TECHNO-ECONOMIC INVESTIGATION OF METHANOL PRODUCTION PLANT USING SOLAR AND WIND ENERGY IN IRAQ

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I certify that in my opinion the presented thesis that has been submitted by Farah Abdalrahman Abdalrzaq ALKHALIDI titled “TECHNO-ECONOMIC INVESTIGATION OF METHANOL PRODUCTION PLANT USING SOLAR AND WIND ENERGY IN IRAQ” is fully adequate in scope and in quality as a thesis for the degree of Master of Science.

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Farah Abdalrahman Abdalrzaq ALKHALIDI

ABSTRACT

Master Thesis

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This study aims to make a techno-economic investigation of a plant that produces methanol using solar and wind energy in Iraq using waste gas from a Fallujah white cement factory. Carbon dioxide in flue gas is captured in the carbon capture plant (CCP) and hydrogen is obtained from the wastewater of the factory in the hydrogen plant (HP) with the help of photovoltaic and wind turbine energy, all of which is combined in the methanol plant (MPP) to produce methanol fuel. Using the Engineering Equation Solver (EES), a calculation was made of the amount of energy required and the number of solar panels or wind turbines that would be required to meet this demand, followed by an investigation of the environmental impact of the methanol plant. The Iraqi Fallujah white cement facility was selected as a case study location. Processes of the systems of CO_2 emissions, heat integration, energy efficiency, and techno-economic performance were all taken into consideration. Renewable energy PV, WT, methanol plants, and methanol fuel showed efficiencies of 0.21%, 0.98%, 0.1626%, and 0.5872%, respectively, and at the optimum density of the electrolyzer, 2.2 kA/m^2, the efficiency of the electrolyzer was 0.782%. This study demonstrates that flue gas is the most significant input parameter affecting the outputs because all process output parameters increase as flue gas levels rise. The entire cost to operate the plant for 30 years for each of the PV plants and wind turbines (WTs) was found to be $9,46 billion and $5,291 billion, respectively, with a production capacity of over 34,530 million tons of methanol, which corresponds to 0.4131 $/kg for the PV plant and 0.2413 $/kg for the WT plant. Environmentally, the rate of captured emissions was approximately 3894 tons per day, and the mitigation rate was approximately 3594 tons per day. According to the results, the existing plant is competitive with other clean synthetic fuel manufacturing facilities.

Key Word : Methanol Production, Carbon Capture, Renewable Energy, Hydrogen Electrolysis, Solar Energy, Wind Energy.
Science Code : 91408

ÖZET

Yüksek Lisans Tezi

IRAK’TA GÜNEŞ VE RÜZGAR ENERJİSİ KULLANILARAK METANOL ÜRETİMİNİN TEKNO-EKONOMİK OLARAK İNCELENMESİ

Farah Abdalrahman Abdalrzaq ALKHALIDI

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Bu çalışma, Irak'ta Felluce'deki bir beyaz çimento fabrikasının atık gazını kullanarak güneş ve rüzgâr enerjisi kullanarak metanol üreten bir tesisin termoekonomik incelemesini yapmayı amaçlamaktadır. Baca gazındaki karbondioksit, karbon yakalama tesisinde (CCP) yakalanır ve tamamı fotovoltaik ve rüzgâr türbini enerjisi yardımıyla elde edilen hidrojen ile birleştirilerek metanol elde edilmektedir. Hidrojen hidrojen tesisinde (HP), fabrikanın atık suyundan elde edilmektedir. Engineering Equation Solver (EES) kullanılarak, gerekli enerji miktarı ve bu talebi karşılamak için gerekli olacak güneş paneli veya rüzgâr türbini sayısı hesaplanmış ve ardından metanol tesisinin çevresel etkisi araştırılmıştır. Irak Felluce beyaz çimento tesisi örnek olay yeri olarak seçilmiştir. Sistemlerin CO_2 emisyonları, ısı entegrasyonu, enerji verimliliği ve termo-ekonomik performans süreçleri dikkate alınmıştır. Yenilenebilir enerji PV, WT, metanol tesisleri ve metanol yakıt sırasıyla %0,21, %0,98, %0,1626 ve %0,5872 verimlilik göstermiştir ve elektrolizörün optimum yoğunluğu olan 2,2 kA/m^2'de elektrolizörün verimliliği %0,782 bulunmuştur. Bu çalışma baca gazı debisinin çıkışları etkileyen en önemli girdi parametresi olduğunu göstermektedir, çünkü baca gazı seviyeleri yükseldikçe tüm proses çıkış parametreleri artmaktadır. Çalışmanın sonucuna göre 34,530 milyon tonun üzerinde metanol üretim kapasitesine sahip olan tesisin 30 yıllık işletme maliyetinin her bir PV santrali ve rüzgâr türbini (WT) için sırasıyla 9,46 bilyon dolar ve 5,291 bilyon dolar olduğu bulundu. PV tesisi için 0.4131 $/kg ve WT tesisi için 0.2413 $/kg. Çevresel olarak, yakalanan emisyonların oranı günde yaklaşık 3894 ton ve azaltma oranı günde yaklaşık 3594 ton bulunuştur. Sonuçlara göre, mevcut tesis diğer temiz sentetik yakıt üretim tesisleri ile rekabet edebilir durumdadır.

Anahtar Sözcükler : Metanol Üretimi, Karbon Tutma, Yenilenebilir Enerji, Hidrojen Elektrolizi, Güneş Enerjisi, Rüzgâr Enerjisi
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SYMBOLS

CRF : capital recovery factor, dimensionless
Cp : specific heat, kJ/kgK
ί : annual interest rate, %
N : annual operating hours, h
n : system lifetime, y
$\dot{Z}$: capital cost rate, $/s
Z : capital cost, $
η : efficiency
ϕ : maintenance factor, dimensionless
$\dot{n}$: Molar Flowrate, kmol/s
$\dot{Q}$: Heat, kW
$\dot{W}$: Work, kW
$\dot{m}$: Mass Flowrate, kg/h
C_C : Factor of Carbon Emissions t C/TJ
H_V : Gross Calorific Value of Coal TJ/kiloton
h : Enthalpy kJ/kg

ABBREVITIONS

CO2 : Carbon Dioxide
PEC : Purchased Equipment Cost
EES : Engineering Equation Solver
MPP : Methanol Production Plant
HP : Hydrogen Plant

CCP : Carbon Capture Plant
PEM : Proton Exchange Membrane
PV : Photovoltaic
WT : Wind Turbine
MEA : Mono Ethanol Amine
IPCC : Intergovernmental Panel on Climate Change

PART 1

INTRODUCTION

Exceptionally environmentally friendly forms of energy are in high demand worldwide. It is now a priority on a global scale to reduce pollution and emissions of greenhouse gases to safeguard the environment in a better manner. Although fossil fuel-derived energy remains accessible. and shows no sign of disappearing soon, the days of abundant, affordable energy are ending. It is therefore of the utmost importance to investigate alternative forms of energy, particularly renewable forms of power, and to address the environmental issues associated with such energy sources.

Energy can be thought of as the capability to act. When a force is applied to an object, that object moves directly due to the pressure being applied. Work can be broken down into three primary components: power, displacement, and causality. Energy refers to the amount of work that must be applied to an object to produce these components. This quantity of work requires power. Even though there is a limited supply of energy in the universe, this resource has been carefully conserved. In spite of the fact that it is capable of being immediately converted into matter, it is not something that can be classified as being material.

In spite of the fact that we hear or read about it very regularly, we never truly make use of any energy. In addition to working on the things it comes into contact with, it can also change states, transform into other things, and transfer across items [1].

1.1. IMPORTANCE OF ENERGY

Energy is essential to life and to all living beings for both their continued existence and their continued development. The sun is the source of all of Earth’s energy, be it directly or indirectly. Although we might not be aware of the full extent to which our activities and decisions regarding energy affect the natural systems of the Earth, it is essential that we proceed with extreme caution whenever we make decisions regarding energy. The real cost of energy is not simply a question of money; rather, it has significant repercussions not only for the economy but also for politics and society as a whole.

The majority of our day-to-day energy requirements are satisfied by fossil fuels, nuclear energy as well as biomass and other renewable energy sources. Multiple types of electrical energy sources are utilized during the production of electricity, regardless of whether it occurs on a large or small scale and whether or not it is connected to a grid. Electricity merits its own category because it serves as a channel for the transmission of energy rather than being a major source of energy.

Coal, oil, and natural gas are just a few of the fossil fuels that are used to produce electricity. Nuclear energy is an example of a non-renewable source of electricity that stands out due to the fact that it does not release carbon dioxide emissions. In nuclear power plants, the process known as fission, which refers to the act of breaking atoms, is used to produce vast amounts of energy, which is then used to heat water. The generation of electricity involves the rotation of a turbine that is driven by the steam that is created [2].

In contrast to the very limited availability of fossil fuels, renewable energy sources like wind, water, and the sun may be found in large quantities (and in the case of solar energy, taking energy directly from the sun). Wind power, hydroelectricity, and geothermal energy are the three primary categories of renewable energy sources.

1.2. RENEWABLES

Energy that can be renewed over time is known as renewable or alternative energy. Solar, wind, and hydroelectric energy are a few examples of this sort of energy, power from hot springs, power from tidal pools, and power from geothermal heat (biofuels). A source of energy that is renewable is one that does not deplete its supply and has an infinite potential for further production, such as the sun. When people discuss "alternative energy," they typically refer to both renewable and non-renewable sources of power. In the context of this discussion, it refers to types of energy that cannot be maintained throughout time, such as coal [3].

Energy access, energy security, and climate change are all global issues that affect sustainable development [4]. Global challenges, such as global warming, have been caused by the world's reliance on fossil fuels and their impact on the global economy and ecology. Carbon emissions, climate change, and increased use of fossil fuels are all such effects. Flue gases produced by burning fossil fuels are a main component of greenhouse gases [5]. All of those issues demand answers, which encourages the move toward renewable energy [6]. When compared to conventional sources, energy from alternative sources including solar, wind, hydropower, and biomass are sustainable, clean, and affordable [7].

1.3. STATUS OF IRAQ

Iraq is located between latitudes 29 and 37 degrees north and covers an area of 437,072 square miles. The southern and central regions of the northern zone of the central area are home to the 58th largest country on Earth. There are many variables that can affect this region, including the angle of the sunlight, radiance, and daylight hours, which can vary greatly from warm summer days (about 14 hrs.) to chilly winter days (roughly 8 hrs.). Wintertime is when climate weather depressive conditions last for six months. in the Mediterranean Sea, causing rainfall and temperature variations [8].

Iraq’s economy already relies heavily on oil exports, which brought in 95% of the government’s revenue and accounted for 70% of the country’s total GDP in 2011. Regarding the oil sector, the speed of Iraq’s recovery depends greatly on production and exports, and how successfully profits are managed. Currently, Iraq’s oil output stands at more than 3 million barrels per day, making it the fourth largest oil exporter in the world. Even the most modest estimates of Iraq’s potential oil production have a significant effect on the nation's economy [9].

Warm, moist winds and showers are brought to Iraq’s central and northern regions by depressions generated by the west wind during the winter passage. These depressions bring rain and warm, humid winds.

As a result of its four distinct seasons, Iraq’s climate exhibits a wide range of climate features. The two longest seasons are summer and winter, and the two shortest are spring and fall. The sun is practically vertical to the northern hemisphere from June to August, which is known as the summer solstice. High-pressure orbital winds, which are prevalent throughout Iraq in the summer, contribute to a lack of rain in some areas, as the dry summer season is extremely hot. The period from December to February is the peak of the winter season’s climatic qualities and can be separated into two distinct periods.

All over Iraq, the temperature dips during the winter; it can fall to below zero degrees in some locations in central and northern Iraq on some winter evenings. As a result, the monthly heat index decreases northwards [10]. When the Mediterranean Sea experiences flight depressions in the winter, western and northwestern winds push from high-pressure zones toward low-pressure areas, passing across Iraq in the process [11].

With regard to wind direction, northwesterly winds are prevalent throughout the year, whereas southeastern breezes are responsible for rainfall during storms, or depressing conditions following the passage of the northwestern winds [12]. This puts Iraq in the top echelon of countries that generate electricity from solar power, with solarity ranging from 1,800 kWh/m^2/year to 2,390 kWh/m^2/year of direct normal radiation [13]. The cheapest form of renewable energy, wind energy, is also the most abundant [14], despite its low cost.

1.3.1. Fossil Fuels in Iraq

Iraq was one of the world’s most fuel-economies in 2010 due to its reliance on fossil fuels, outdated technology, and a lack of energy efficiency regulations. Nevertheless, Iraq is on track to reduce its carbon intensity by 25% by 2035. Improved energy efficiency in Iraq is partly the result of the country’s rapid economic expansion (supported by large-scale investments in new machinery) [15], but shifting patterns of energy consumption have also had an impact. With natural gas taking the place of liquid fuels in electricity generation, this is the most critical of these changes. Fuel derived from fossil sources includes natural gas, coal, naturally produced petroleum products, and crude oil [11].

Table 1.1. Fossil fuels in Iraq

No.	Fossil used in Year	Percentage	Inc / Dec	First used
1	2014	94.98%	0.7% Decrease	2013
2	2013	96.67%	0.89% Decrease	2012
3	2012	97.57%	0.1% Increase	2011
4	2011	97.67%	0.12% increase	2010
5	2014	96%	Decrease	1995

1.3.2. Renewables in Iraq

Some locations in Iraq, such as Muthanna and Anbar provinces, have some of the country’s most appealing solar irradiation values at 1,899 kWh/m^2 in the west and south. As demand for electricity exceeds supply during the peak summer months, solar power provides the advantages of being built quickly, cost-effectively, and in support of Iraq’s efforts to become self-sufficient by lowering electricity and gas imports. Baghdad spends between $2.5 billion and $2.8 billion a year on these imports, with results as follows:

1.3.2.1. Solar Energy Potential

In this research, the potential for the use of renewable energy sources in Iraq as well as the opportunities for the application of technology for concentrated solar power to assist with the generation of electricity in Iraq are both investigated. Solar power in Iraq is not being utilized to its full potential at the moment. However, considering that the global solar radiation averages between 2,000 and 2,500 kWh/m2 per day on an annual basis, this source of power has the potential to play a significant role in Iraq's overall energy output.

