub>2</sub> to CO<sub>2</sub> ratios of 2.5, 3.0 and 3.5 are shown in **Figures 5-7** respectively. On average the amounts of CH<sub>4</sub> produced when the H<sub>2</sub> to CO<sub>2</sub> ratios of 2.5, 3.0 and 3.5 are 0.625, 0.75 and 0.875 kmol/hr, respectively. It's observed that increasing the H<sub>2</sub> to CO<sub>2</sub> ratio in the feed increases the production rate of methane (CH<sub>4</sub>) as is depicted in **Figure 4** through **Figure 7**.



**Figure 5.** Molar flow of CH<sub>4</sub> produced at different temperature and pressure for [H<sub>2</sub>/CO<sub>2</sub>] = 3.5.



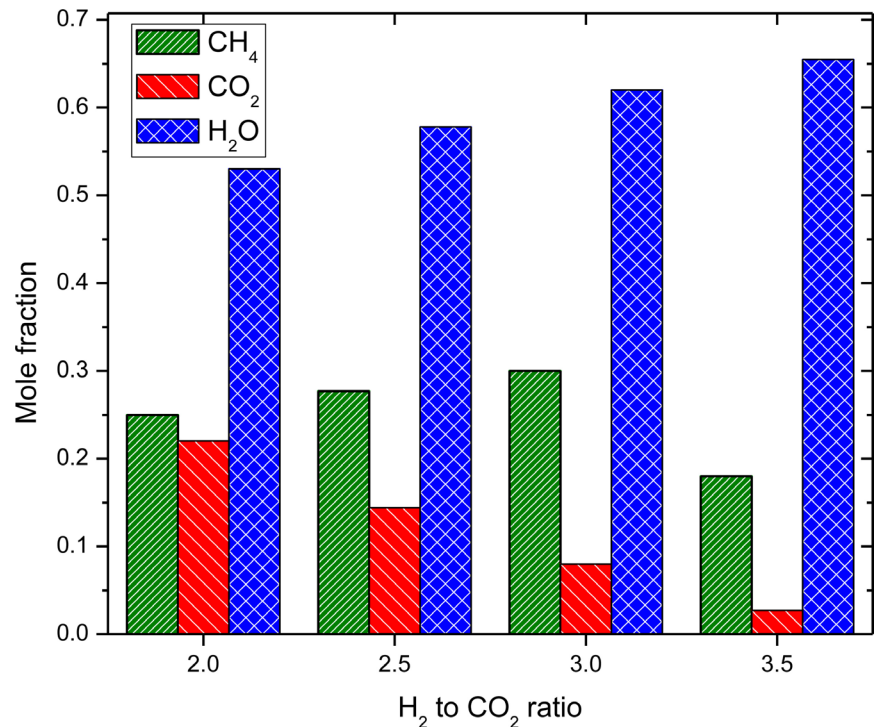
**Figure 6.** Molar flow of CH<sub>4</sub> produced at different temperature and pressure for [H<sub>2</sub>/CO<sub>2</sub>] = 4.



**Figure 7.** Molar flow of  $H_2$  produced at different temperature and pressure for  $[H_2/CO_2] = 4$ .

As the product ( $CH_4$ ) will be used as fuel, it should free of any  $H_2$ , because of its explosive nature. The product ( $CH_4$ ) stream is free of  $H_2$ , for  $H_2$  to  $CO_2$  ratios are less than 4. If the  $H_2$  to  $CO_2$  ratio is increased to 4 and above, there will be a considerable amount of  $H_2$  in the product stream. The molar flow of  $CH_4$  produced per kmol of  $CO_2$  for  $H_2$  to  $CO_2$  ratio of 4.0 is shown in **Figure 6**, which is approximately 0.95 kmol/hr. The associated amount of  $H_2$  in the product side for  $H_2$  to  $CO_2$  ratio of 4.0 shown in **Figure 7** that is about 0.2 kmol/hr. Further increase of the  $H_2$  to  $CO_2$  ratio increases the amount of  $H_2$  in the product stream (not shown here for the ratio of higher than 4). As the  $CH_4$  product will be used as fuel, it needs to be free of  $H_2$  because of the explosion nature of  $H_2$ . Thus, the optimal ratio of  $H_2$  to  $CO_2$  in the feed stream is 3.5 that gives the maximum possible amount of  $CH_4$  with no  $H_2$ . These simulation results are in agreement with Koschany [17], where the  $CO_2$  to  $CH_4$  conversion is approximately 100% for  $H_2$  to  $CO_2$  ratio of 4 at low temperatures 200°C - 300°C.

The molar fraction of different components in the product stream is analyzed for different temperatures and pressures considered in this simulation. The amount of  $CH_4$  is observed to increase upon increasing the  $H_2$  to  $CO_2$  molar ratio, a similar trend is observed on the amount of water produced. The average molar fraction of components in the product stream is shown in **Figure 8**. The amount of  $CO_2$  is observed to decrease upon increasing  $H_2$  to  $CO_2$  molar ratio. The amount of CO is negligibly small in the product stream, not shown in **Figure 8**. These results are in good agreement with results reported in the literature by J. Gao *et al.* [18] and R. Stefan *et al.* [5] for the considered range of temperatures and pressures.



**Figure 8.** Average molar fraction CH<sub>4</sub>, H<sub>2</sub>O and CO<sub>2</sub> in the product stream for [H<sub>2</sub>/CO<sub>2</sub>] molar ratios = 2.0, 2.5, 3.0, and 3.5 at the range of temperature and pressure considered.

## 6. Conclusion

The present work represents the first part of the simulation of an NGCC Power Plant for the production of electricity from CO<sub>2</sub> emissions. In this paper, the feed of the methanation reactor is the CO<sub>2</sub> stream from the capture unit of the power plant. The optimal conditions of methanation process are identified through the present simulation studies. Based on the simulation results, The [H<sub>2</sub>/CO<sub>2</sub>] ratio is the most influential parameter that highly affects the production rate of CH<sub>4</sub>. It is found that the production of CH<sub>4</sub> is directly proportional to the [H<sub>2</sub>/CO<sub>2</sub>] ratio at the different temperatures and pressures under consideration. However, increasing the H<sub>2</sub> to CO<sub>2</sub> ratio higher than 3.5 results in the presence of H<sub>2</sub> in the product stream, which is not recommended due to safety in the plant. Thus, the optimum amount of CH<sub>4</sub> is obtained for [H<sub>2</sub>/CO<sub>2</sub>] ratio equal to 3.5. Moreover, low temperature (250°C - 270°C) and high pressures [30 - 40 atm] also enhance the production of methane. CH<sub>4</sub> production.

## Acknowledgements

The authors would like to thank the Higher Colleges of Technology (UAE), for supporting this applied research.

## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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