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Optimal Carbon Dioxide Methanation using Green Hydrogen

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The surge in demand for energy has resulted in a significant transformation of the worldwide energy sector, causing a shift toward the advancement of energy sources that are both efficient and sustainable. In order to address environmental issues and advance a sustainable energy future, renewable energy (RE) sources and carbon dioxide (CO_2) utilisation are crucial. Greenhouse gas (GHG) emissions increments are driven by economic and population growth, which are increasing. The rise in growth has led to an increase in the atmospheric concentration of CO_2. Due to this situation, carbon capture, utilisation, and storage (CCUS) seems to be a promising approach to reducing CO_2 emissions. Among all the carbon utilisation strategies available, CO_2 methanation is promising for producing fuel for future energy. This project aims to develop an optimisation model for a mobile pilot facility for CO_2 methanation using green hydrogen (H_2) generated from solar photovoltaic (PV). In this project, an energy model for the design of a solar energy source for hydrogen production integrated with battery energy storage to ensure optimum usability of the renewable energy source for CO_2 utilisation will be developed.

1. Introduction

Climate change has become a severe global challenge, and there is no exception for Malaysia. Reducing carbon emissions under rapid economic growth and social development has been identified as one of the macro challenges in the 12th Malaysia Plan (EPU, 2021). The impact of anthropogenic carbon emissions on climate change cannot be ignored because 95% of climate changes result from human activities (World Bank, 2020). Power plants contribute to 54% of carbon emissions in Malaysia. Transitioning to the decarbonisation of power plants is very challenging.

The valorisation of CO_2 into methane by reacting with H_2 is one of the options that mitigate carbon emissions and promote green energy (Nicola Pierro et al., 2023). Sibai (2019) examines CO_2 methanation at a variety of application levels, including chemical kinetics, reactors, and the entire process, in the context of power-to-grid applications. Energy storage is a crucial part of any renewable energy system due to the intermittent nature of renewable sources. Power-to-gas technology (P2G) effectively stores excess renewable energy on a large scale and for durations ranging from hours to months. Since natural gas transportation and storage infrastructure are already in place in many nations, turning renewable electricity into hydrogen (H_2) and synthetic natural gas (SNG) via CO_2 methanation seems to be an appealing P2G process option.

Integrating solar PV, a battery energy storage system (BESS), an electrolyser, and H2 storage for CO2 methanation is not easy. Mathematical modelling is a powerful framework often used to identify processes and optimise operations. Uebbing et al. (2020) optimised the dual objectives model by maximising the exergetic efficiency and minimising the investment cost via Pareto optimal solutions. A superstructure optimisation approach to power-to-methane processes containing 13 potential process technologies in seven levels is now in the development stage of power-to-methane.

Saad and Alnouri (2022) presented the mixed integer linear programme (MILP) as a rapid evaluation tool to find the optimal choice(s) among reported thermocatalytic carbon monoxide (CO) hydrogenation processes. Using the MILP model, the author sizes and costs four major types of chemical units (compressor, heat exchanger,

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reactor, and distillation column) in a network optimisation of 29 literature processes. Wang et al. (2018) created a multi-objective optimisation platform that uses component models that have been experimentally calibrated along with an integrated heat cascade computation. The model looked at (1) system-level heat integration; (2) effects of operating factors such as operating voltage, reactant utilisation, anode/cathode feed ratio, and operating pressure of the methanation reactor and membrane on system performances; (3) competitiveness of the electrolyser operation with pure oxygen production; and (4) the possibility of avoiding electrical heating, which is required for thermoneutral operation to heat up the electrolyser fee.