Due to the fact that Iraq receives more than 3,300 additional hours of daylight on a yearly basis on average, the country is an outstanding site for the generation of solar electricity. Solar radiation has an effect on the desert regions of Iraq, which today account for more than 60% of the overall land of the country. It is possible to calculate that a total area of 437,072 square kilometers is covered by the energy that is produced in the country as a whole.

It is common knowledge that Iraq enjoys extensive stretches of daylight throughout the year. In a typical year, there are approximately 3000 hours of daylight in Baghdad. The hourly solar intensity in January is 416 W/m2, but in June, it reaches 833 W/m2 [16]. With regard to the number of sunny days per year, Iraq actually outperforms Spain [17]. The utilization of solar technology is quite limited despite the fact that Iraq possesses a significant deal of untapped potential. The desert in western Iraq can provide the highest amount of solar irradiation for the generation of electric power anywhere in the world, with an annual average horizontal surface irradiance of 170 W/m2. The barren deserts of Iraq have a mean power density of up to 290 watts per square meter [18,19], and they have the potential to achieve a peak power density of 2,310 kWh/m2 per year.

The deserts of Iraq take up 31% of the total land area of the country. However, Iraq has managed to keep its place as one of the leading suppliers of fossil fuels to the world [20]. Because of this, there is little interest in utilizing solar electricity. The value of renewable sources of energy is not being recognized by either the Iraqi government or the Iraqi people as a result of this. It is necessary to advance renewable energy technologies in this region; however, this must be accomplished solely via the efforts of private citizens and non-governmental organizations, and not by means of state policy. In the past ten years, it has been abundantly evident that today energy is a complex problem with many facets. Despite the substantial amount of fossil fuel resources available in the country, Iraq suffered from a severe energy shortage when it was completely destroyed in 1991. It is anticipated that fossil fuels will finish by the next century due to their limited availability. In this uncertain future, solar energy will be the only reliable source of renewable energy that will also contribute to the reduction of CO2 emissions caused by a wide sources of fossil fuels and biofuels in various forms. Because of the potential positive effects on the climate, it is worth considering solar energy as soon as possible [21].

1.3.2.2. Wind Energy Potential

Around the world, policies and investments in renewable energy have concentrated most of their attention on the electricity sector. As a direct result of this, renewable sources of power generation have been ranked as the source with the highest rate of growth worldwide. In spite of the fact that it is the renewable energy source with the lowest cost, wind power has a tremendous amount of untapped potential and, according to some studies, it has the capacity to satisfy 20 times the amount of electricity that is consumed globally [22].

The wind resources in Iraq can be categorized as low, moderate, or high according to their intensity [23]. 48% of Iraq’s total land area has an annual wind speed that is 3.1-4.9 meters per second or less, 35% has an annual wind speed that is 3.1-4.9 meters per second or higher, and 8% has a relatively high annual wind speed. Wind speed (WS) is one of the most important factors to consider while producing electricity from the wind [24]. Data from a measuring station that was installed in the same location as the site in question need to be reviewed and explained before an accurate assessment of the potential for wind energy at the location can be made. The data may be categorized on a daily, monthly, or yearly basis, depending on preferences. When the wind energy potential has been precisely determined, only then will it be possible to analyze accurately the efficiency of any proposed WTs [25].

1.3.2.3. Other Sources of Energy

Iraq’s utilization of solar power would help the nation achieve its aim of reducing the CO2 emissions brought on by the burning of fossil fuels. Solar power is an obvious alternative for Iraq as a source of renewable energy. As a potential remedy for the issue of climate change, solar power is receiving increasingly more attention.

The Iraqi government must make every effort to decrease pollution in the country’s air, water, and land in order to reduce environmental harm. Furthermore, it is crucial that the government attempts to identify the best strategies to utilize renewable energy sources. One of the most crucial factors that must be taken into account when selecting new energy sources is the availability of renewable energy sources that are also ecologically sound. In Iraq, solar energy has the capacity to meet all of these needs. With certain places producing more than 2200 kWh of solar energy per square meter per year, the nation boasts one of the greatest solar energy densities in the world. This is an ideal option because it is completely free, never ceases, and is environmentally friendly. Iraq’s government should devote a sizeable percentage of its sizable wealth from oil production to research into alternate types of power generation because of the country’s huge desert areas, high solar radiation levels, and numerous dawn hours (3300 on average annually).

1.4. METHANOL PRODUCTION

Methanol is an important chemical compound that is used in a wide range of applications such as fuel, solvents, and chemicals for the production of plastics and other materials. While methanol can be produced from non-renewable sources such as natural gas and coal, there has been growing interest in methanol production from renewable energy sources to cut the release of greenhouse gases and dependence on non-renewable resources. Methanol is an important chemical compound that is used in a wide range of applications, including fuel, solvents, and chemicals for the production of plastics and other materials. With the increasing demand for clean energy and the need to reduce greenhouse gas emissions, there has been growing interest in producing methanol from renewable sources of energy, particularly solar and wind energy. In this study, we discuss different methods of methanol production from solar and wind energy.

1.4.1. Solar Thermal Methanol Production

Solar thermal methanol production involves using solar energy to heat a reactor that contains a feedstock such as biomass; It is subsequently transformed into methanol through a procedure called biomass gasification. This method has the advantage of producing methanol from a renewable energy source, and it is particularly suited for using wood chips, agricultural waste, and other forms of organic waste as feedstock.

1.4.2. Synthesis Gas-Based Methanol Manufacturing

A variety of CO/H_2 combinations are referred to as syngas in the scientific literature. Mineral oil fractions, coal, and natural gas fractions can all be utilized as the base materials for the production of synthesis gas. Because of their high hydrogen contents, natural gas and light oil fractions are perfect for synthesis gas production. Because natural gas is used as a raw material in this study to make methanol, we investigated different ways to make synthesis gas from natural gas. These strategies fall into three categories with production methods for syngas generation being influenced by natural gas prices and composition, acceptance for exporting energy, and the capacities of plants.

Steam Reforming

Steam reforming of natural gas accounts for the majority of methanol facilities in use today. The following is a description of the reaction:

$$CH_4 + H_2 \rightarrow CO + 3H_2 \qquad \Delta H(298K) = 247kJ/mol$$

The equation demonstrates a surplus of hydrogen. There is an excess of hydrogen in the system because more hydrogen is produced than is necessary to convert carbon oxides into methanol. The endothermic reaction of the turbo reformer makes it work more effectively at higher temperatures. However, the maximum temperature of the reformer is constrained by the materials used to construct it, which must be heat resistant. Tubular reformers are now able to handle brick layers at temperatures of up to 1,050℃ due to new tube materials. It is highly likely that reformer output temperatures can be reduced while keeping the exchange rate constant to below 700℃. The figures on steam reformation processes are as follows:

$$CO + H_2O \rightarrow CO_2 + H_2 \qquad \Delta H(298K) = -47kJ/mol$$

To accomplish this, carbon dioxide can be injected. Syngas comprising carbon oxides and hydrogen in stoichiometric proportions is created by adding CO2 to balance off any excess hydrogen, and as a result of this change, feed and fuel requirements per ton of methanol would be reduced. With today's CO2 politics, one would be compensated for utilizing the gas, hence releasing more CO2 may result in a net economic benefit. There are several secondary reforming reactions available for controlling the syngas's hydrogen-to-carbon ratio. These include ox reforming and autothermal reforming.

Steam reforming and ox reforming are used in conjunction to create autothermal reforming (ATR), which is commonly used to modify the synthetic ratio by using oxygen as a reactant. Oxygen, or oxygen-rich air, is injected into the reformer, where it undergoes the following reactions with natural gas methane:

$$2CH_4 + O_2 \rightarrow 2CO + 4H_2 \qquad \Delta H(298K) = -36kJ/mol$$

Because this reaction is exothermic, it is thermodynamically more productive than steam reforming. The stoichiometric ratio for the generation of methanol from carbon monoxide is 2, and ox reforming produces syngas with this ratio. In order to avoid huge levels of nitrogen as an inert in the system, one must first remove oxygen from the air [24,25]. The expense of air separation might be high.

As a starting point, CO_2 is used in the following reaction:

$$CH_4 + CO_2 \rightarrow 2CO + 2H_2 \qquad \Delta H(298K) = 206kJ/mol$$

The equation suggests that the CO_2/CH4 ratio of 1 is the best feed gas proportion for carbon dioxide (CO_2) reformation, leading to the maximum synthesis gas output. Given that the process is highly exothermic, its rate of conversion increases with increasing reaction temperature. Then achieve the necessary gas compositions, steam reforming may be preferable to CO_2 reforming in some cases. Thermodynamic considerations dictate that thermodynamically reforming will only partially convert CH4, and the process economics are highly sensitive to the pressure and value of CO_2 present in the synthesis plant. This allows for the coupling of steam and CO_2 reforming. With natural gas's low price and the fact that it contains carbon dioxide (CO_2), this could become a reality. It is widely accepted that the CO_2 reforming economics are comparable to the steam reforming economics [26,27].

Biosynthesis

Enzymes termed methane monooxygenases catalyze the transformation of methane into methanol [20]. These enzymes, called mixture oxygenases, are essential for both the production and oxygenation of water [28]. There have been extensive efforts made, the vast majority of which have been fruitless, to duplicate this sensitivity [29,30]. In most cases, the reactions are not selective because methanol may be oxidized more readily than the fuel, which is methane. These problems can be solved using a variety of approaches. These systems do have a number of effects on metalloenzyme processes despite the fact that they do not exactly mirror such processes. Examples of this include Shilov systems and zeolites that include iron and copper [31,32]. The active sites of enzymes are notoriously unpredictable due to their extreme variability. In the Fe-zeolite, the MMO enzyme is thought to have a mononuclear iron (alpha-oxygen) protein complex as opposed to a dinuclear active site [33].

1.4.3. Renewable Methanol

Methanol is a tool that may be utilized to help to achieve the aims of reducing emissions of greenhouse gases, boosting the use of renewable energy sources (RES), and improving the efficiency of the energy system through the storage of energy [34].

It is a chemical with an extremely low carbon footprint, and it can be produced from sustainable biomass. This makes methanol a renewable source for methanol. Methanol is produced either from carbon dioxide and hydrogen, both of which are produced throughout the process, or from renewable sources of electricity. The same international requirements apply to the generation of methanol from renewable sources as they do to the production of methanol from fossil sources., according to IMPCA [35].

1.5. CARBON CAPTURE METHODS

Pre-combustion, post-combustion, and oxyfuel are the three basic types of carbon capture and storage (CCS) technologies that could potentially aid in reducing emissions from power plants and other industrial sites.

1.5.1. Post-Combustion

According to this technique, CO_2 is removed from the power plant’s flue gas by bubbling it over an absorber column suspended in a liquid solution (such as ammonia). In the most common technique, once the absorber column’s chemicals have reached saturation, a stream of superheated steam is pushed through it at a temperature of approximately 120°C. When the restricted CO_2 is released, it can be moved and stored elsewhere. Requiring saltwater to collect the gas and afterwards dumping the resulting mixture back into the ocean for extended storage is one of the experimental methods being tested to remove carbon dioxide from flue gases without using the two-step procedure. So far, however, these techniques have been shown to be less effective and dependable.

1.5.2. Pre-Combustion

In general, coal-gasification consolidated power plants will use this technique. To create a synthetic gas from hydrogen and carbon monoxide, the coal is gasified. More hydrogen and CO2, which are then captured, are produced when the first is mixed with water. The hydrogen can be directed toward a turbine so that it can be burned there to produce electricity. As an alternative, part of this gas may be vented and used to fuel hydrogen fuel cells in automobiles.

The pre-combustion approach has the drawback that it cannot be retrofitted to older pulverized coal power plants, which account for a large portion of the installed base of fossil fuel energy around the globe. Synthetic gas is initially created by reacting methanol with steam to generate carbon dioxide and hydrogen, which is then used in normal gas stations. However, it has yet to be demonstrated how this approach is more cost-effective than post-combustion.

1.5.3. Oxyfuel

CO_2 comprises approximately 3% to 15% of the waste gas produced when coal, oil, or natural gas are burned in regular air, and its separation is labor- and energy-intensive. Additionally, the fuel can be burned with solely pure oxygen. A great deal of the waste gas in this situation will be made up of CO2 and water vapor. Whereas the former could be piped or shipped straight to a storage unit, the latter could be condensed out.

In the oxyfuel system, substantial volumes of air must be split into liquid energy sources, vapor nitrogen, argon, along with additional minor gases. Up to 15% of a station’s output can be consumed in this process [36].

1.6. CURRENT STUDY

This current study is a techno-economic and environmental investigation of a plant that produces methanol fuel by means of solar and wind energy. In this study, a techno-economic investigation of a plant that produces methanol by hydrogenating carbon dioxide in the waste gas from a white cement facility using renewable energy was carried out.

The carbon dioxide in the flue gas is captured in the carbon capture plant, and the hydrogen obtained from the wastewater from the cement facility in the hydrogen plant with the help of photovoltaic and wind energy is combined in the methanol plant to produce methanol fuel. Afterwards, the environmental impact of the methanol plant is investigated.

