Bitlis Eren Üniversitesi Fen Bilimleri Dergisi
BİTLİS EREN UNIVERSITY JOURNAL OF SCIENCE
ISSN: 2147-3129/e-ISSN: 2147-3188
VOLUME: 11 NO: 2 PAGE: 490-498 YEAR: 2022
DOI: 10.17798/bitlisfen.1036026

Performance Assessment of a Combined Coal Gasification and Methanation System with Particle Swarm Optimization Method

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Keywords: Carbon dioxide hydrogenation, Particle swarm optimization, Coal gasification, Methane production

Abstract

Carbon dioxide hydrogenation is a promising method of producing alternative fuels in an environmentally friendly way. Researchers in the current literature have mainly investigated the performance of carbon dioxide hydrogenation systems that use carbon dioxide from various sources and hydrogen from water electrolysis units. In the present study, the performance of a combined coal gasification and methanation unit is investigated to produce methane and power. The carbon dioxide and hydrogen for the methanation unit are provided by the coal gasification system. A Particle swarm optimization (PSO), an optimization-based artificial intelligence method, is applied to optimize the carbon dioxide and hydrogen values here. Therefore, the water electrolysis unit, which needs high amounts of energy, effectively is removed from the system. The results from the studied system showed that it is possible to produce ~225 kilotons of methane annually by using ~946 kilotons of coal per year. In addition, the results revealed that annual carbon dioxide utilization of ~624.3 kilotons is possible. The system efficiency is estimated at around 49%.

1. Introduction

It is significantly important to investigate and develop novel and alternative energy conversion systems because of the increasing energy requirements and adverse environmental effects of fossil fuels [1], [2]. Producing alternative fuels from various sources including coal, biomass, renewable sources, etc., is one of the solutions for governments to enhance energy security, energy independence and the clean production of fuels. One of the most promising ways to produce alternative fuels from different sources is carbon dioxide hydrogenation. Various fuels, including methane, methanol, ethanol, 1-Butanol, 2-Butanol, iso-octanal, dimethyl ether, polyoxy dimethyl ether, synthetic gasoline, paraffinic diesel, and paraffinic kerosene can be produced via carbon dioxide hydrogenation [3]. Various carbon dioxide sources that are produced from coal gasification power plants, coal-fired power plants, gas-fired power plants, refineries and natural gas processing, steel mills, cement production, biogas plants, and direct air capture have been mainly used for carbon dioxide hydrogenation systems in the literature [4]. In addition, the hydrogen requirement for carbon dioxide hydrogenation has been provided by employing water electrolysis [4].

Dieterich et al. [4] reviewed the state of the art of the conversion of hydrogen and carbon dioxide to liquid fuels via power-to-liquid (PtL) processes. They investigated the feasibility of the production of methanol, dimethyl ether, and Fischer-Tropsch fuels via carbon dioxide hydrogenation and PtL processes. Schemme et al. [5] provided a comprehensive overview of the synthesis possibilities and potential of hydrogen and carbon dioxide based alternative fuels for the transport sector. They explained the promising synthesis pathways as well as the technical aspects of the adopted processes to produce alternative fuels (methanol and higher alcohols) for the transport sector. Schemme et al., in their other paper [3], conducted a study to understand the

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Received: 13.12.2021, Accepted: 02.06.2022