Mah et al. (2021a) developed a cascade analysis method for targeting and scheduling microgrid energy systems with energy sources from renewables and using a liquid organic hydrogen carrier as energy storage. The proposed framework can help provide a better estimation in selecting the energy system capacity. Mah et al. (2021a) focused on equipment sizing and finding sufficient capacity but did not optimise the sizing from an economic perspective. Mah et al. (2021b) developed a comprehensive optimisation framework to optimise the microgrid's design and operation, consisting of an intermittent energy source and multiple electricity and hydrogen loads. A mathematical model was designed to reduce the cost of a microgrid with hydrogen and electrical loads by selecting the optimum equipment capacity. Mah et al. (2021b) also studied the economic feasibility of the PV system under different configurations, such as tilt angle adjustment and solar tracking system, but only focused on one energy storage.

Due to the fluctuation in solar irradiance, the hourly solar power generation, hourly H_2 generation, and hourly H_2 methane are hard to predict. Different options for storing energy will affect the overall cost of the CO_2 methanation system. In this study, both hydrogen and battery energy storage are included in the mathematical model. This study will minimise the overall cost of the power system to convert all of the CO_2 into CH_4 via General Algebraic Modeling System (GAMS) modelling.

2. Problem identification

Today's energy derives from fossil fuels, which results in increased CO_2 concentrations in the atmosphere, causing global warming through the greenhouse effect. Significant efforts are being made to replace conventional fossil fuels with renewable and new energy sources such as methanation. In this study, the model was developed based on the existing Janamanjung Power Plant to determine the solar energy supply required for optimal H_2 production. The system would be integrated with BESS to react with CO_2 flow rate via methanation. The CH_4 produced would be consumed in situ as part of the fuel needed to operate the site. The model's applicability was demonstrated using the Janamanjung power plant with 0.214105 kg CO_2/h. A mathematical model was formulated using mixed integer linear programming (MILP) and solved using CPLEX 12.6.3 in GAMS. The objective of this mathematical model is to minimise the total cost of methanation, which consists of renewable energy technologies, electrolysers, hydrogen production, and methanation. Several equality and non-equality constraints are developed to define the model's boundary. The equality constraint of the model mainly consists of the energy and mass balance of each operating unit, while non-equality constraints consist of limitations on resources and the requirement to convert CO_2 to CH_4.

3. Methodology

Figure 1 shows the superstructure of a power plant utilising solar energy for H_2 generation to be reacted with CO_2 via the CO_2 methanation process. Solar energy is susceptible to weather intermittency. The weather conditions considered in this study are high and low intensity for solar irradiation. The solar irradiation values were extracted from a daily solar irradiance for a month, where the days with the highest (6.14 kW/m2/d) and lowest (1.04 kW/m2/d) solar irradiance within the month were considered as high and low solar irradiations in this study, respectively. Battery and H_2 storage were also being considered to deal with the intermittency of energy supply. It was assumed that high and low solar irradiance occurred almost evenly throughout the day over the year. The solar irradiation trends for high and low solar irradiance were the same. Tables 1 to 3 depict the secondary data assumptions for equipment costs, process-related information, and solar and CO_2 methanation technology data.

Table 1: Equipment cost data assumptions obtained from secondary sources

Technology	Capital Cost	Fixed Operational Cost	Source
Solar power	574.5 USD/kW	11.69 USD/m^2 (2 % Capex)	(Maleki et al., 2020)
Li-ion Battery	500 USD/kWh	-	(Dinesh et al., 2018)
Hydrogen Compressor	5,439,525 USD/unit	-	(Yousefi et al., 2023)
Hydrogen Storage	1,250 USD/kg H_2	-	(Cruz-Soto et al., 2022)