The Iraqi Fallujah White Cement Plant has been selected as the case study location. The system's processing of CO_2 emissions, heat integration, energy efficiency, and techno-economic performance were all taken into consideration.

The results of the current study provide cement factories with a way to reduce CO_2 emissions while also producing something with high added value (i.e., methanol). This study compares this computation to other research that has been carried out in other nations, as well as the applicability of economic values and the effect of this output on the environment.

PART 2

LITERATURE REVIEW

The generation of novel fuels (biofuels) has received recent support from the European Union as one of the key objectives for the year 2020 [37] to reduce the pollution-emitting emissions of traditional fossil fuels. Although it only possesses nearly half the energy density of gasoline (20.1 MJ/kg for methanol, compared to 44.3 MJ/kg for gasoline), methanol is a fuel that has outstanding combustion qualities [38]. The influence of a high compression ratio and the addition of hydrogen on the performance and emissions of a lean burn results in an ignition engine fueled by ethanol-gasoline [39]. The octane rating of methanol is higher (108) than gasoline (95). This allows for a larger compression ratio, leading to improved combustion efficiency and lower emissions of CO and CO_2 relative to conventional gasoline [38,40] compared with conventional fuels (gasoline and diesel). Methanol plays a vital role in producing a number of chemicals, such as formaldehyde, MTBE, and acetic acid.

Samimi, F., et al. (2019), in their study, two approaches to producing methanol through the inverse water gas shift (RWGS) as a consequence of incidental (CO_2) conversion were analyzed and compared. The first approach involved an RWGS reactor with a $Fe_2O_3/Cr_2O_3/CuO$ catalyst to convert CO_2 into a synthesized gas. After passing through a condenser to eliminate any water, the resulting product was forwarded to a reactor for methanol production; this, however, hinders the methanol synthesis. The second experiment utilized a water perm selective membrane in the RWGS reactor, while the overall process remained similar to the first experiment.

This scenario eliminated the need for a separate water removal step before the methanol synthesis reactor, as the water generated from the RWGS reaction was separated by the membrane.

The combination of these processes was numerically modeled by optimizing methanol production through the use of the Differential Evolution (DE) method for variance evolution.

The production of methanol was investigated by comparing two different scenarios and the traditional method (CR) in a study. The study's findings revealed that the membrane reactor utilizing RWGS generated a higher CO_2 conversion rate and CO yield, in addition to a synthesis gas composition that is more favorable with water removal. Additionally, the methanol production rate increased by 50.23% (109 tons/day) compared to the first scenario, and by 4.15% (13 tons/day) compared to CR. For the second experiment, methanol synthesis occurred in a reactor. The process, in fact, produced less water than the first scenario (a 17% reduction) [41].

The reactor's output, Stream 13, is combined with the hydrogen and carbon dioxide supplies that have been compressed. A portion of the reactor's output, 60%, is used to warm the reactor feed, Stream 4, close to a temperature of 210°C. The reactor contains a catalyst filled fixed bed with a volume of 6.98 m^3 and a weight of 7,432 kg, made of $Cu/ZnO/Al_2O_3$. At 284°C, the reactor product is divided into two streams: Streams 4 and 5. The latter is utilized to warm the reboiler and preheater of the distillation column, and the two streams are later combined and cooled to 40°C with HX-6. Drum 1, the initial knockout drum, isolates the unreacted gases, Stream 12, from the methanol/water mixture, which yields Stream 11. To prevent the stockpile of inert gases and by-products, Stream 12 undergoes a 1% partial purging. Stream 13, which contains the remaining unreacted gases, is recycled and mixed with the feed streams before re-entering the reactor. Increasing the pressure of Liquid Stream 11 (crude methanol) to 1.2 bars using VLV-1 results in the separation of most of the unreacted gases in Drum-2. The liquid from Drum-2 is preheated to 70°C (D1) with HX-7 before entering the 30-tray distillation column, where a 1:1 reflux ratio is employed. The bottom stream, consisting primarily of water and containing 967 wt-ppb of methanol, exits the column at 102°C and 1.1 bars. The filtered methanol, along with 57 wt-ppm of water and selected unreacted gases, is present in the top gaseous stream (64°C and 1.0 bar), in Stream 18, which is then further purified by undergoing compression and chilling to 40°C in Drum-3, eliminating any remaining unreacted gases [42].

Yao, Y., et al. (2018) evaluated the viability of producing methanol from CO_2 captured by a CCS system and hydrogen obtained through water electrolysis in their study, which took into account three different economic scenarios. The feasibility of the facility would be most affected by the price of electrical energy, with the current high capital cost of the electrolyzer being a secondary factor. It would be reasonable to expect a reduction in construction costs in the near future as the technology advances. A 30% decrease in real costs could lead to a 10% reduction in the Profit Before Taxes (PBP). The sale of oxygen is crucial for the financial viability of the plant, with the “base point” (O_2 at 150 euros per ton and MeOH at 400 euros per ton), indicating that oxygen sales revenue would comprise approximately 40% of the plant’s total profitability. A 30% increase in the value of oxygen could result in a 20% decrease in PBP. Moreover, there is an expectation that the price of methanol would rise due to its use as a fuel in the automotive industry.

The price of methanol is affected by various factors, including its use as fuel, energy content, and environmental impact. An increase in the value of methanol to 800€/kg could result in a reduction of its Profit Before Taxes by over 50%. Another significant consideration is the environmental consequences associated with the production of methanol, as the recycling of CO_2 through a 63 MW methanol plant may lead to significant financial savings due to the CO_2 European market value of approximately 7€ per ton. Increasing CO_2 taxes will make this factor even more relevant in the future. However, it is crucial to assess both the benefits and drawbacks of methanol production and its use, such as its effect on air quality and the high energy requirement to produce methanol from fossil fuels. An extensive evaluation of the advantages and disadvantages is necessary to make informed decisions with regard to using methanol as a fuel [42].

In summary, CO_2 serves as the principal carbon source in the production of industrial methanol, while hydrogen and CO are also used as inputs. There are various methods for producing methanol using CO_2 and hydrogen, including traditional as well as the latest catalysts. A new facility is being built that utilizes a sustainable electrolysis process to produce methanol from CO_2 that would otherwise be released into the atmosphere. The field of science is continuously evolving, with new ideas and processes expected to emerge, including the exploration of novel materials and eco-friendly methods of creating copper-based catalysts. One such approach is the avoidance of solvents in the preparation process, as recent studies have shown that catalysts can be produced following anti-solvent approaches, such as supercritical CO_2 or gas-phase CVI, to achieve the desired result [43].

Human-generated CO_2 emissions have increased in the past century, leading to potential business opportunities for utilizing captured CO_2. Aspen Plus software simulation is used to model the production of fuel-grade methanol from captured CO_2, as proposed in this paper. Chemical absorption is used to capture CO_2 from thermal power plant flue gases, while carbon-free water electrolysis generates hydrogen. The methanol plant contributes 36% of the thermal energy essential for CO_2 capture, resulting in a considerable decrease in the costs of capture. According to the CO_2 stability of the process, the sale of the oxygen by-product can reduce 1.6 t of CO_2 per ton of methanol created, or 1.2 t if not sold [44].

The cost of producing methanol is influenced by feedstock and plant expenses. A 1 million ton/year plant can save approximately 10 million USD in investment costs, resulting in a reduction of 2 USD/ton in production costs with a typical payback period. Operating costs are expected to decrease by approximately 2 USD/ton of methanol based on a natural gas cost of 1 USD/MM BTU and a demineralized water cost of 1 USD/m^3, leading to a total decrease of approximately 4 USD/ton in the net methanol production cost. However, without free CO_2, the point at which the cost of CO_2 equals the income generated by it, it is estimated to be approximately 15 USD/ton [45].

Monnerie et al. (2020) made a techno-economic evaluation of a solar thermochemical cycle of cerium oxide for the purpose of creating H_2 and CO_2. The process was modeled at the system level, with a solar sensor using large-scale solar heat to create synthesized gas (hydrogen and carbon monoxide). Methanol was produced from the synthesis gas in plug-flow reactors, without emitting CO_2. A MW-scale methanol manufacturing facility was used to simulate the process using process simulation software. The reactor settings were optimized, and the study mentions that the solar methanol production plant was planned in Spain. A cost assessment was conducted, which showed that a 350 MWh solar barbican can produce 27.81 million liters of methanol. To operate the plant under unfavorable conditions, the facility would require 880,685 m^2 of mirrors and a solar tower height of 220 m. The estimated production cost would be 1.14 euros per liter of methanol [46].

M. Nizami, et al. (2022) evaluated two scenarios: grid-powered PV electrolysis with a battery and PV electrolysis without a battery. The study describes an investigation that focuses on the production of methanol using CO_2 hydrogenation. The tools and software used in the study or analysis are related to a proton exchange membrane electrolyzer. Kinetic models were developed to simulate methanol production from CO and CO_2. The study conducted a process of economic analysis and a CO_2-equivalent emissions study to evaluate its environmental impact and economic viability, with levelized costs being determined. The consolidated hydrogen generation and methanol synthesis respectively had overall energy efficiencies of 48.39% and 55.16%. The study describes a process or analysis that involves the use of a heat exchanger network (HEN) for heat integration and makes a comparison of results before and after the integration. It was found that methanol production would cost $1,040.17 per tonne-MeOH for the PV-grid scenario and $1,669.56 per tonne-MeOH for the PV-battery scenario. The PV-grid scenario produced 0.244 kg-CO_2-eq/MJ-MeOH, while the PV-battery scenario resulted in −0.016 kg-CO_2-eq/MJ-MeOH [47].

Firmansyah et al. (2018) conducted a study comparing arrangements for production. The study describes a process or system that is used to produce power and methanol from biomass using solar and wind energy. It also describes a study or analysis that considered three different biomass conversion technologies in the context IGCC, oxy-fuel burning, and syngas conversion are methods of harnessing sun and wind energy to produce power and methanol from biomass. The study considered solar and wind energy-powered water electrolysis to generate hydrogen for methanol production.

The study evaluated the technological and economic feasibility of the proposed technologies, and the results showed that the economic feasibility was limited and suggests this could be related to the high cost of solar and wind energy systems. Additionally, the technical and economic performance of the systems varied across locations, with interest rates having a greater effect on economic performance. Mentions are made of a number of factors (capital costs, fuel costs, and electricity prices) that are considered or analyzed in a particular context, such as the economic viability or feasibility of a process, system, or project.

The study found that Beijing outperformed Gotland and Denver in terms of economic success, although it is not clear from the input what specific criteria were being used to define economic success in this context. Overall, it appeared that the study aimed to compare different classifications for production. It describes a process or system that is used to produce power and methanol from biomass using solar and wind energy and to provide insights into their technical and economic feasibility. However, further information is needed to fully understand the scope and results of the study [48].

Techno-economic measures evaluated the viability of a tri-reforming process for methanol. Empirical kinetic calculations simulated the process with flue gas from an incinerator. It describes a sensitivity analysis that was conducted to regulate the impact of the feed composition and temperature on the results of a process or system aimed at reducing CO_2 emissions. The economic viability of the methanol plant modeled in the study was evaluated using key dials such as Net Current Fraction. The study also describes some financial metrics (External Rate of Return, Payback Period, and break-even) [49].

Schorn, F, et al. (2021) investigated the use of an energy storage system that included a battery and a power-to-methanol unit in order to create a renewable energy storage solution. To determine the minimum-cost battery and power-to-methanol capacities, a nonlinear programming model was used. The study evaluated four different configurations of the renewable energy system, and the cost was analyzed with and without energy storage units. Based on the published data, the proposed model demonstrated that value-adding units, such as PtMs, are crucial for ensuring stable renewable energy systems. The study’s findings are expected to aid in the development of policies for managing electricity supply and demand and renewable energy storage.

The study that analyzes the importation of renewable methanol to reduce dependence on fossil-based energy carriers. The net production costs of methanol are determined based on the expenses for hydrogen and carbon dioxide, which are evaluated through a simulation model. The study compared the import costs of methanol and hydrogen for different country combinations, taking into account the production and distribution costs of hydrogen, and found that renewable methanol can be cost-competitive with the current fossil market price of 400 €/t under certain conditions. The study also noted that hydrogen and methanol have comparable energy-specific import costs of 18-30 €/GJ within a range of carbon dioxide prices, and the decision to produce methanol in the origin or destination country depends on the relative costs of carbon dioxide in each location. Finally, the study concluded that were the price of carbon dioxide in the host country to be 181-228 €/t less than in the origin country, the higher shipping expenses for hydrogen could always be mitigated [50].

Sharma, I, et al. (2022) suggested utilizing wind energy to electrolyze water, producing hydrogen with a cell, and also utilizing carbon industrial processes and atmospheric ozone. The study describes a process to produce methanol, in which CO_2 and hydrogen are combined and burned in a reactor to create methanol and water. The byproducts are then separated via distillation. Even though this approach has potential, inefficient electrochemical cells and high production costs would pose significant cost and efficiency challenges. Furthermore, capturing CO_2 is expensive. Nevertheless, storing excess wind energy as methanol instead of transferring it to the grid would still be beneficial. This method is more resource and carbon efficient than traditional methods, and the researchers proposed various wind energy simulations for methanol manufacturing, with evaluations of their viability and future potential. The reactor would burn CO_2 and hydrogen to create methanol and water, with the byproducts being purified through distillation [51].