economic feasibility of the production of various fuels via carbon dioxide hydrogenation. Herdem et al. [6] suggested a novel combined oxyfuel combustion biomass gasification and solar photovoltaic system to produce methanol in an environmentally friendly way. They used carbon dioxide hydrogenation for methanol synthesis. The hydrogen for the methanol synthesis was provided by an alkaline water electrolysis system, while the power requirement of the alkaline water electrolysis system was supplied by the solar photovoltaic and biomass gasification plants, and the remaining power was provided from the electrical grid. Furthermore, the carbon dioxide for the methanol synthesis was provided by the oxyfuel combustion biomass gasification system. Zhang et al. [7] studied the techno-economic optimization of green methanol production from the carbon dioxide hydrogenation system with an integrated solid-oxide electrolysis process. They simulated the system using Aspen Plus and used multi-objective optimization for the techno-economic optimization. Kotowicz et al. [8] performed a thermodynamic analysis of a carbon dioxide hydrogenation system for environmentally friendly methanol production. Hydrogen for the methanol synthesis was provided by water electrolysis. The power requirement of the water electrolysis was provided by a 40 MW wind farm during the night valleys. They [8] also used the captured carbon dioxide from a power plant`s flue gas for renewable methanol production. Eveloy [9] investigated a hybrid solid oxide electrolyzer and oxyfuel combustion system for methane production via carbon dioxide hydrogenation. The system was conceptually designed for synthetic natural gas (methane), power, and heat production. Eveloy developed a thermodynamic model to investigate the operation characteristics and energetic and exergetic performance of the system. Momeni et al. [10] investigated the performance of a synthetic natural gas (methane) production system based on carbon dioxide hydrogenation. They used the carbon dioxide from a natural gas power plant while employing a water electrolysis unit in the system for hydrogen production to produce synthetic natural gas. They estimated the energy and environmental performance of the system as well as the cost of the system. Synthetic fuels and electro-fuels for the transport sector have also been reviewed in terms of production processes and cost in [11] and [12]. However, the estimation of these system inputs sometimes does not produce adequate and accurate results. The use of more up-to-date mathematical models and applications has become essential to increase the efficiency of methane production. Recently, artificial intelligence technologies have been used to make effective and accurate coal gasification and methanation systems and to obtain statistical results [13], [14]. Today, with the discovery of optimization-based technologies such as genetic algorithms and PSO, artificial intelligence methods such as machine learning, artificial neural networks, and even deep learning with feature selection are frequently used for coal methaneization and gasification. In addition, it enables effective energy production and the use of alternative energy sources in life. Azarhoosh et al. [15] simulated and optimized the auto-thermal reforming of methane to synthesis gas using a genetic algorithm. Shamsi et al. [16] presented process simulation and optimization of the coal gasification process in a moving-bed reactor using Pittsburgh No. 8 coal as feed. A simulation was used to estimate solid and gas temperature status and gas composition in the reactor. The methods such as optimization methods, artificial intelligence, and machine learning are applied in many application areas such as health, agriculture, education, sport, finance as well as obtaining optimum energy sources. It has become indispensable for efficiency in various fields to produce the best information from big data or to extract the best or optimum values from energy data [17]. In addition to artificial neural networks (ANNs), machine learning algorithms, ensemble models, and hybrid models could be used to high prediction performance to assess coal gasification and methanation applications. Deep learning algorithms have also been used to predict coal methanation parameters [18]. Due to the high performance of machine learning methods in different disciplines, these methods have been used frequently in various energy fields, especially in the last decade. Researchers have used machine learning algorithms in prediction, and estimation of factors affecting match results [19].

In this study, a preliminary analysis was performed to show the energetic performance of a combined coal gasification and carbon dioxide hydrogenation unit for methane and power production using optimization based Particle Swarm Optimization (PSO). The reason for using PSO as the optimization algorithm in this study is that particle motions are suitable for the optimization of carbon dioxide and hydrogen data. Also, PSO is the most well-known of all metaheuristic methods. Adaptation of this method in this study has already allowed and validated the optimal and optimal results. In addition, a parametric study was conducted to understand the effects of various parameters on the performance of the methanation unit. The simulation of the system was conducted using Aspen Plus.

The innovative contributions and highlights of this study can be listed as follows.

- The main novelty of this study is that the hydrogen produced from the coal gasification system is used as a hydrogen source for carbon dioxide hydrogenation instead of using water electrolysis, as in the other studies in the literature.
- The carbon dioxide is also provided from the coal gasification system for the carbon dioxide hydrogenation unit.
- In this coal gasification and methaneization system, the PSO method has been applied in order to use the carbon dioxide and hydrogen data feeding the reactors in the best and balanced way. In this way, the most effective results were obtained.

The data regarding the coal gasification system was extracted from previous work [20]. The main focus of this study is to investigate the energy efficiency of the combined coal gasification and methanation system and the effects of different operation parameters on the methanation unit. The present study will be useful for researchers as a guide for developing alternative fuel production systems.