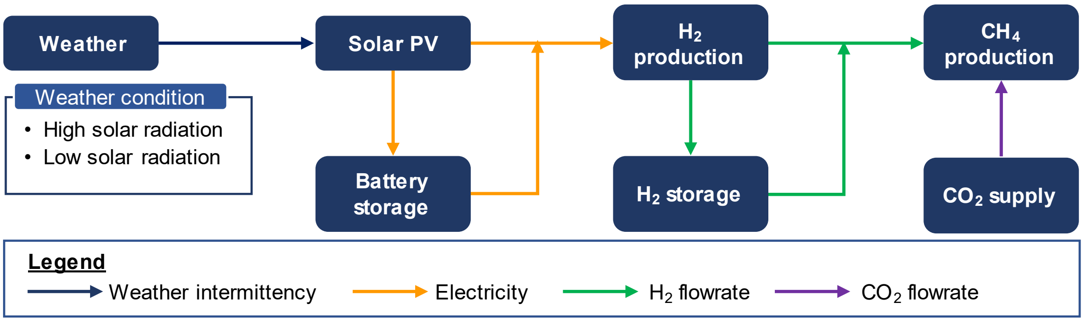

Figure 1: Superstructure of the CO_2 methanation process at the power plant

Table 2: Process-related information and data obtained from secondary sources

Process information	Value (Unit)	Source
H_2 Electrolysis Rate	0.015037594 kg/kWh	(Zhuk et al., 2022)
Ratio of H_2 to CO_2	4 mol of H_2 = 1 mol of CO_2	(Jensen et al., 2021)
Battery Efficiency	85 %	(Dinesh et al., 2018)
CO_2 flowrate	636,323 kg CO_2/h	TNBR

Table 3: Technologies data assumption obtained from secondary sources

Technology	Value (Unit)	Source(s)
Solar Panel		
Solar Efficiency	12 %	(Maleki et al., 2020)
Solar Area	Unlimited m^2	-
Solar Panel Life Time	25 y	(Cruz-Soto et al., 2022)
CO_2 methanation		
Electrolyzer Pressure	30 bar	(Shiva Kumar and Lim, 2022)
Storage Pressure	350 bar	(Ni, 2006)
Compressor Energy Consumption	23.25 kWh/kg H_2	-
Compressor Power Capacity	5,000 kWh/kg H_2	(Yousefi et al., 2023)