A facility that combines the direct synthesis of methanol, bioethanol-induced CO2 capture, and hydrogen generation based on wind energy was the subject of a techno-economic analysis by Matzen et al. (2015). The study used the ASPEN Plus software to simulate the facility and evaluate its performance. It was found to have generated 97.01 metric tons of methanol per day while consuming 138.37 metric tons of CO_2 and

18.56 metric tons of H_2. The economic analysis was performed using a discounted cash flow diagram, and a feasibility analysis was conducted using a multi-criterion decision matrix to compare methanol production from renewable and non-renewable sources in accordance with economical and environmentally friendly indicators. The renewable methanol was found to have an energy efficiency of about 58% and would reduce CO_2 equivalent emissions by −1.05 CO_2 per kilogram of methanol. The price of electrolytic hydrogen production is the most substantial economic factor for the facility. The multi-criterion feasibility analysis suggested that renewable methanol production could be a viable option [52].

Bos, M, et al. (2020) assessed the efficiency and capital requirements of a process that converts 100 MW of wind power to methanol. The amount of hydrogen generated would depend on the capacity of the electrolysis process, while direct air capture would be used to obtain CO_2 for methanol production. The costs for each stage are calculated and combined, including utilities for CO_2 capture, with two processes, hydrogen production, and methanol synthesis, being commonly used in power-to-fuel technologies. The estimated conversion efficiency of power to methanol is 50%. The cost of methanol is approaching 300 euros per ton without the cost of wind turbines, and approximately 800 euros per ton including wind turbines. The facility’s total price, excluding the 100 MW wind turbine cost, would be 200 million euros. The electrolyzers, CO_2 capture equipment, and methanol synthesis system have operating costs of 45%, 50%, and 5%, respectively. According to the conceptual design and evaluation, it is becoming feasible to produce renewable methanol using CO_2 from air, water, and renewable electricity. This can be achieved at a cost of 750-800 euros per ton [53].

Decker, M, et al. (2019) examined short-term integration of systems for electro fuel production. To optimize design parameters and simulate yearly operations, a list was made of components in a power-to-fuel system located in Germany, which included an electrolyzer, storage of hydrogen, CO2 source, wind farm, and synthesis facility. The researchers developed a model to evaluate production costs for different cases and sites and suggested that off-grid systems would be feasible for short-term implementation. In the reference case, the net fabrication prices of methanol would be

1.73 €/lGE. The study contained a sensitivity analysis to evaluate the effect of different economic assumptions on a power-to-fuel system, which found that optimal wind farm sites could decrease production costs to 1.32 €/lGE, and the methodology and results could also be applied in other regions [54].

PART 3

MATERIALS AND METHODS

In the current study, to meet the requirements of the process, there are several factors that should be determined, as shown below.

- Resources and characteristics related to waste gas, such as:
  - ✓ Temperature
  - ✓ Volumetric flow rate
  - ✓ Composition
- The type of renewable energy that is closest to the plant’s location
- Selecting a CO_2 capture technique from waste gas
- Composition method of H_2 atoms with C atoms
- Selection of the appropriate software to solve the energy and economy equations

The White Cement Plant in Fallujah's data and operational circumstances were used in this chapter's thermodynamics analysis of the process, with flue gas having a temperature of 380℃, 1.2 bars of pressure, and a 126.56 kg/s gas flow rate. The flue gas from the plant comprises a mix with a molecular composition of CO_2 (26.2%), CO (0.6%), N_2 (68.8%), and O_2 (4.4%) [55]. Electricity is generated to run the facility by two options: solar panels and wind turbines that are connected to all units of the plant. For CO_2 emissions from the plant, we employed a post-combustion capture (PCC) as the CO_2 capture unit. The Engineering Equation Solver (EES) was the program selected to solve the equation involving energy and economy.

3.1. PROPOSED METHANOL PRODUCTION SYSTEM

In the present work, we designed a process for the conversion of waste gases into valuable products at a white cement plant for the purpose of finding a practical solution that would allow the cement industry to achieve green and low-carbon development. The process design of the methanol plant is based on previous studies conducted by H. Özcan and E. Kayabaşı [5], and Kiss et al. [56]. As shown in Figure 3.1, the suggested methanol production plant consists of four key parts.

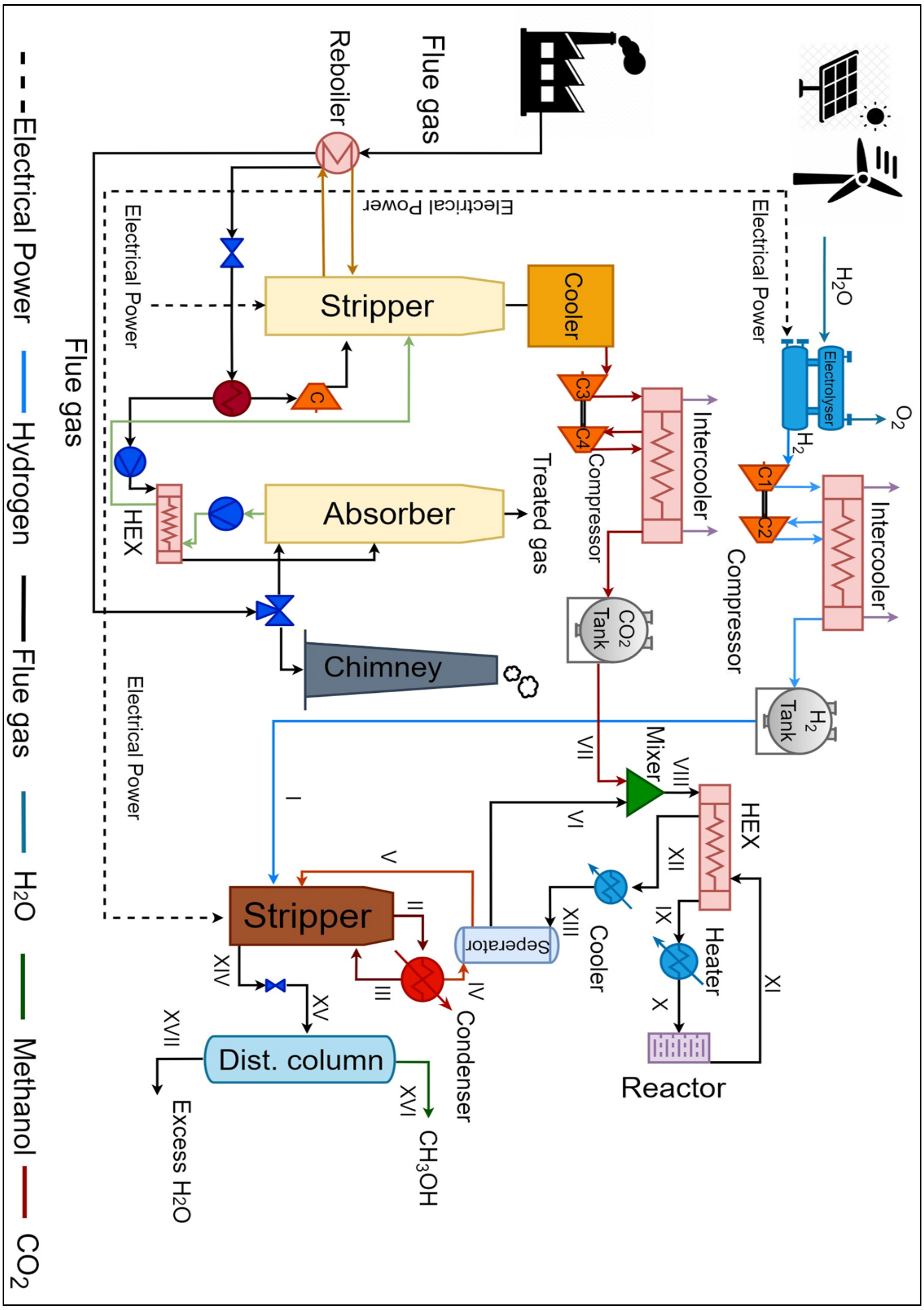

Figure 3.1. Detailed flow diagram of the Methanol production plant.

3.1.1. Photovoltaic Plant (PV)

To do this process, it is necessary to have a power source. Solar panels were used to generate power for the factory. We assumed that ground-mounted, large-scale panels would be installed near the factory on the ground. The panels are approximately 1000 m and on an area of 1 m^2. The location was determined at to be at 33°22’26.3”N 43°50’56.3”E, and the data was obtained from Global Solar Atlas [57]. Figure 3.2 shows the installation locations of the panels and the cement factory, with Table 3.1 showing information about location data.

Figure 3.2. The installation locations of the panels [57].

Table 3.1.Information about the location data [57].

Map data	Per day
Direct normal irradiation DNI	4.905 kWh/m^2
Diffuse horizontal irradiation DIF	2.217 kWh/m^2
Global horizontal irradiation GHI	5.352 kWh/m^2
The optimal tilt of PV modules OPTA	31 / 180º
Global tilted irradiation at optimal angle GTI opta	6.027 kWh/m^2
Terrain elevation ELE	45 m
Air temperature TEMP	24.8 °C

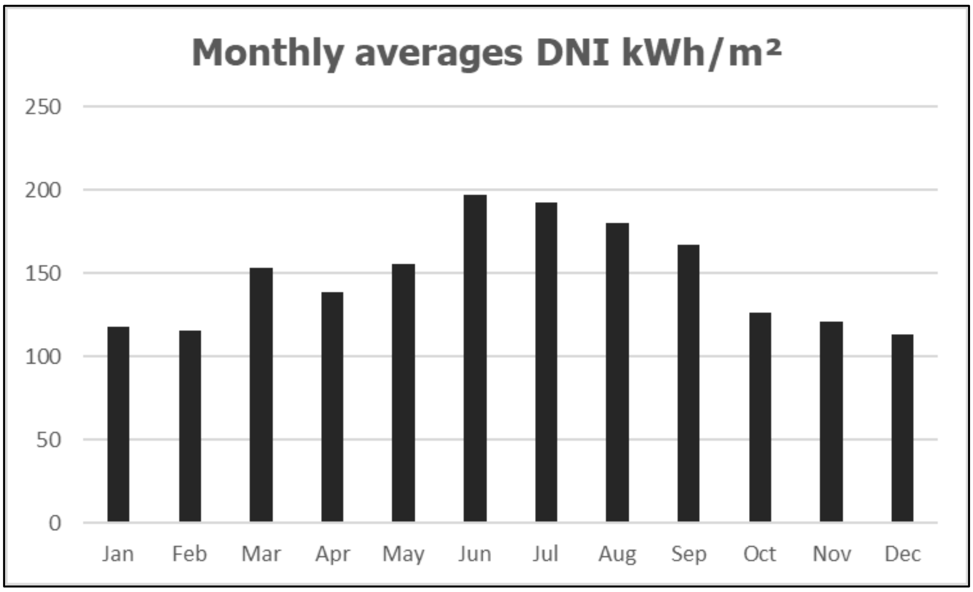

Figure 3.3. Monthly averages of direct normal irradiation [57].

Figure 3.3 shows the monthly averages of direct normal irradiation, with May, June, July, August and September having the highest radiation levels. The radiation rate is low in October, November, and December up to February. Table 3.2, which displays the average hourly direct normal irradiations, also includes rate hours for solar radiation.

Table 3.2. Average hourly profiles DNI [Wh/m²] [57].

Hrs.	**Jan**	**Feb**	**Mar**	**Apr**	**May**	**Jun**	**Jul**	**Aug**	**Sep**	**Oct**	**Nov**	**Dec**
5 - 6	0	0	0	1	24	52	31	2	0	0	0	0
6 - 7	0	0	22	110	185	281	240	166	102	33	0	0
7 - 8	53	106	246	275	303	426	387	354	355	245	189	61
8 - 9	309	316	395	383	414	536	498	471	478	369	392	334
9 - 10	417	423	497	466	498	616	583	561	571	463	471	431
10 - 11	490	513	590	533	551	666	633	624	642	540	533	487
11 - 12	532	559	635	562	575	689	658	650	666	551	552	515
12 - 13	538	548	617	547	564	687	661	650	655	528	535	511
13 - 14	507	528	576	505	534	669	645	636	634	490	506	482
14 - 15	460	473	517	446	476	619	600	587	574	422	446	435
15 - 16	380	400	438	374	397	540	520	506	480	324	349	339
16 - 17	111	247	331	281	297	430	410	388	340	117	65	62
17 - 18	0	11	81	137	179	301	281	208	81	0	0	0
18 - 19	0	0	0	2	22	59	50	11	0	0	0	0

3.1.2. Wind Turbine (WT)

In the proposed plant, wind energy is used to produce electricity and to generate power for the factory. Fallujah, Iraq was selected for the location of the wind turbine farm at 33°22’26.3”N 43°50’56.3”E. Its annual mean wind velocity is illustrated in Figure 3.4 [58].

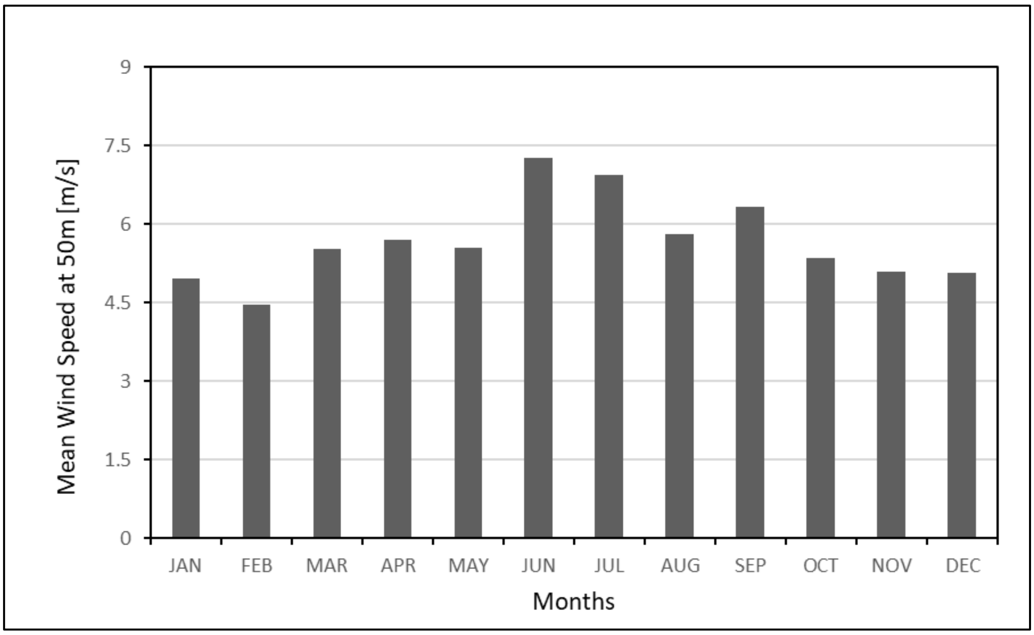

Figure 3.4. Annual mean wind speed at 50m. [58]

Table 3.3 displays the specifications chosen for the wind turbines. The chosen wind speed represents the location's annual average value.

