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# Methanol Production from $CO_2$ Emissions: Simulation and Environmental Analysis

**Khloud Souleman T. Souleman[a,c,*], Mohamed fathy[b], Eman A. Emam[c]**

[a]*Canal Higher Institute for Engineering and Technology, Egypt.*

[b]*Mostorod Refinery Plant, Egyptian Refining Company (ERC), Egypt.*

[c]*Refining and Petrochemical Engineering Department, Faculty of Petroleum and Mining Engineering, Suez University, Egypt*

**Abstract**

It is very exciting to obtain methanol from $CO_2$ emissions as a by-product, especially when this by-product causes world environmental catastrophes and health problems. This paper is organized to present applicable solution for reduction $CO_2$ emissions through converting $CO_2$ emissions of refining plant to methanol by hydrogenation technology. Therefore, Aspen HYSYS simulation program was used for simulation of $CO_2$ capture plant and methanol production plant. The results achieved that 99% of $CO_2$ emissions from refining plant were captured. As well as production of methanol with 99.99% purity of methanol; in addition, that $CO_2$ tones/one tone methanol of our work is less than previous work by 82.3%. Therefore, this paper presented an actual solution for reduction of $CO_2$ emissions and enhancing methanol production.

*Keywords:* Carbon dioxide; $CO_2$ emissions; $CO_2$ capture; Methanol production; Simulation plant; Aspen HYSYS; Environmental analysis.

## 1. Introduction

Nowadays, all worlds suffer from environmental problems of greenhouse gases which lead to global warming and climate change. It is found that carbon dioxide emissions contribute with the largest percent of greenhouse gases. Carbon dioxide emissions resulted by human activity such as manufacturing of cement and steel, combustion of fossil fuel such as coal and natural gas, generation electricity from power plant, refining plant as a by-product, ships and other transportation [1]. In Egypt, main source of carbon dioxide emission is refinery plants [2]. Carbon dioxide emissions increase, as refining plant capacity increases [3]. Although carbon dioxide emissions have negative impacts on health and environment, there are a lot of utilizations of carbon dioxide as a raw material for producing chemicals in most processes. Major industrial process that utilizes carbon dioxide as a raw material is methanol production [4]. Therefore, it is exciting to convert carbon dioxide emissions (by-product) into value-added product such as methanol.

Methanol is main member of the alcohol group which has several uses and applications. It can be used as a feedstock for chemical syntheses such as formaldehyde, acetic acid and other important products. Methanol can also be used as a fuel for Otto Engines (gasoline). It is important to mention that research octane number of methanol is higher than gasoline. In direct methanol fuel cell (DMFC), methanol or methanol solutions is used as fuel at an ambient temperature. In this process, methanol reacts with air to generate electricity from carbon dioxide and water. Due to low freezing point of methanol, it used in refrigeration systems and used as antifreeze in heating and cooling circuits. Additionally, methanol is used to protect natural gas pipelines against the formation of gas hydrates at low temperature. In Rectisol process, methanol is also used as an

*Corresponding author e-mail: Khloudsouleman@gmail.com.; (Khloud Souleman T. Souleman).
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absorption agent in gas scrubbers to removal of $CO_2$ and $H_2S$ at low temperature [5].

Hydrogen is main raw material, used to produce methanol from $CO_2$. There are two main routes for production of methanol from carbon dioxide depending on method of hydrogen production: conventional route (source of hydrogen production is fusel fuel such as natural gas) and green route (source of hydrogen production is renewable source such as water). After comparison between conventional route and green route, it is found that green route emitted lower emission than conventional route due to low emissions of green $H_2$. Conventional route produced methanol with lower price than green route due to higher price of green $H_2$ [6]. In conventional route, there are two main technologies: direct hydrogenation of $CO_2$ and indirect hydrogenation of $CO_2$. After comparison between direct hydrogenation of $CO_2$ and indirect hydrogenation of $CO_2$, it is found that indirect hydrogenation of $CO_2$ was superior to direct hydrogenation of $CO_2$ due to achieving 20.8 % increase in methanol production rate. Therefore, the indirect hydrogenation of $CO_2$ is feasible as a green route to produce methanol in a large scale [7].

The main step for simulation of methanol production plant is modeling carbon dioxide capture plant. There are several technologies for carbon dioxide capturing such as absorption, adsorption and membrane. The most mature technology is absorption technology. Monoethanolamine (MEA) is used as a chemical solvent in absorption process because it increases the efficiency of $CO_2$ capturing. Additionally, MEA has high $CO_2$ absorption capacity, and achieve high recovery of $CO_2$ [8]. Aspen HYSYS used as a software simulation program for modeling and simulation of carbon dioxide capture plant [9].

In $CO_2$ capture plant simulation, it was used a standard amine-based $CO_2$ capture process as a process configuration. The amine package "Acid Gas - Chemical Solvents" is used as a fluid package in Aspen HYSYS program. In absorber tower, total flue gas and MEA inlet temperature is 40°C, total flue gas inlet and MEA pressure is 100-150 KPa, number of stage is 12-24. In heat exchanger, $\Delta T_{min}$ is 10-15°C. in regenerator, number of stages is 6-10, and pressure is 150-200 KPa [10].