3.1 The mathematical formulation for the economic decision analysis model

In this study, a mixed integer linear programming mathematical model was developed to optimise the total cost of the CO_2 methanation at the power plant by adjusting the solar install area, energy storage capacity and hydrogen storage to meet the hydrogen demand of the system. The objective function Eq(1) is to minimise the total cost of the system, (TCost), which includes grid cost ($\mathrm{Cost}^{\mathrm{G}}$), solar system cost ($\mathrm{Cost}^{\mathrm{S}}$), battery cost ($\mathrm{Cost}^{\mathrm{BT}}$), compressor cost ($\mathrm{Cost}^{\mathrm{C}}$) and hydrogen storage cost ($\mathrm{Cost}^{\mathrm{HS}}$). Eq(2) is to determine the $\mathrm{Cost}^{\mathrm{G}}$ by summing up the grid energy used to produce H_2 ($\mathrm{Grid}^{\mathrm{H2}}_{\mathrm{T,D}}$) and grid energy used to charge the battery ($\mathrm{Grid}^{\mathrm{BESS}}_{\mathrm{T,D}}$), which is then multiplied with the weather day type ($\mathrm{Day}_{\mathrm{D}}$). Eq(3) is to determine the $\mathrm{Cost}^{\mathrm{S}}$ by summing the amortised solar capital cost and solar operation cost. The solar capital cost is determined by multiplying the solar installed area ($\mathrm{Solar}^{\mathrm{Area}}$) with solar area unit cost ($\mathrm{Solar}^{\mathrm{UP}}$) and then amortise the cost with interest rate (IR) and solar panel lifetime (LTS). Eq(4) is to determine the $\mathrm{Cost}^{\mathrm{BT}}$ by multiplying energy storage capacity ($\mathrm{BESS}^{\mathrm{Ins}}$) with the battery unit price ($\mathrm{BESS}^{\mathrm{UP}}$) and then amortise with the battery life time (LTB) and IR. Eq(5) is to determine $\mathrm{Cost}^{\mathrm{C}}$ by multiplying compressor unit ($\mathrm{Comp}^{\mathrm{Unit}}$) with compressor unit cost ($\mathrm{Comp}^{\mathrm{UP}}$) and then amortise with the compressor lifetime (LTC) and IR. Eq(6) is to determine $\mathrm{Cost}^{\mathrm{HS}}$ by multiplying hydrogen storage capacity ($\mathrm{HS}^{\mathrm{Cap}}$) with the hydrogen capacity unit cost ($\mathrm{HS}^{\mathrm{UP}}$) and then amortise with the hydrogen storage lifetime (LTHS) and IR. Eq(7) is to determine H_2 produced by multiplying the summation of the solar energy for H_2 production ($\mathrm{Solar}^{\mathrm{H2}}_{\mathrm{T,D}}$) and battery energy for H_2 production ($\mathrm{BESS}^{\mathrm{H2}}_{\mathrm{T,D}}$) with the H_2 conversion rate ($\mathrm{H}_2^{\mathrm{CR}}$) with the unit of kg H_2/kWh. Eq(8) is to determine the solar energy generated ($\mathrm{Solar}^{\mathrm{Gen}}_{\mathrm{T,D}}$) by multiplying the solar radiation ($Solar^{Rad}_{T,D}$) with the $Solar^{Area}$, solar efficiency ($Solar^{Eff}$) and solar binary ($Solar^{Binary}$). Eq(9) is to distribute the $Solar^{Gen}_{T,D}$ to battery storage ($Solar^{Bess}_{T,D}$), $Solar^{H2}_{T,D}$, excess energy ($Solar^{Ex}_{T,D}$). Eq(10) is to determine the state of charge in battery storage ($BESS^{SOC}_{T+1,D}$) by summing up the import energy and deducting with $BESS^{H2}_{T,D}$. The import energy will have to multiply with the battery efficiency ($BESS^{Eff}$) first. Eq(11) is to ensure the $BESS^{SOC}_{T,D}$ is less than $BESS^{Ins}$. Eq(12) is to determine the hydrogen storage level ($HS^{LVL}_{T,D}$) . $H_{2}{}^{Dem}_{T,D}$ is an input parameter and hydrogen demand of the power plant, and the model is required to fulfil the $H_{2}{}^{Dem}_{T,D}$. Eq(13) is to ensure that $HS^{LVL}_{T,D}$ will always be less than the HS^{Cap}. Eq(14) is to ensure that the sufficient unit of compressor ($Comp^{Unit}$) is installed to fulfil the compressor power. $Comp^{Cons}$ is the power required for the compressor to compress the H_2 with the unit of kW/kg H_2, while $Comp^{PUnit}$ is power per compressor unit.

$$\min TCost = Cost^{G}+Cost^{S}+Cost^{BT}+Cost^{C}+Cost^{HS}s \quad (1)$$

$$Cost^{G}=\sum_{T,D}\left(Grid^{H2}_{T,D}+Grid^{BESS}_{T,D}\right)\times Day_{D} \quad (2)$$

$$Cost^{S}=\left(Solar^{Area}\times Solar^{UP}\times\frac{IR\times(1+IR)^{LTS}}{(1+IR)^{LTS}-1}\right)+\left(Solar^{Area}\times Solar^{OMUP}\right) \quad (3)$$

$$Cost^{BT}=BESS^{Ins}\times BESS^{UP}\times\frac{IR\times(1+IR)^{LTB}}{(1+IR)^{LTB}-1} \quad (4)$$

$$Cost^{C}=Comp^{Unit}\times Comp^{UP}\times\frac{IR\times(1+IR)^{LTC}}{(1+IR)^{LTC}-1} \quad (5)$$

$$Cost^{HS}=HS^{Cap}\times HS^{UP}\times\frac{IR\times(1+IR)^{LTHS}}{(1+IR)^{LTHS}-1} \quad (6)$$

$$H_{2}{}^{Pro}_{T,D}=\left(Solar^{H2}_{T,D}+BESS^{H2}_{T,D}\right)\times H_{2}^{CR} \quad (7)$$

$$Solar^{Gen}_{T,D}=Solar^{Rad}_{T,D}\times Solar^{Area}\times Solar^{Eff}\times Solar^{Binary} \quad (8)$$