Table 3.3. the specifications for windmills.

Parameter	Value	REF
Wind speed (m/s)	6.85	[59]
Air density (kg/m^3)	1.25	[60]
Power Coefficient (Cp)	0.55	[60]
Rotor diameter (m)	110	[60]

3.2. THERMODYNAMIC MODEL

The plant has been examined using thermodynamic and techno-economic analysis techniques. The Engineering Equation Solver (EES) was used to complete the thermodynamic model [5]. The thermophysical characteristics of the flue gas were obtained from a plant.

The energy and mass balance are calculated with the following equations [61]:

$$\dot{Q} - \dot{W} = \sum m_{out} \cdot h_{out} - \sum m_{in} \cdot h_{in} \quad (3.1)$$

$$\sum \dot{m}_{in} = \sum \dot{m}_{out} \quad (3.2)$$

Heat and workflow are denoted by $\dot{Q}$ and $\dot{W}$. The thermal efficiency of the plant is obtained and calculated by [62]:

$$\eta = \frac{W_{net}}{Q_{in}} \quad (3.3)$$

Two compressor units compress pure CO_2 into the tank. The following equations were used to compute the power for this two-stage procedure:

$$\dot{W}_{c3,co2} = \dot{m}_{co2}\left(h_{2,out} - h_{1,in}\right) \quad (3.4)$$

$$\dot{W}_{c4,co2} = \dot{m}_{co2}(h_{4,out} - h_{3,in}) \quad (3.5)$$

where $\dot{W}$is the compressors’ power and $\dot{m}_{co2}$ is the mass flow rate of carbon dioxide. A PEM-type electrolyzer that operates at a low temperature (400 K) and at medium pressure (10,000 kPa) has produced hydrogen. Using Eq. 3.6, power consumption can be determined.

$$\dot{W}_{C1,H2} = \dot{m}_{H2}\left[h_{6,out} - h_{5,in}\right] \quad (3.6)$$

$$\dot{W}_{C2,H2} = \dot{m}_{H2}\left[h_{8,out} - h_{7,in}\right] \tag{3.7}$$

where $\dot{m}_{H2}$ is the mass flow rate of hydrogen. The total cell potential is calculated using Eq. 3.8.

$$E_{tot} = E_{rev} + E_{act} + E_{ohm} + E_{con} \tag{3.8}$$

Reversible, activation, ohmic, and concentration, respectively, are indicated as E_{rev}, E_{act}, E_{ohm} and E_{con} [63,64]. Eq. 3.9 was used to compute the reversible cell voltage [65].

$$E_{rev} = E_o - 85 \times 10^{-4}(T_{cell} - T_o) + 4{,}3085 \times 10^{-5}(T_{cell}) \ln\left(\frac{P_{H2}P_{O2}^{0.5}}{P_{H_2O}}\right) \tag{3.9}$$

$\mathrm{E_o}$ is given as $(-\Delta\mathrm{G}/\mathrm{zF})$. Here, $-\Delta\mathrm{G}$ refers to Gibbs energy of the reaction of water splitting, F is Faraday's constant, and z is the number of the transferred electrons. The activation cell voltage, ohmic cell voltage, and concentration cell voltage overpotentials are defined and calculated as follows:

$$E_{act} = \left(\frac{\alpha_a+\alpha_c}{\alpha_a\alpha_c}\right)\frac{RT_{cell}}{zF}\frac{J}{J_o} \tag{3.10}$$

R represents the universal gas constant, T_{cell} represents cell temperature, α_c and α_a are change coefficients. J_o is exchange current density and defined as follows:

$$J_o = 1.08 \times 10^{-17} \exp\left(0.086T_{cell}\right) \tag{3.11}$$

The ohmic cell voltage is estimated with the use of Eq. 3.12.

$$E_{ohm} = J\frac{t_{mem}}{\sigma_{mem}} \tag{3.12}$$

Where σ_{mem} and t_{mem} represent membrane conductivity and thickness. Cell voltage concentration can be calculated from:

$$E_{con} = J\left(\beta \frac{J}{J_c}\right)^{\beta} \tag{3.13}$$

Where β represents a constant as cell temperature and pressure function, J_c is limiting current density [66]. The hydrogen rate was calculated using by:

$$\dot{n}_{H2} = \frac{\dot{W}_{elec}}{E_{tot} \times Fz} \tag{3.14}$$

To calculate the efficiency of the electrolyzer, we use the following equation:

$$\eta_{elec} = \frac{-DG_t}{E_{tot} \times Fz} \tag{3.15}$$

The heat load in the components of the methanol plant is calculated with the following:

$$\dot{Q}_{heating} = \dot{Q}_{st} + \dot{Q}_{het} + \dot{Q}_{CO2} \tag{3.16}$$

$$\dot{Q}_{cooling} = \dot{Q}_{dc} + \dot{Q}_{cond} + \dot{Q}_{col} + \dot{Q}_{rea} \tag{3.17}$$

Where $\dot{Q}_{heating}$ and $\dot{Q}_{cooling}$ refer to the heat and cold utility. $\dot{Q}_{dc}$, $\dot{Q}_{st}$, $\dot{Q}_{cond}$, $\dot{Q}_{col}$, $\dot{Q}_{het}$ and $\dot{Q}_{rea}$ refer to heat loads for each distillation column, stripper, condenser, cooler, heater, and reactor, respectively. The fuel efficiency of a methanol production plant (MPP) may be expressed as follows:

$$\eta_{fuel} = \frac{\frac{m_{45}}{3600} LHV_{met}}{\dot{W}_{Renewable}} \tag{3.18}$$

The plant efficiency is calculated as follows:

$$\eta_{MP} = \frac{m_{45}h_{45} + m_{46}h_{46}}{(m_{30}h_{30} + m_{36}h_{36} + \dot{W}_{comp,CO2}\dot{W}_{comp,H2}) \times 3600} \tag{3.19}$$

The factors that determine wind turbine power include [60]:

$$P_{WT} = 0.5 \times C_P \times \rho_{air} \times A_{WT} \times U^3 \tag{3.20}$$

Where ρ_{air} is the air density, C_P is the power coefficient, which dictates how much of the wind's power can be converted into mechanical energy, and has a maximum permissible value of 0.593 (Lanchester-Betz limit), A is the rotor area, U is the velocity of the wind.

3.3. TECHNO-CONOMIC ANALYSIS

The initial design of thermal systems must take into account the system investment cost [67]. Using the EES software, a thermodynamic model was created for this investigation. In addition to employment and operational costs, economic evaluations also took into account annual operation time, plant life, interest rates, and maintenance costs.

Every component capital cost rate is denoted as Ż, and defined thus [5]:

$$\dot{Z}_{tot,Renewable} = CRF\frac{\phi}{\tau}PEC_{tot,Renewable} \tag{3.21}$$

Where CRF is the capital recovery factor, τ represents annual operating time, ϕ represents the maintenance factor, and PEC is the equipment purchase cost for each component in the plant. CRF was calculated by Eq. (3.22):

$$CRF = \frac{i_{eff}(1+i_{eff})^n}{(1+i_{eff})^n-1} \tag{3.22}$$

In the current study, the effective interest rate (i_{eff}), the plant life (n). Assumed to be 10% for interest rate and 30 years for plant life. $PEC_{tot,Renewable}$ for each of the photovoltaic plant (PV) and wind turbines (WT) were calculated using Eq (3.23, 3.24):

$$PEC_{PV,total} = PEC_{PV} + PEC_L \tag{3.23}$$

$$PEC_{WT,total} = PEC_{WT} \tag{3.24}$$

Where $PEC_{PV,total}$, $PEC_{WT,total}$, PEC_{PV}, PEC_{L}, PEC_{WT} are the equipment purchase cost for the PV plant and WT. The PV plant cost PEC_{PV} is calculated as a function of rated power P_{PV} and the WT cost PEC_{WT} is calculated as a function of rated power P_{WT} [68]. The purchase equipment cost values of system components have been shown in Table 3.3.

Table 3.3. Purchase equipment costs of system components

Components	Cost Correlation	REF
PEM Electrolyser	$PEC_{elc} = 940\dot{W}_{electrolyser}$	[69]
Compressors CO_2, H_2	$PEC_{comp} = \frac{711\dot{m}}{0.9\eta_s} Pr \ln(Pr)$	[70]
CCP	$PEC_{ccp} = \frac{172.95\dot{V}_{fg}3600}{10}$	[69]
MPP Separator and Splitter	$PEC_{sep} = \frac{1773\left(\frac{dailymethanol}{0.7}\right)}{350}$	[56]
Catalytic Reactor	$PEC_{sep} = \frac{6582\left(\frac{dailymethanol}{0.7}\right)}{350}$	[56]
Distillation	$PEC_{sep} = \frac{4350\left(\frac{dailymethanol}{0.7}\right)}{350}$	[56]
PV Panels	$PEC_{PV} = 1500 \times P_{PV}$	[68]
Inverter of PV panels	$PEC_{L} = 180 \times P_{PV}$	[68]
WT	$PEC_{WT} = 3500 \times P_{WT}$	[68]

Electricity, carbon dioxide, hydrogen, and methanol product costs are estimated using Eqs. 3.25-3.28 [5]:

$$\dot{Z}_{elec} = \frac{\sum \dot{Z}_{tot,Renewable}}{\dot{W}_{Renewable}} \tag{3.25}$$

$$\dot{Z}_{H2} = \frac{\sum \dot{Z}_{Renewable} + \sum \dot{Z}_{elec}}{\dot{m}_{H2}} \tag{3.26}$$

$$\dot{Z}_{CO2} = \frac{\sum \dot{Z}_{CCP}}{\dot{m}_{CO2}} \tag{3.27}$$

$$\dot{Z}_{CH3OH} = \frac{\sum \dot{Z}_{Total}}{\dot{m}_{CH3OH}} \tag{3.28}$$

Where $\dot{Z}_{tot,Renewable}$, $\dot{Z}_{elec}$, and $\dot{Z}_{CCP}$ represent total cost rates of the PV plant, WT turbines, electrolyzer, and CCP whereas $\dot{Z}_{Total}$ represents the cost rate of the whole plant. The cost of electricity has been expressed in \$/kWh, whereas other prices are expressed in units of \$/kg.

3.4. ENVIRONMENTAL ANALYSIS

Counting the contaminants released into the atmosphere requires environmental analysis. Moreover, cutting emissions can lower environmental costs [71,72]. Therefore, CO_2 procedures must reduce CO_2 emissions, thereby necessitating calculations of the total amount of CO_2 emissions.

The carbon emission factors that are utilized may differ significantly between, and even within, the various basic fuel types. The composition of natural gas, which, when supplied, is primarily composed of methane but may also contain trace amounts of ethane, butane, propane, and other heavier hydrocarbons, affects the gas’s carbon emission factor. Flared natural gas at the production site is “wet,” which refers to a higher content of hydrocarbons other than methane. The carbon emission factor will therefore vary as well. In comparison to fully refined fuels such as residual fuel oil, lightly refined products such as gasoline frequently have a lower carbon content per unit of energy. The amount of carbon per ton of coal depends significantly on the quantity of carbon, sulfur, hydrogen, oxygen, ash, and nitrogen.

The amount of fuel utilized, and the average emission factor are used to estimate emissions from all combustion sources. The carbon emissions factor from coal was calculated using the IPCC Tier 1 approach, as in Eq. 3.29 [73]:

$$C_C = 32.15 - (0.234 \times H_V) \tag{3.29}$$

where C_C is the carbon emissions factor in t C/TJ, and H_V the gross calorific value of coal, with a calorific value between 31 and 37 TJ/kiloton on a dry mineral matter-free basis.

Due to the system's extensive carbon dioxide consumption, GHG emissions are significantly reduced. However, because the system relies heavily on thermal energy, there are many indirect greenhouse gas emissions. The system's ability to reduce CO_2 can then be calculated using Eq. 3.29:

$$ER_{net} = ER_{utilization} + ER_{substitution} - ER_{generation} \tag{3.30}$$

where ER_{net} is the net amount of CO_2 emissions, $ER_{utilization}$ the amount of CO_2 used in the system processes, $ER_{substitution}$ the amount of CO_2 reduction and $ER_{generation}$ the amount of CO_2 generated by the process.

3.5. ENGINEERING EQUATION SOLVER (EES)

The EES can be thought of as a general program equation solver that is used to solve nonlinear algebraic equations as well as systems of differential equations. Additionally, this software is used to execute optimization, unit conversion, and unit verification. The software also performs linear and nonlinear regression, provides uncertainty analyses, solves differential and integral equations, and generates graphs.