2. Material and Method

The simplified schema of the studied system is illustrated in Figure 1. The coal gasification plant is explained in detail in our previous study [20]. The system consists of a coal gasifier unit, an air separation unit, a water gas shift reactor unit, hydrogen sulfur, and carbon dioxide removal units, a pressure swing adsorption unit, an alkaline electrolyser unit, a heat recovery steam generator unit, and a power generation unit. Hydrogen is produced in the system by using the pressure swing adsorption unit, and the alkaline water electrolyser unit, which is powered by the power generation unit. In this study, it is assumed that the hydrogen is produced via the pressure swing adsorption unit; thus, the coal gasification system produces power, hydrogen, and carbon dioxide as well as sulfur as a by-product. All the produced hydrogen and a certain amount of produced carbon dioxide in the coal gasification unit are used in the methanation unit. In addition, the power requirement for the methanation unit is provided by the power generated in the coal gasification unit [21].

The methanation unit integrated into the coal gasification plant is shown in Figure 2. Methane is produced in the methanation unit via the carbon dioxide hydrogenation reaction. The carbon dioxide hydrogenation for methane production is known as the Sabatier reaction, which is given in Eq.(1) [17]. The amounts of the reactants are estimated based on the reaction stoichiometry.

$$4H_2 + CO_2 \rightarrow CH_4 + 2H_2O \; H_r^o = -206\, kJ/mol \quad (1)$$

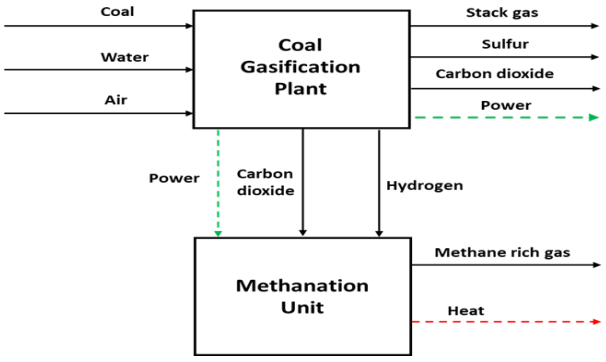

Figure 1. A simplified scheme of the studied system in this study. The coal gasification plant is explained in detail in [20]

Various types of reactors can be used for carbon dioxide hydrogenation, including multitubular reactors [22] and micro-channel reactors [23]. In this study, the effects of different parameters on the performance of carbon dioxide hydrogenation for methane production are estimated using the Gibbs free energy minimization method without considering any specific type of reactor. This method is useful in understanding the thermodynamic limits of different parameters on carbon dioxide hydrogenation. After that, the PSO method is used to optimize the carbon dioxide and hydrogen parameters and to achieve the desired limitation. PSO is a metaheuristic-optimization method in which the behavior of various birds in nature is artificially tackled to obtain a desired target or optimum value [24]. In a flock, a bird always flies towards a better position in its surroundings. Each individual in the PSO is like a bird, following various rules and interacting with other individuals around it in order to complete the final task. In a PSO algorithm, each individual in the swarm is represented as a particle. The particles follow several simple rules and benefit from the experience of neighboring particles or their own during swarm updates. They update their position to head to the destination and their speed to arrive at the destination just in a given time [24]. The velocity and position equations of the basic PSO algorithm are given in Eqs. (2) and (3).

$$v_i(t+1) = \omega v_i(t) + c_1 r_1(t)(o_b(t) - x_i(t)) + c_2 r_2(t)(g_b(t) - x_i(t)) \quad (2)$$

$$x_i(t+1) = x_i(t) + v_i(t+1) \quad (3)$$

where v_i and x_i are the velocity and position of the particle i at time t, respectively. Also, c_1 and c_2 are acceleration constants that are positive numbers used in the contribution of cognitive and social components to rate the updates. Random numbers r_1 and r_2 can take various values between 0 and 1. The inertia weight ω controls the inertia of a particle, and measures the effect of the velocity of the previous instant on the next displacement. $o_b(t)$ and $g_b(t)$ are the optimal positions calculated by the particle itself and all particles in the population, respectively. All particles know the population information. Each particle moves towards the global optimal solution and aims to find the optimal solution in the population. Before the update, the particle decides whether the reached location is better than the known location or the location known by someone else. Otherwise, the particles retain the previous optimal values and continue to move. The PSO algorithm only terminates when a successful solution is found or the iteration count reaches its maximum value.