$$Solar^{Gen}_{T,D}=Solar^{Bess}_{T,D}+Solar^{H2}_{T,D}+Solar^{Ex}_{T,D} \quad (9)$$

$$BESS^{SOC}_{T+1,D}=BESS^{SOC}_{T,D}+\left(Solar^{Bess}_{T,D}+Grid^{BESS}_{T,D}\right)\times BESS^{Eff}-BESS^{H2}_{T,D} \quad (10)$$

$$BESS^{SOC}_{T,D}\leq BESS^{Ins} \quad (11)$$

$$HS^{LVL}_{T+1,D}=HS^{LVL}_{T,D}+H_{2}{}^{Pro}_{T,D}-H_{2}{}^{Dem}_{T,D} \quad (12)$$

$$HS^{LVL}_{T,D}\leq HS^{Cap} \quad (13)$$

$$H_{2}{}^{Pro}_{T,D}\times Comp^{Cons}\leq Comp^{Unit}\times Comp^{PUnit} \quad (14)$$

4. Results and discussions

GAMS version 24.4.6 encoded the objective function, variables, parameters, and constraints. The mixed integer linear programming model was optimised using the CPLEX solver. The model used an i7 processor and a 12 GB RAM system. The optimal result was obtained with zero tolerance. The findings showed that the ideal cost for converting 636,323 kg/h of CO_2 through methanation is 2,649 billion USD per year.

Figure 2 and Figure 3 show the hydrogen- and energy-related results for the high solar radiation scenario, and Figure 4 and Figure 5 show the hydrogen- and energy-related results for the low solar radiation scenario. The peak energy generation during the low solar radiation scenario was 3,015 GWh/h; for H_2, it was 45 million kg/h. During the high solar radiation scenario, peak energy generation was identified as 6,031 GWh/h, and 18,465 GWh/d of solar energy was overproduced and wasted. Due to reliance on only solar PV technology, which is intermittent by nature, the solar PV have to be sized to cater for the worst-case scenario when solar radiation is low (rainy days), as shown in Figure 4 and Figure 5. The phenomenon of solar PV being overdesigned only happened during high solar irradiance days, as there would be excess solar energy, as shown in Figure 3. As shown in both figures, since solar is only available during the day, H_2 storage is mandatory to store solar energy during the day to be utilised at night to continuously process CO_2, which is assumed to be constant throughout the day. Despite some energy losses during the electricity conversion into H_2, the mathematical model decided to use H_2 storage as the only storage option due to energy losses during charging and discharging into the BESS. The H_2 stored in advance will be used for CH_4 production when the instantaneous H_2 production is insufficient to satisfy the production of CH_4 (Hour 18 of Figure 2 and Figure 4). H_2 production is only available during the daytime as it follows the availability of solar radiation. The H_2 generated will be prioritised for CH_4 production rather than stored in the H_2 storage.