The primary benefit of the EES is its extremely precise thermodynamic and transport possession database, which is made available for hundreds of substances in a manner that enables their use with the ability to solve equations. Moreover, fundamental features include:

- Instantaneous multi-equation calculation at extremely high speeds
- May be entered equations and coefficients in any order
- The capacity for both single- and multi-variable optimization
- Professional contour plotting in 2-D, 3-D, and with automated updating
- MATLAB, Excel, Python, C/C++, Fortran, and other links

EES incorporates a wide range of mathematical and thermophysical features, and because it creates a database by categorizing fluids, its thermodynamic calculations are quite precise.

The dependent variables are determined once the user defines the input for the EES application. It is a helpful program because it may resolve a variety of fundamental issues in thermodynamics, heat transfer, fluid mechanics, and other more difficult issues. EES is a valuable and practical all-purpose engineering solution. The proposed system and every component of the methanol production plant were analyzed and calculated in this study using the EES [74].

PART 4

RESULTS AND DISCUSSIONS

This proposed process for the synthesis of methanol using solar and wind energy in Iraq, and the results of the efficiency of a methanol plant (η_{MP}), electrolyzer (η_{elec}), fuel efficiency (η_{fuel}), renewable net power ($\dot{W}_{Renewable}$), purchased equipment costs (PEC), renewable generation costs ($\dot{Z}_{tot,Renewable}$), costs of the methanol plant, methanol production, daily CO_2 capture, and hydrogen product were analyzed. The needed calculations were made using Fallujah white cement plant flue gas measurement data. The system's calculated outcomes and the results attained are listed below section by section.

4.1. THERMODYNAMIC ANALYSIS

In order to determine how the system would behave given the operating pressure, temperature, and mass flow, the thermodynamic analysis is crucial. Therefore, using the criteria established by the first and second laws of thermodynamics is the best way to assess a system's performance. This helps provide specific information about the system's present state.

In this section, thermodynamic analysis was obtained according to the varying mass flow rate of 7,161,000 to 19,820,000 kg/h, enthalpy of 6,053 to 2,684 kJ/kg, pressure of 45 to 1.1 bars, and temperature of 443 K to 377.9 K, in addition to the energy and material balance of the methanol production plant, as shown in Table 4.1. The energy duties of the subsystem are presented in Table 4.2.

Table 4.1. Methanol Production Plant energy and material balance.

State	Enthalpy (kJ/kg)	Mass Flow Rate (kg/h)	Pressure (bar)	Temp. (K)
I	6053	22120	45	443
II	2456	33159	45	320
III	-740.6	748.4	45	303
IV	2372	32410	45	303
V	-646.1	175576	45	303
VI	466.4	871803	50	315.1
VII	-264.5	143167	100	293
VIII	381.9	1.015E+06	50	301.2
IX	903.7	1.015E+06	50	498
X	903.7	1.015E+06	50	498
XI	862.4	1.015E+06	50	523
XII	484.6	1.015E+06	50	366.9
XIII	328.1	1.015E+06	50	304
XIV	-465.2	165286	45.2	365.2
XV	-484	165286	5.066	360.6
XVI	-1120	104063	1.013	312
XVII	2684	61223	1.1	377.9

Table 4.2. Energy duties of the plant

Component	Value
CCP	
CCP heat load	32770 kW
CCP workload	4055 kW
HP	
Daily H_2 production	530874 kg/day
Cell voltage	1.57 V
MPP	
CO_2 Compressor power	10561 kW
H_2 Compressor power	44471 kW
Cooler heat duty	-44111 kW
Reactor heat duty	-11656 kW
Distillation column heat duty	-35508 kW
Stripper heat duty	4262 kW
Condenser heat duty	-1423 kW
Daily methanol production	2498 ton/day

Figure 4.1 shows the daily production of methanol at different flue gas levels during the course of the process. Methanol production rises with flue gas production, reaching a maximum of 6390 tons per day.

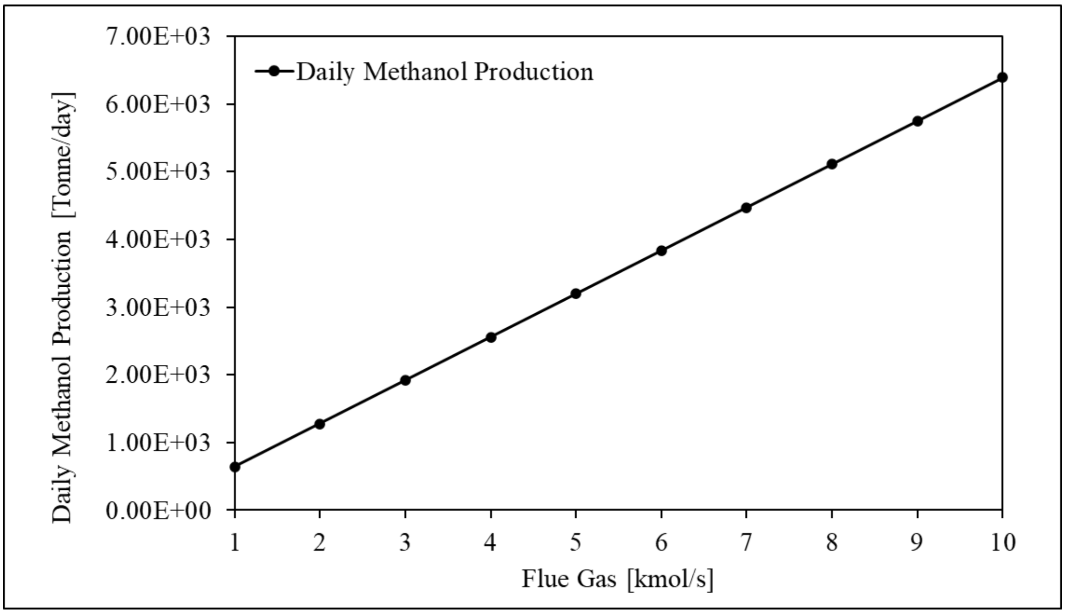

Figure 4.1. Effects of Increasing flue gas on daily methanol production.

Figure 4.2 shows flue gas rates versus hydrogen production, indicating that hydrogen production increases to 1,358 million kg/day at the highest flue gas rates.

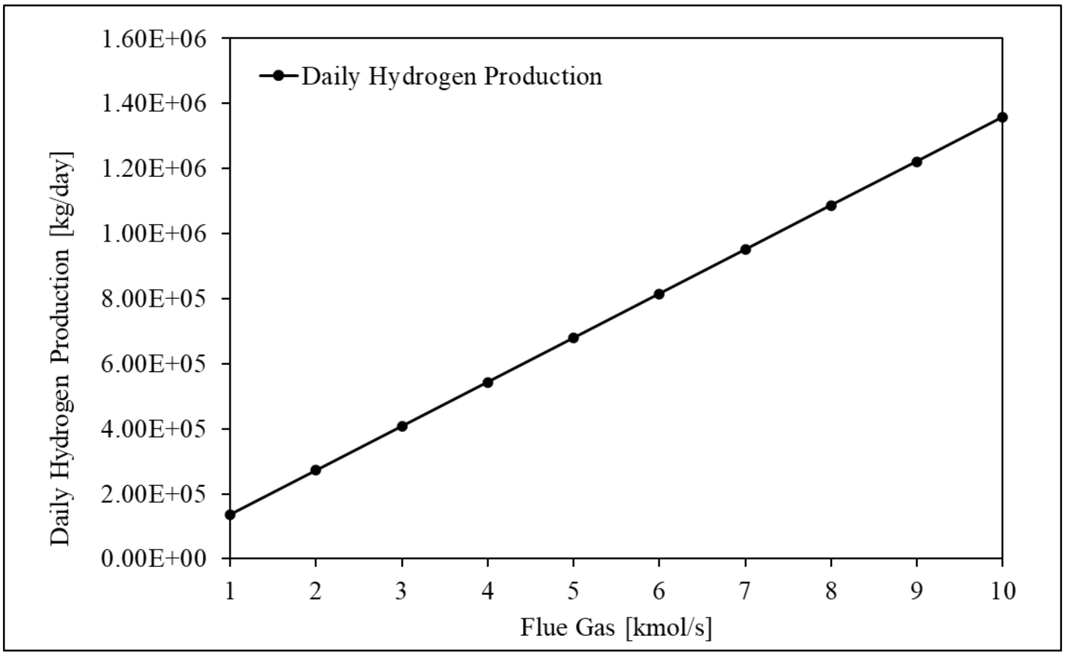

Figure 4.2. Effects of increasing flue gas on hydrogen production

The daily amount of carbon dioxide captured during the process is shown in Figure 4.3. As flue gas levels rise, the amount of carbon dioxide captured rises as well, peaking at 9962 tons per day.

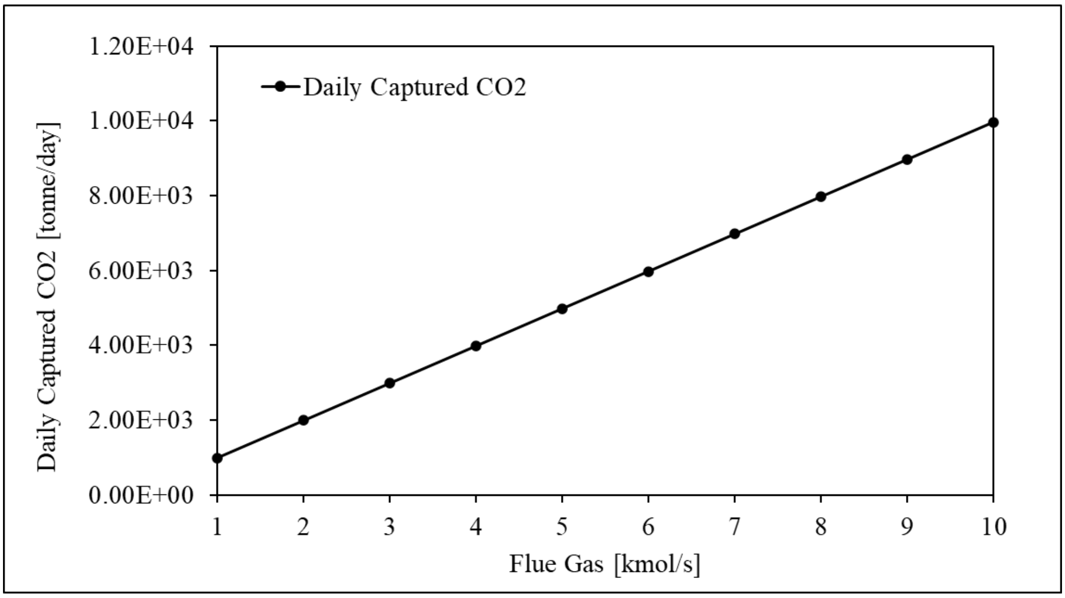

Figure 4.3. Effects of Increasing flue gas on daily captured CO_2

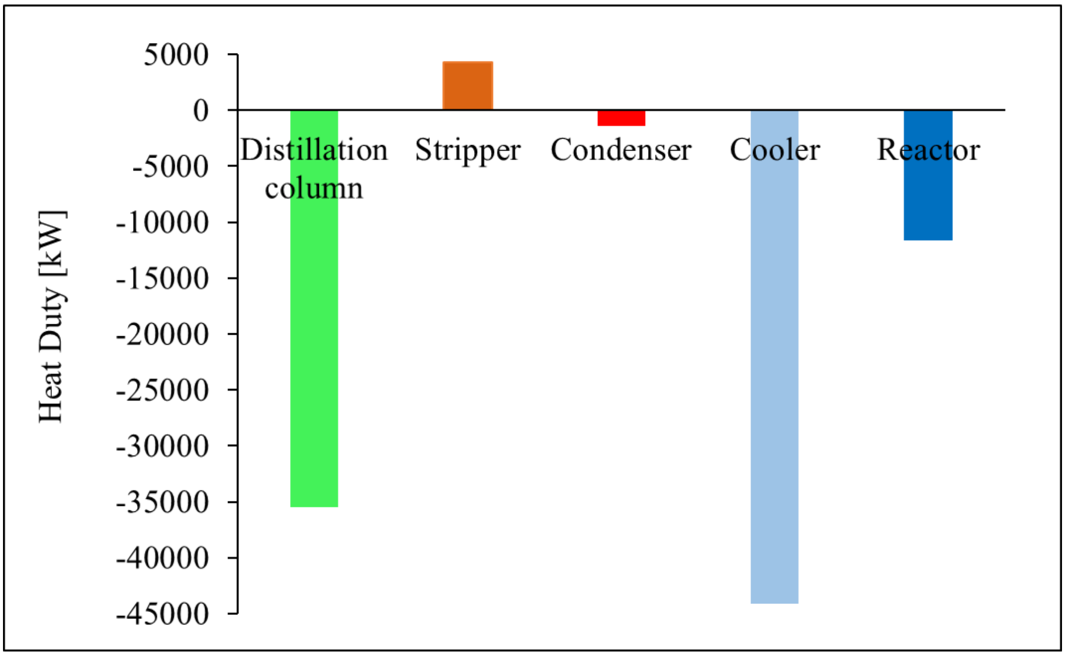

Figure 4.4. Heat duty for each unit in MPP.