Therefore, $(G^t)_{T,P}$ is created for fitness function $min_{n_i}(G^t)_{T,P}$ given in Eq. (4). The function is minimized until the best reactor values are selected according to this equation. In PSO, c_1 and c_2 values selected as 1 and 2, respectively. The population number was chosen as 50 in PSO method.

$$minimize_{n_i}(G^t)_{T,P} = \min_{n_i} \sum_{i=1}^{M} n_i \left(G_i^o + RTln\left(\frac{\bar{f}_i}{f_i^o}\right)\right) \quad (4)$$

In this study, four moles of hydrogen are used per one mole of carbon dioxide. The inlet conditions of the reactants are given in Table 1. The effects of reaction temperature and pressure, and reactant inlet temperature to the reactors on the carbon monoxide conversion, the amount of heat removal requirement for the first reactor and methane production are found from the simulation. The carbon dioxide conversion for the first reactor is calculated as in Eq.(5).

$$X_{CO2,R1} = \frac{\dot{n}_{CO2,4} - \dot{n}_{CO2,5}}{\dot{n}_{CO2,4}} \times 100 \quad (5)$$

where $\dot{n}_{CO2,4}$ is the mole flow rate of the carbon dioxide at stream 4 (see Figure 2) while $\dot{n}_{CO2,5}$ is the mole flow rate of the carbon dioxide at stream 5. In addition, the overall carbon dioxide conversion in the methanation unit is estimated as in Eq.(6).

Table 1. Carbon dioxide and hydrogen feed streams to the methanation unit.

Parameter	CO_2 gas	H_2 gas
Flowrate (kg/h)	71268.7	13058.6
Temperature (°C)	25	25
Pressure (bar)	1.5	20

An RGibbs reactor in Aspen Plus is used for the Gibbs free energy minimization method. The list of the chemical components used in the simulation are H_2, CO_2, CH_4, and H_2O. Thermodynamic physical properties in the simulation are estimated using the Peng-Robinson equation of state with Boston-Mathias modification (PR-BM) [21]. Two reactors for the carbon dioxide hydrogenation are used in the system illustrated in Figure 2. Note that the CO_2 and H_2 feed in Figure 2 are given as an optimized input to the system thanks to the PSO.

The first reactor is an isothermal reactor that requires heat removal to control the reactor temperature while the second reactor is an adiabatic reactor. A similar strategy (one tubular reactor and one adiabatic reactor in series) is suggested in [21] for methanation of coke oven gas to improve the system efficiency and increase the catalyst lifetime. Using a multitubular reactor and an adiabatic reactor in series can also be useful for carbon dioxide hydrogenation to decrease the system cost and increase the efficiency. The obtained results in this study can be expanded in future studies to understand the benefits of this method.

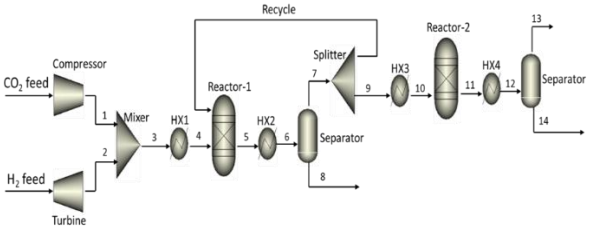

Figure 2. Methanation unit where carbon dioxide hydrogenation takes place. The figure is modified from [21].

$$X_{CO2,Overall} = \frac{\dot{n}_{CO2,4} - \dot{n}_{CO2,11}}{\dot{n}_{CO2,4}} \times 100 \quad (6)$$

where $\dot{n}_{CO2,11}$ is the mole flow rate of the carbon dioxide at stream 11. The system efficiency of the combined coal gasification and methanation system is found after the parametric analysis. The efficiency of the system is calculated as in Eq.(7).

$$\eta_{sys} = \frac{\dot{W}_{net}+\dot{m}_{H2}LHV_{H2}+\dot{m}_{CH4}LHV_{CH4}}{\dot{m}_{Coal}LHV_{Coal}} \quad (7)$$

where $\dot{W}_{net}$ is net power generation of the combined coal gasification and methanation system while LHV_i is the lower heating value of the hydrogen, methane, and coal. In addition, $\dot{m}_i$ refers to the mass flow rate of the hydrogen, methane and coal. Further explanation about the system is given in the Section 3.