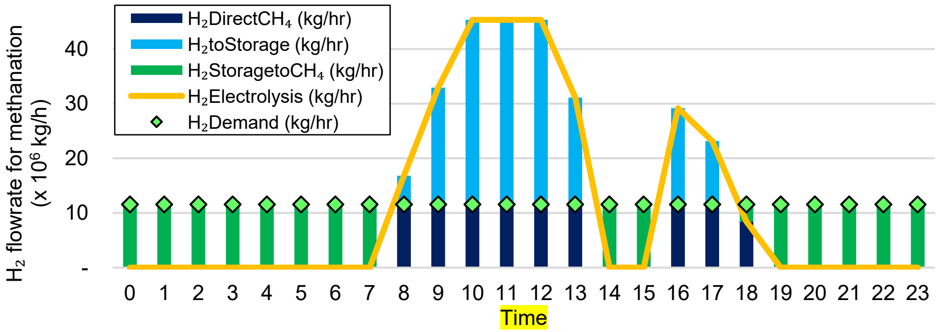

Figure 2: Hydrogen-related results for high solar radiation scenario

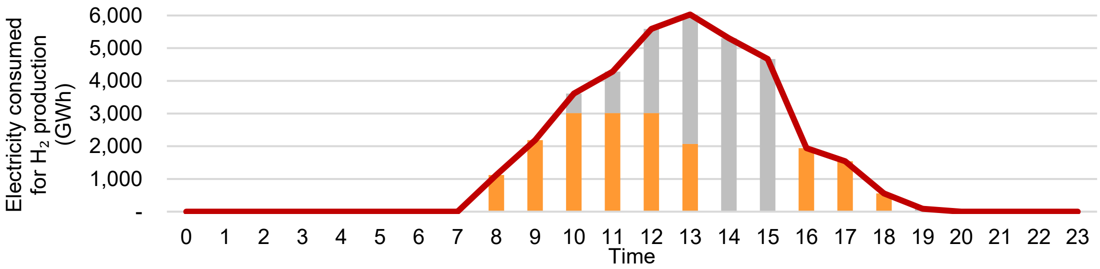

Figure 3: Energy-related results for high solar radiation scenario

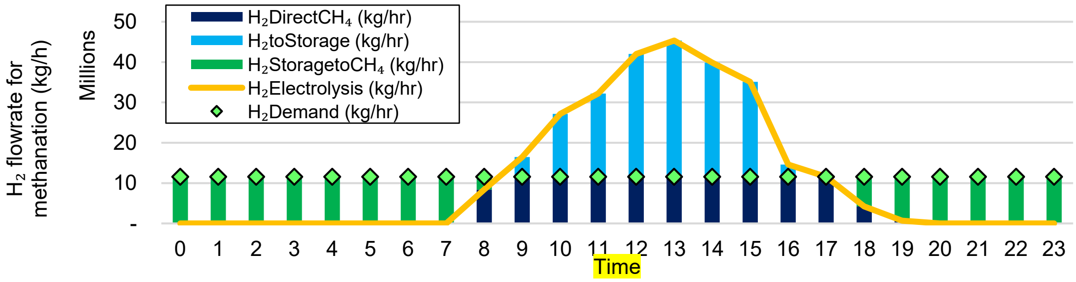

Figure 4: Hydrogen-related results for low solar radiation scenario

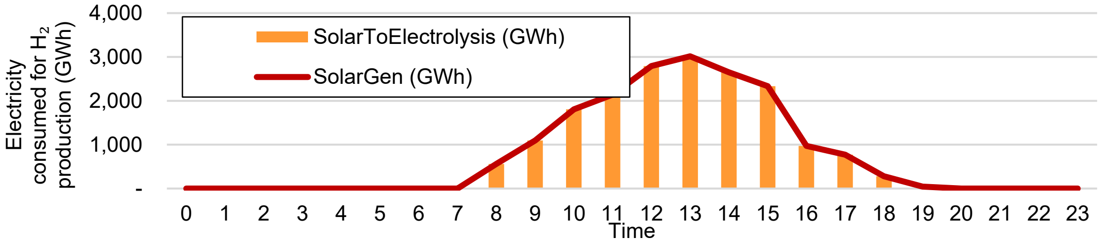

Figure 5: Energy-related results for low solar radiation scenario

5. Conclusions

In this project, an energy model for designing a solar system for hydrogen production integrated with battery energy storage to ensure optimum usability of the renewable energy source for CO_2 utilisation via the methanation process has been developed successfully. The model has been demonstrated using a mobile pilot facility for CO_2 methanation using green hydrogen. The results revealed that the total optimal cost for the conversion of CO_2 with an amount of 636,323 kg/h via the methanation process is 2,649 billion USD/y, and the model prefers to store energy in H_2 storage instead of using a battery energy storage system. The result also indicated that fully depending on green energy to supply the energy demand of the process, regardless of weather conditions, will generate much excess energy during high solar irradiation days. This happens as the pieces of equipment are designed to also tackle the energy demand during low solar irradiation days. In future studies, the energy supply from the RE sources and grid energy should be mixed together to achieve the highest CO_2 emission.

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