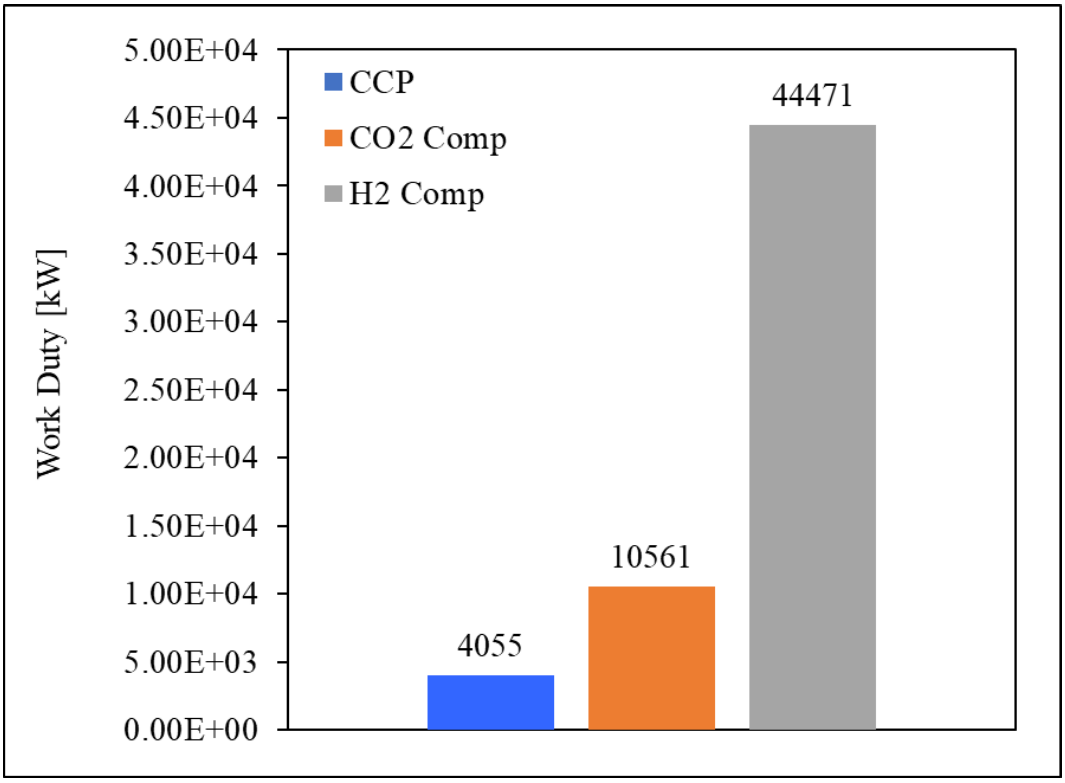

Figure 4.5. Work duty for the unit in the system.

4.2. TECHNO-ECONOMIC ANALYSIS

The cost of each product and the annual operating costs of the plant are calculated using a component-based cost analysis. The results of a thermodynamic analysis are used to determine costs, with power-consuming and energy-producing components essentially considered as functions of how much energy they consume or produce. The size of the plant also affects the costs of the CCP and MPP. For plants, a 30-year lifespan is assumed. In Table 4.3, the major findings of the economic study are presented.

Figure 4.6 shows how the cost of the plant decreases over the course of the plant's life. For example, the costs of the plant at 30 years, which is the time period for the plant's life that was taken into account in the accounts, are \$8,991 billion for the PV plant and \$5,259 billion for the wind plant, while the value is roughly \$8,720 billion for the PV plant and \$5,100 billion for the wind plant at 40 years.

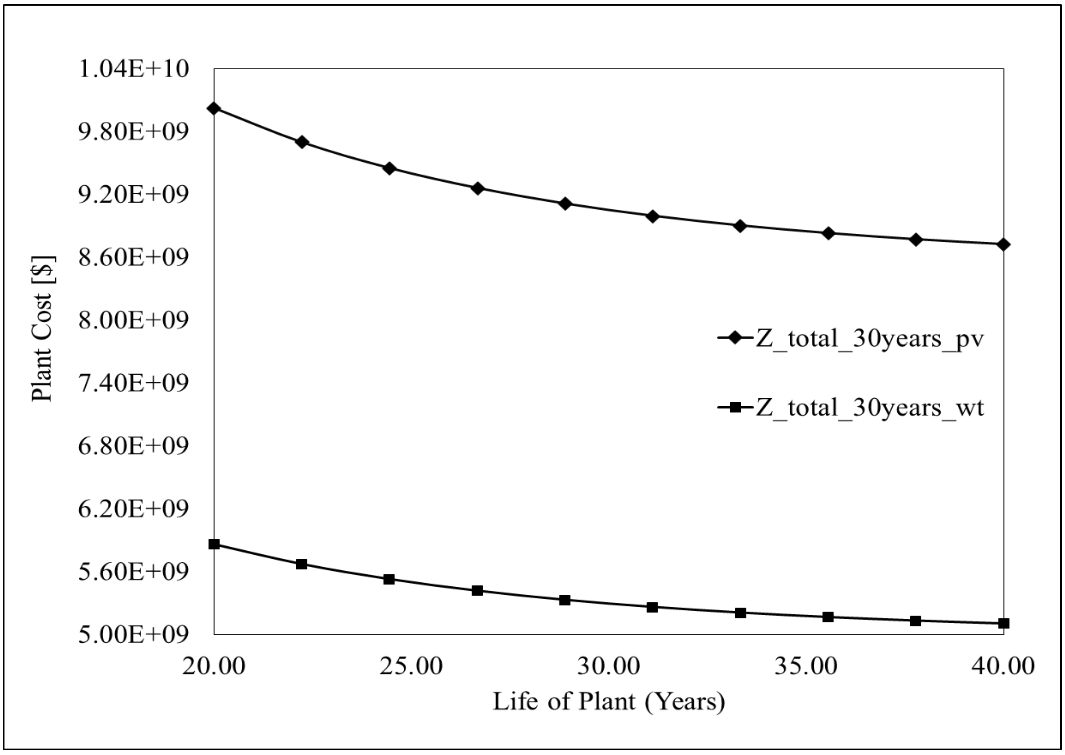

Figure 4.6. Effects of increasing the life of a plant on plant costs.

Figure 4.7 shows the area of the PV panels and the cost of equipment for the PV panels versus levels of flue gas. The maximum area of the PV panels is 26116 m^2, and the maximum cost is $4,211 billion.

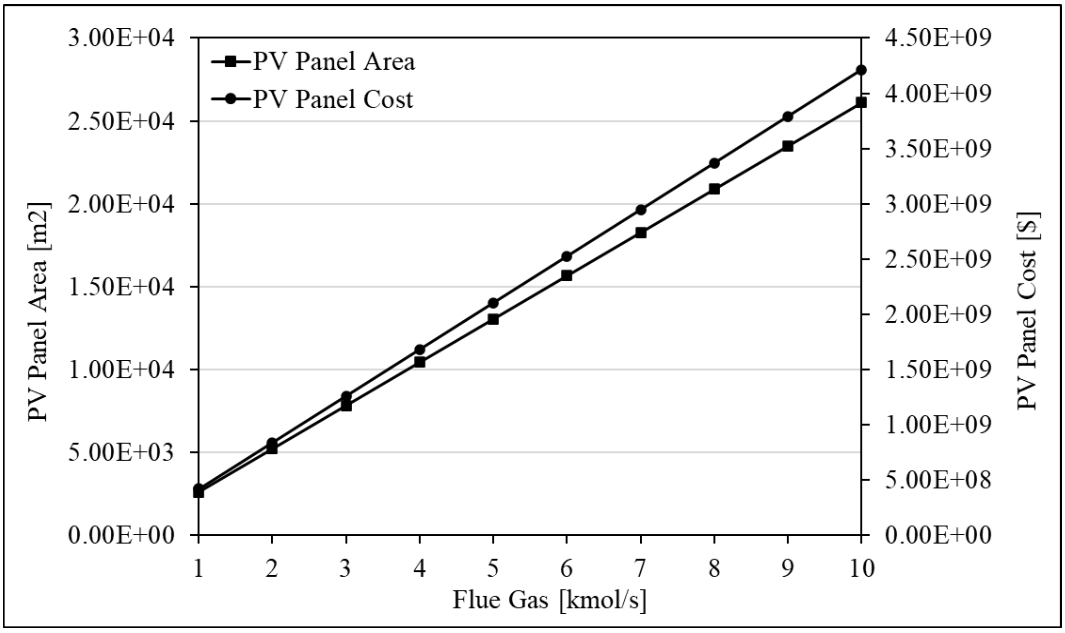

Figure 4.7. Effects of increasing flue gas on PV panel area and PV panel costs.

Figure 4.8 shows the area of the wind plant and the cost of equipment for the wind plant versus the levels of flue gas. The maximum area of the wind panels is 170498 m^2, and the maximum cost is \$1,515 billion.

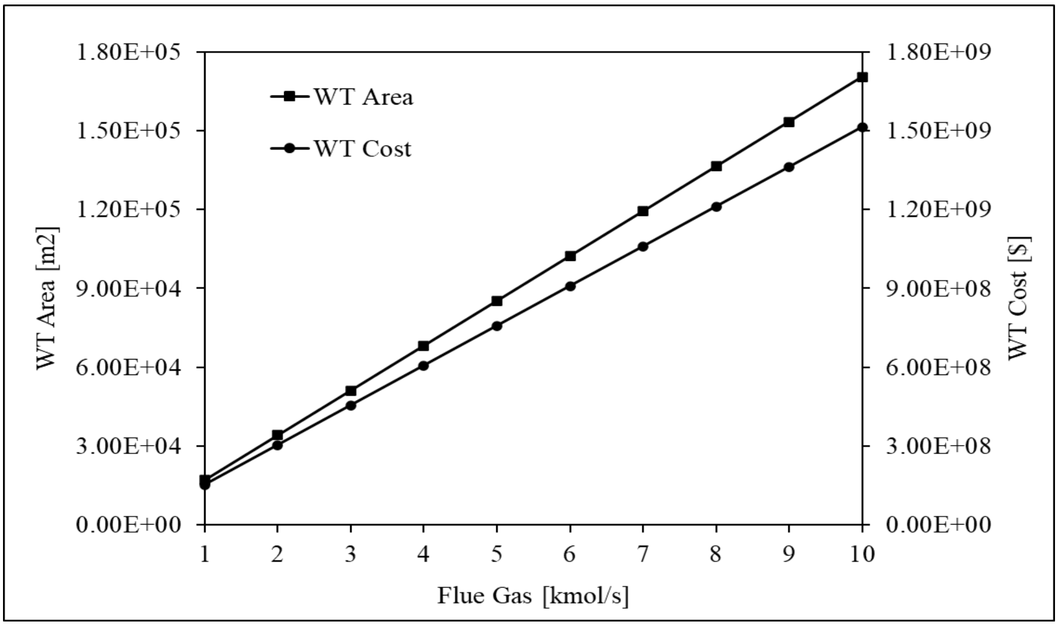

Figure 4.8. Effects of increasing flue gas on wind plant area and wind plant costs.

Figure 4.9 shows the total cost of the PV panels ($\dot{Z}_{tot,PV}$) and the total cost of the methanol ($\dot{Z}_{Methanol,PV}$) as the plant's life changes, with the total cost of the PV panels at the 30th point of the plant's life being \$7.712 per second and the cost of methanol being \$0.416 per kg, indicating that costs decrease with an increase in the plant's life.

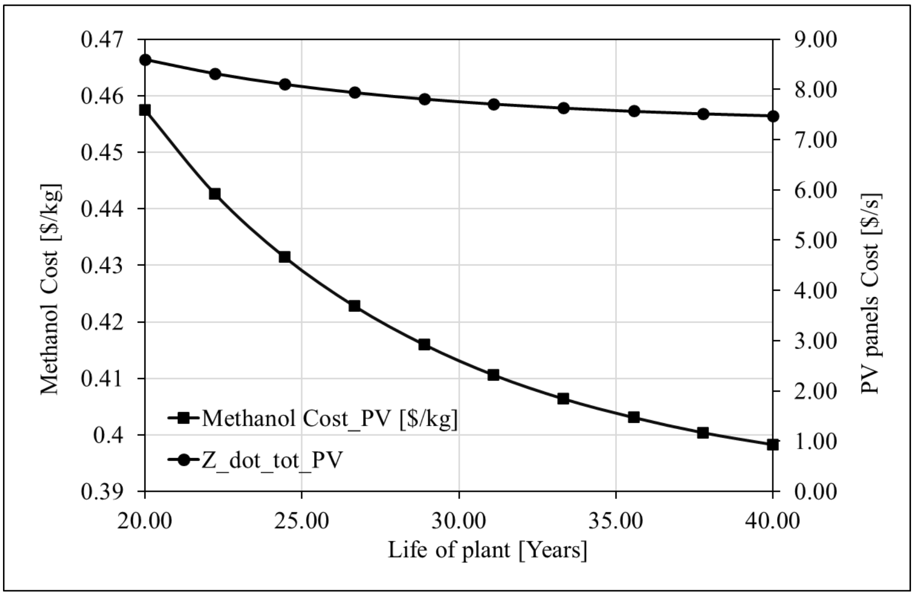

Figure 4.9. Effects of increased plant life on Methanol Costs and Total PV panels Costs

Figure 4.10 shows the total cost of the wind turbine ($\dot{Z}_{tot,WT}$) and the total cost of methanol ($\dot{Z}_{Methanol,WT}$) as the plant's life changes, with the total cost of the wind turbine at the 30th point of the plant's life being $2.811 per second and the cost of methanol being $0.243 per kg, indicating that costs decrease as the plant's life increases.