3. Results and Discussion

The change in the carbon dioxide conversion for the first reactor with variation of the reactor temperature and pressure is shown in Figure 3. The reactor temperature changes from 150°C to 400°C. In addition, there are different reactor operation pressures: 3 bar, 10 bar and 50 bar which are used to understand the effect of the operation pressure on the carbon dioxide conversion. As shown in the figure, the carbon dioxide conversion increases with lower reactor temperature as expected. The methanation reaction (Eq.(1)) is highly exothermic; thus, the reaction shifts to the left with an increase in temperature according to Le Chatelier`s Principle [25].

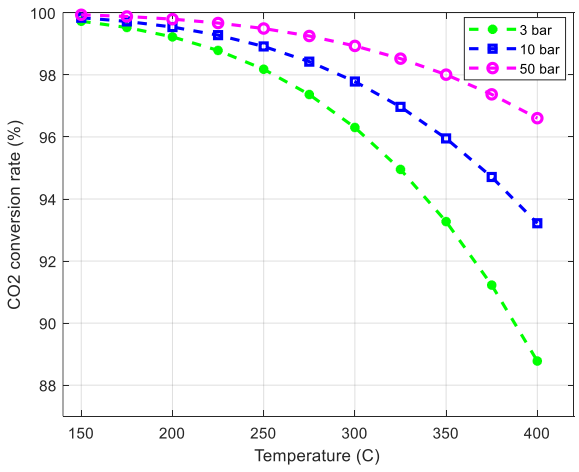

Figure 3. The change in the carbon dioxide conversion for the first reactor with variation of the reactor temperature and pressure.

The low reaction temperature is thermodynamically favourable for the carbon dioxide hydrogenation; however, the reaction kinetics and the catalyst used for carbon dioxide hydrogenation should be considered to define the optimal reaction temperature. The reactor temperature is generally higher than 280°C for carbon dioxide hydrogenation in practical applications [23]. The carbon dioxide conversion also increases with an increase in pressure. In particular, the effect of pressure on the conversion significantly increases with relatively high reactor temperature. For example, the carbon dioxide conversion is equal to ~96% at 300°C and 3 bar while it is ~99% at 300°C and 50 bar. On the other hand, the carbon dioxide conversion is equal to ~88.5% at 400°C and 3 bar while it is ~96.5% at 400°C and 50 bar. Although the carbon dioxide conversion can be increased with elevated pressures, the balance of plant of the system can also significantly increase with an elevated operation pressure. Therefore, the carbon dioxide conversion and the balance of plant of the system should both be considered to select the optimum operation pressure of the methanation unit.

One of the most important issues for carbon dioxide hydrogenation to produce methane is to control the reactor temperature because the carbon dioxide hydrogenation reaction is highly exothermic. Therefore, it is critical to understand the change in the heat removal requirement of the reactor with the variation of different parameters. The change in the amount of heat removal requirement from the reactor with variation of the reactor temperature and pressure, and the reactant inlet temperature into the reactor is shown in Figures 4 and 5, respectively.

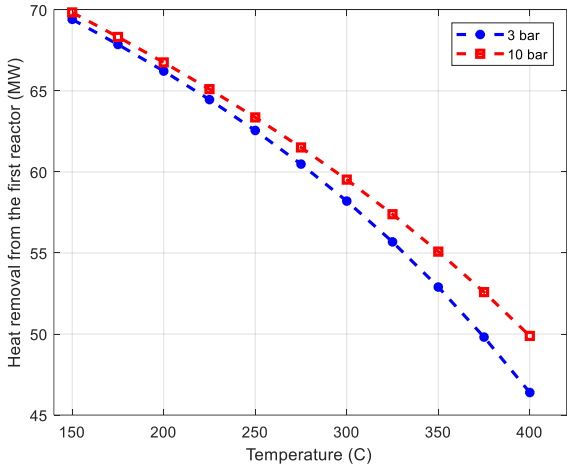

Figure 4. The change in the heat removal requirement from the first reactor with variation of the reactor temperature, pressure and reactant inlet temperature. The reactant inlet temperature is 50°C.