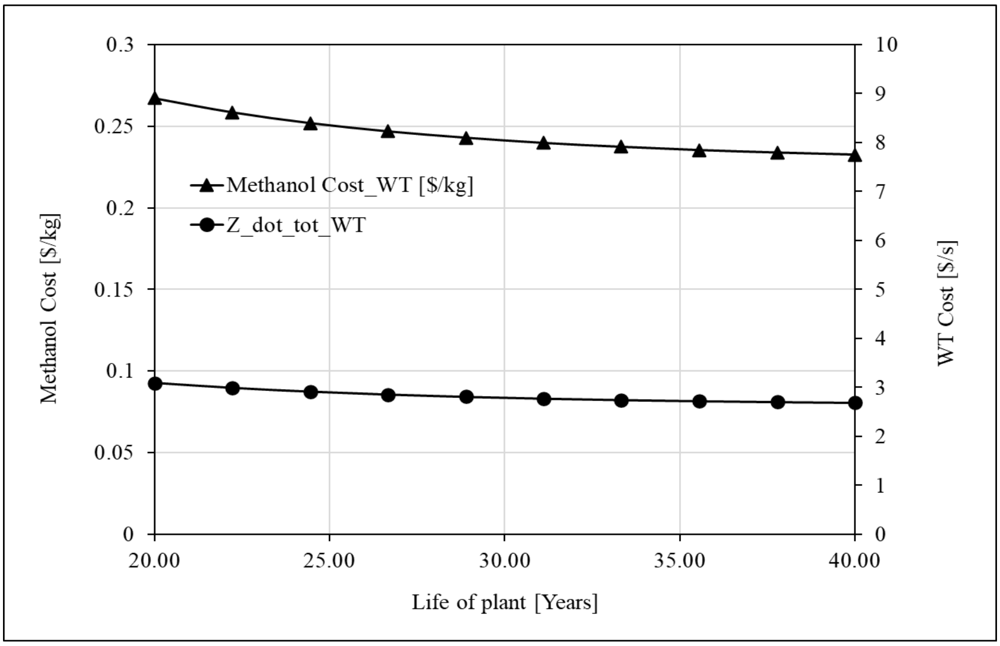

Figure 4.10. Effects of increased plant life on Methanol Costs and Total wind turbine Costs

Table 4.3. Economic analysis results

Parameter	**Value**
Renewable cost (PV)	195,5 M $/y
Renewable cost (WT)	70,350 M $/y
Electricity cost (PV)	0.02851 $/kWh
Electricity cost (WT)	0.01026 $/kWh
CCP cost	1,228 M $/y
Electrolyser cost	104 M $/y
CO_2 production cost	0.0016 $/kg
Hydrogen production cost (PV)	1.936 $/kg
Hydrogen production cost (WT)	1.127 $/kg
MPP cost	790,825 $/y
Methanol production cost (PV)	0.4131 $/kg
Methanol production cost (WT)	0.2413 $/kg

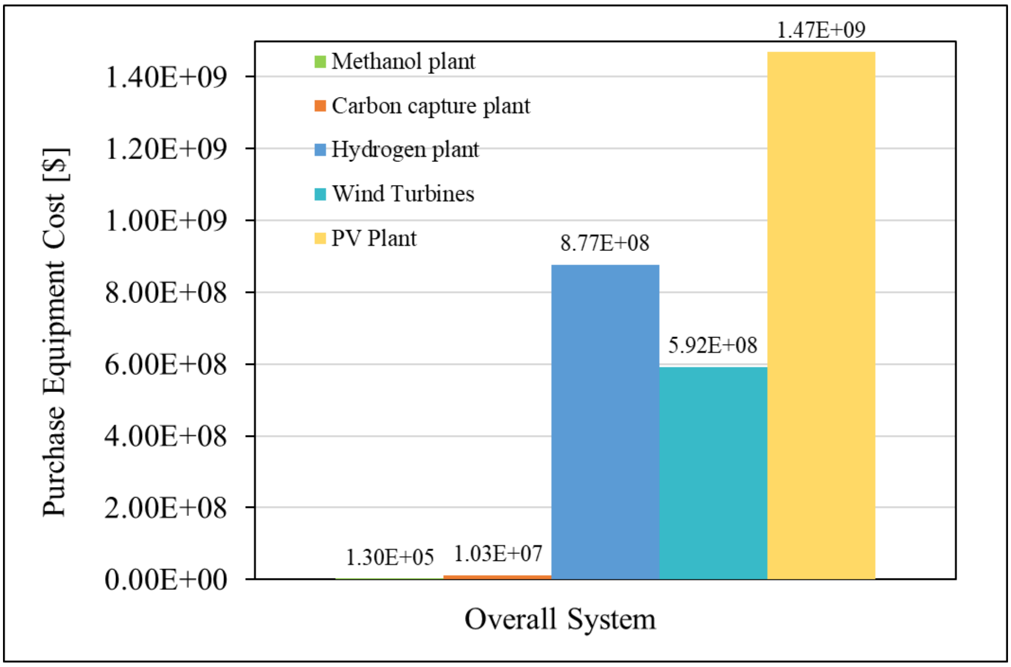

Figure 4.11. The effect of variation on the overall system's purchase equipment cost.

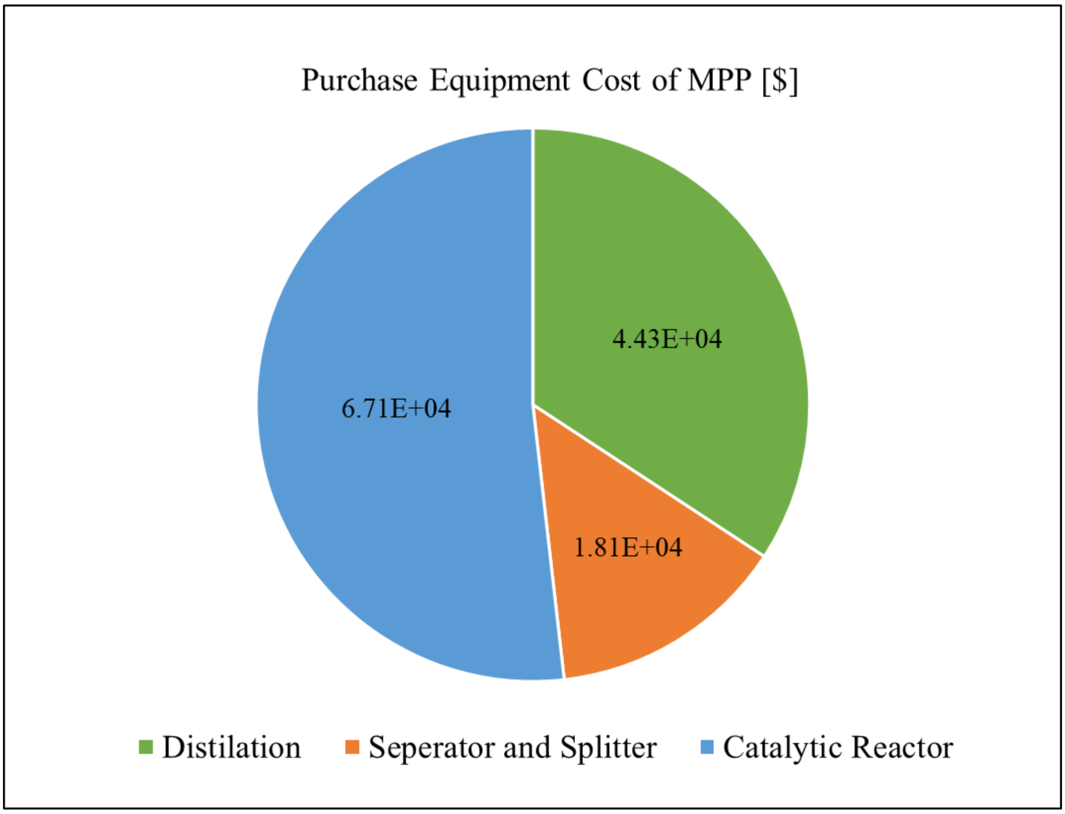

Figure 4.12. Effect of variation on equipment purchase cost for a methanol production plant.

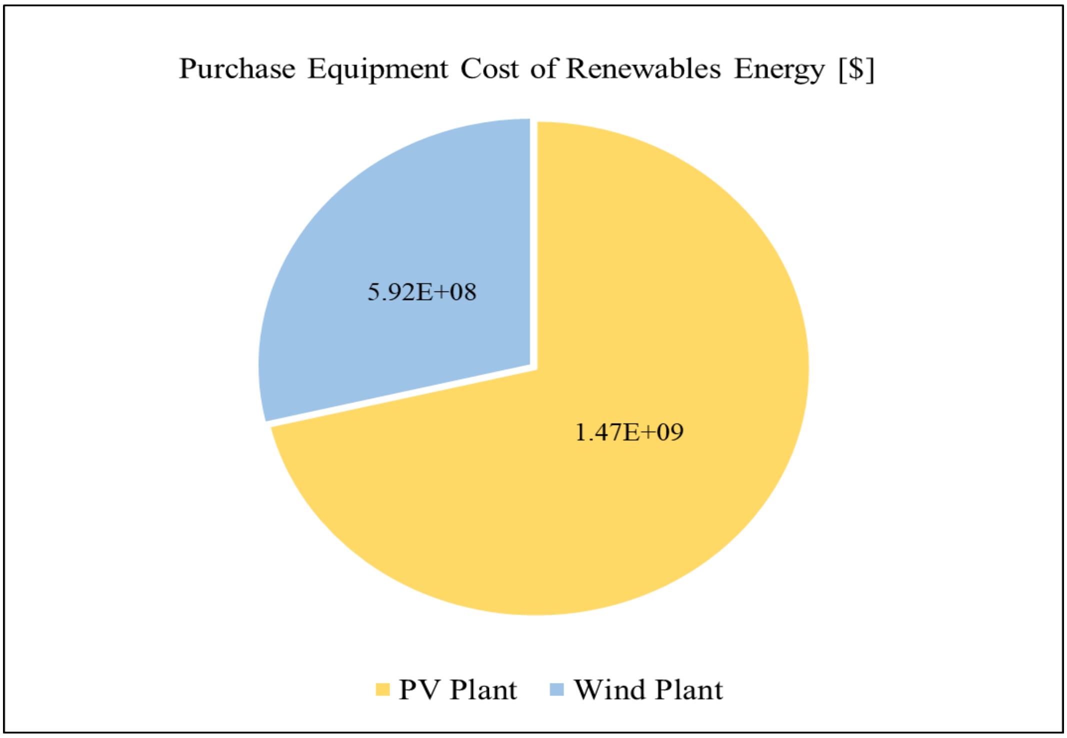

Figure 4.13. Impact of variation on the purchase equipment cost of renewables.

4.3. ENVIRONMENTAL ANALYSIS

In this section, we discuss calculated CO_2 emissions from the production plant and methods for reducing them.

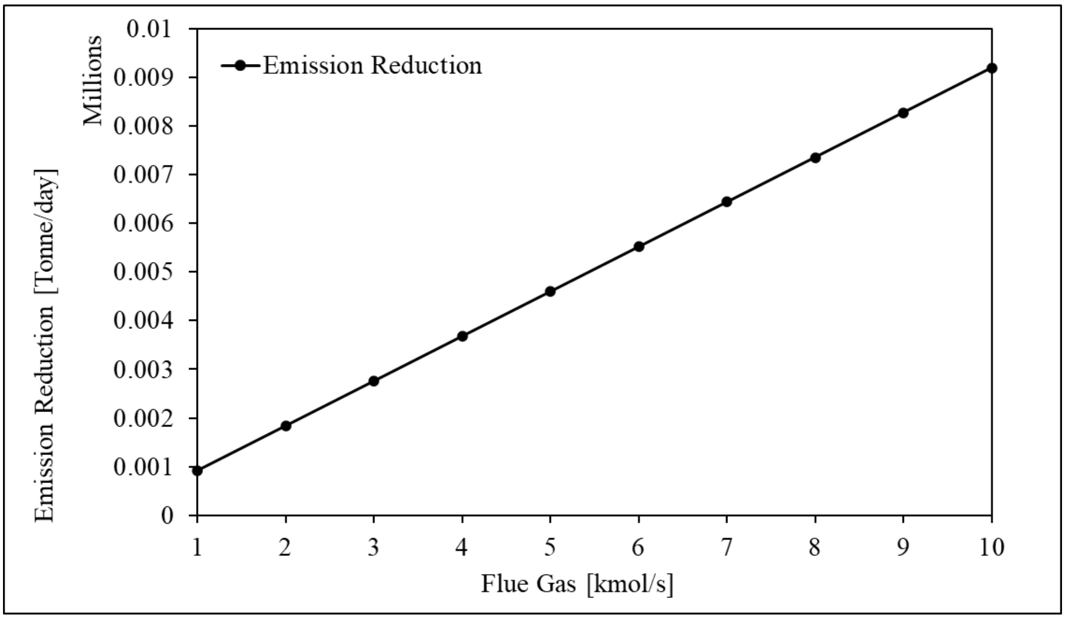

Figure 4.14. Effects of increasing flue gas on emission reduction.

Figure 4.14 shows the link between flue gas levels and the reduction of emissions. At the maximum flue gas level, the greatest emission reduction is 9194 tons per day.

PART 5

CONCLUSIONS

This study makes a techno-economic and environmental investigation of methanol production plant using solar and wind energy and using waste gases from a white cement plant.

Following is a summary of the study's main conclusions:

- The amount of captured CO_2 has been estimated at 3894 tons/day, and the heating load of the CCP has been estimated at 32770 kW in the case where the H/C ratio has been assumed as being stoichiometric.
- At the reactor's ideal temperatures and pressure, 2498 tons of methanol can be produced daily, according to estimates.
- PEM electrolyzer cell efficiency was measured to be at a maximum of 0.782% at a 400 K cell temperature and 2.2 kA/m^2 current density. Under those circumstances, a daily production of hydrogen at a rate of 530874 kg/day has been noted.
- According to calculations, the plant's overall efficiency reached 0.1626%, and the MPP fuel efficiency 0.5872%.
- The total plant cost for 30 years of operation for each of the PV and wind turbine (WT) plants are \$9,46 billion and \$5,291 billion, respectively, which can result in the production of over 34,530 million tons of methanol, which corresponds to 0.4131 \$/kg for the PV plant and 0.2413 \$/kg for the WT plant.
- The rate of captured emissions was approximately 3894 tons per day, and the mitigation rate was approximately 3594 tons per day.

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