As seen in the figures, there is no significant effect of the operation pressure on the amount of heat removal from the reactor. The heat removal requirement increases with elevated reactor temperature as expected because carbon dioxide

conversion is higher at the elevated reactor temperatures. One of the easiest ways to control the heat removal requirement of the reactor is to manipulate the reactant inlet temperature. A heat exchanger (HX1 in Figure 2) is used to control the reactant inlet temperature. As seen from Figures 4 and 5, the heat removal requirement from the first reactor increases ~27% at 350ºC and 3 bar with variation of the reactant inlet temperature from 50ºC to 250ºC.

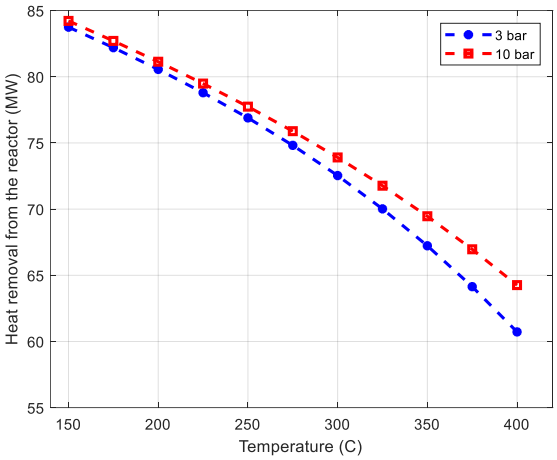

Figure 5. The change in the heat removal requirement from the first reactor with variation of the reactor temperature, pressure and reactant inlet temperature. The reactant inlet temperature is 250ºC.

The changes of the overall carbon dioxide conversion and methane production in the methanation unit variation of the first reactor temperature and the reactant inlet temperature into the second reactor are shown in Figures 6 and 7. The results are obtained for 3 bar operation temperature of the methanation unit. As illustrated in Figure 6, it is possible to achieve an overall carbon dioxide conversion higher than 96% for all parameters used in the present study. As expected, the higher overall conversion is found for the lower reactant inlet temperature of the second reactor. The reaction kinetics and hot spot formation in the reactor should be considered for the final decision of the reactor temperature and the reactant inlet temperature of the reactor. As can be shown from Figures 6 and 7, the thermodynamically maximum methane production is obtained at almost 100% carbon dioxide conversion. The maximum methane production is around 25972 kg/h at ~100% carbon dioxide conversion while it is ~25000 kg/h at ~96% carbon dioxide conversion, as seen in Figure 7. The efficiency of the combined coal gasification and methanation unit and methane production from the system are estimated for 3 bar and 20 bar operation pressure of the methanation unit after the parametric analysis and optimization method. These operation pressures are selected while considering hydrogen output pressure from the pressure swing adsorption unit and the carbon dioxide inlet pressure to the methanation unit.

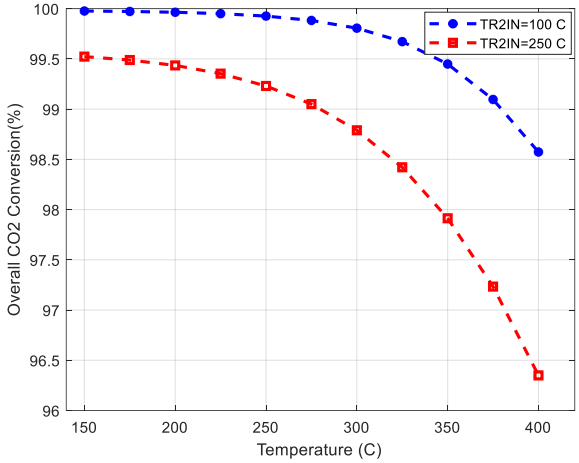

Figure 6. The change in the total carbon dioxide conversion with the variation of the temperature of the first reactor and the reactant inlet temperature of the second reactor.

The carbon dioxide inlet pressure is increased to the operation pressure of the methanation unit by using a compressor. A single compressor is used to increase the pressure of the carbon dioxide feed stream for 3 bar of the operation pressure of the methanation unit while a multistage compressor is selected to increase pressure of the carbon dioxide feed stream for 20 bar of the operation pressure of the methanation unit. In addition, a turbine is used to decrease the hydrogen pressure and produce extra power for 3 bar of the operation pressure.

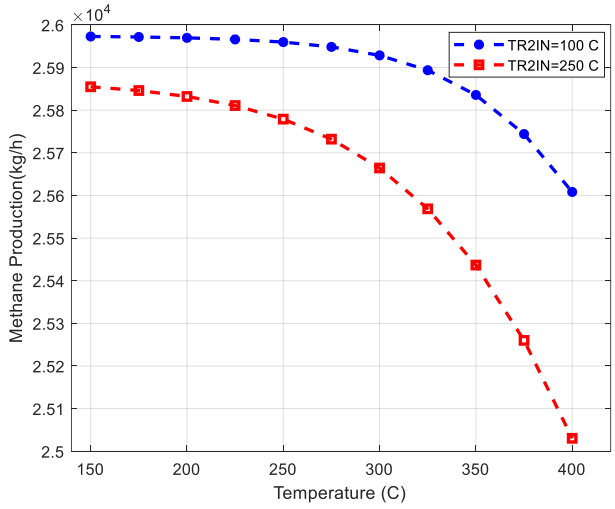

Figure 7. The change in the methane production rate with the variation of the temperature of the first reactor and the reactant inlet temperature.

The isentropic efficiency of the compressors and turbine is assumed to be 0.8. After applying the

PSO and parameters, the results for carbon dioxide and hydrogen feed streams to the methanation unit are listed in Table 2.

Table 2. Carbon dioxide and hydrogen feed streams to the methanation unit

Parameters	CO_2	H_2
Operation pressure of the methanation unit (bar)	3	20
Power generation from the coal gas gasification plant (MW)	26.1	26.1
Compressor power requirement in the methanation unit (MW)	-5.77	-10.07
Hydrogen turbine power generation in the methanation unit (MW)	5.2	0
Net power generation (MW)	25.6	15.4
Overall carbon dioxide conversion (%)	98.8	99.6
Hydrogen rate in the product (kg/h)	158.85	53.72
Methane production (kg/h)	25664	25870
System efficiency (based on LHV) (%)	49.88	48.5

As shown from the table, the increase in methane production is only 0.8% with increasing operation pressure of the methanation unit from 3 bar to 20 bar. Reactor values are optimized by PSO method. However, the compression work significantly increases with higher operation pressure of the methanation unit. Therefore, lower pressure can be preferred to increase the system efficiency. The power generation and methane production from the system are equal to ~25.6 MW and ~25664 kg/h, respectively for 3 bar operation pressure and 108000 kg/h coal input (Illinois#6 coal is used in the coal gasification system and the LHV of the coal is equal to 25.88 MJ/kg [20]).

4. Conclusion and Future Work

A novel system based on combined coal gasification and carbon dioxide hydrogenation is proposed in this study to produce power and methane using PSO method. A parametric analysis was conducted to understand the effects of various parameters on the performance of the methanation unit. In addition, the reactor feeds were optimized by applying the PSO method. The results showed that it is possible to produce ~25.6 MW of power and ~25664 kg/h methane for 108000 kg/h coal by using a combined coal gasification and methanation unit. The results also showed that the system efficiency is ~50%. This efficiency was estimated by assuming that the produced methane is directly injected into the available methane pipeline. The advantage of the PSO method here cannot be overlooked either.

In future studies, the methanation unit will be analyzed in detail by developing Multiphysics models while considering the reaction kinetics and hot spot formation in the reactors to optimize methane production. In addition, various scenarios to produce different fuels including ammonia, methanol, methane and diesel from the combined coal and biomass systems will be explored. Furthermore, deep learning techniques for techno economic assessment of the system should be performed in future studies.

Contributions of the authors

All authors contributed equally to the study.

Conflict of Interest Statement

There is no conflict of interest between the authors.

Statement of Research and Publication Ethics

The study is complied with research and publication ethics.

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