In methanol production plant simulation, “A process of methanol production with two reactors in series” was used as a process configuration. "Peng-Robinson” was chosen as a fluid package per Aspen HYSYS software simulation program recommendation. The optimal operating conditions can be used as follows; inlet pressure to the first reactor is 57.8 bar, inlet temperature to the first reactor is 183.6°C, outlet pressure of valves is 8 bar, inlet temperature to the first distillation column is 51.8°C [11].

Prapatsorn Borisut and Aroonsri Nuchitprasittichai [12] estimated amount of methanol production to be 31036 kg/h with 99.5% purity using 3 moles of $H_2$ per 1 mole of $CO_2$. In another study, Tuan B.H. Nguyen and Edwin Zondervan [3] estimated $CO_2$ tones/one tone methanol to be in range of 1.394-1.467 through methanol production of three different capacities; 300, 1500, and 3500 ton/day with 99.5% purity.

The main objectives of this paper are: i) present applicable solution for reduction of $CO_2$ emissions; ii) production of methanol from $CO_2$ emissions; iii) measuring environmental efficiency. iii) Comparison the obtained result with previous work.

To achieve these objectives, this paper is organized as following: i) methodology of simulation, which included calculation the amount of $CO_2$ emissions, simulation of $CO_2$ capture plant, simulation of methanol production plant; ii) methodology of environmental analysis, which included environmental analysis of $CO_2$ capture plant, environmental analysis of methanol production plant and finally present the results and compared the obtained results with previous work that mentioned in introduction.

## 2. Methodology of simulation

In this study, the $CO_2$ emissions of an Egyptian refining plant are converted to methanol. There are

two main sources of $CO_2$ emissions: $CO_2$ emissions produced from complete combustion of emitting fuel gases from fired heaters and flue gasses from hydrogen production unit (HPU). The source of hydrogen used for production methanol is HPU from the same refining plant. Aspen HYSYS V.12 was used as a simulation software program.

The objective of this paper study is achieved through several steps as the following: calculation the amount of $CO_2$ emissions, simulation of $CO_2$ capture plant, and then simulation of methanol production plant.

### *2.1. Calculation the amount of $CO_2$ emissions*

The data used in this case, is designed data of Egyptian refining plant. In fired heater, $CO_2$ emissions produced from complete combustion of emitting fuel gases from fired heaters in 20% excess air. In HPU, $CO_2$ emissions produced as a flue gases.

From fired heaters, the emitting fuel gases are $CH_4$, $C_2H_6$, $C_3H_8$, $C_2H_4$, $C_3H_6$, $C_4H_8$, i-$C_4$, n-$C_4$, i-$C_5$, neo-$C_5$, $C_6H_{14}$, $N_2$, $CO_2$, $H_2O$ and little few amounts of $H_2S$ and $H_2$. Microsoft Excel program is used in calculation of $CO_2$ emissions produced from complete combustion of emitting fuel gases of fired heaters. Therefore, the emitting flue gases are $CO_2$, $H_2O$, $N_2$ and $O_2$. The flow rate of flue gases resulting from complete combustion of emitting fuel gases from fired heaters is 16471Kg mole/h. The composition of emitting flue gases from fired heaters after complete combustion is shown in Table 1.

**Table 1**
The composition of emitting flue gases from fired heaters after complete combustion

| Flue gas from fired heaters | Mole fractions |
|---|---|
| $CO_2$ | 0.1054 |
| $H_2O$ | 0.1650 |
| $N_2$ | 0.7024 |
| $O_2$ | 0.0272 |
| Total | 1 |

From HPU, the emitting flue gases are $CO_2$, $H_2O$, $N_2$, Argon and $O_2$. The flow rate of flue gases emitting from HPU is 9651 Kg mole/h. The composition of emitting gases from HPU is shown in Table 2.

**Table 2**
The composition of emitting gases from in HPU

| Flue gas from HPU | Mole fractions |
|---|---|
| $CO_2$ | 0.1832 |
| $H_2O$ | 0.194 |
| $N_2$ | 0.601 |
| Argon | 0.0072 |
| $O_2$ | 0.0146 |
| Total | 1 |

By summation flow rate of flue gas from HPU and fired heaters, the result (Total flue gases) is approximately 26122 Kg mole/h. The total flue gases which is calculated, is the input stream of $CO_2$ capture plant. The composition of total flue gases is shown in Table 3.

**Table 3**
The composition of total flue gases

| Total flue gas | Mole fractions |
|---|---|
| $CO_2$ | 0.1341 |
| $H_2O$ | 0.1757 |
| $N_2$ | 0.6649 |
| Argon | 0.0027 |
| $O_2$ | 0.0226 |
| Total | 1 |

### *2.2. Simulation of $CO_2$ capture plant*

Aspen HYSYS V.12 is used as simulation program software for all process simulations. For choosing fluid package, the amine package "Acid Gas - Chemical Solvents" is chosen per the recommendation of Aspen HYSYS V.12.

#### *2.2.1. Process description*

There are two main steps in $CO_2$ capture plant: absorption of $CO_2$ and then purification of $CO_2$ as shown in Figure (1).

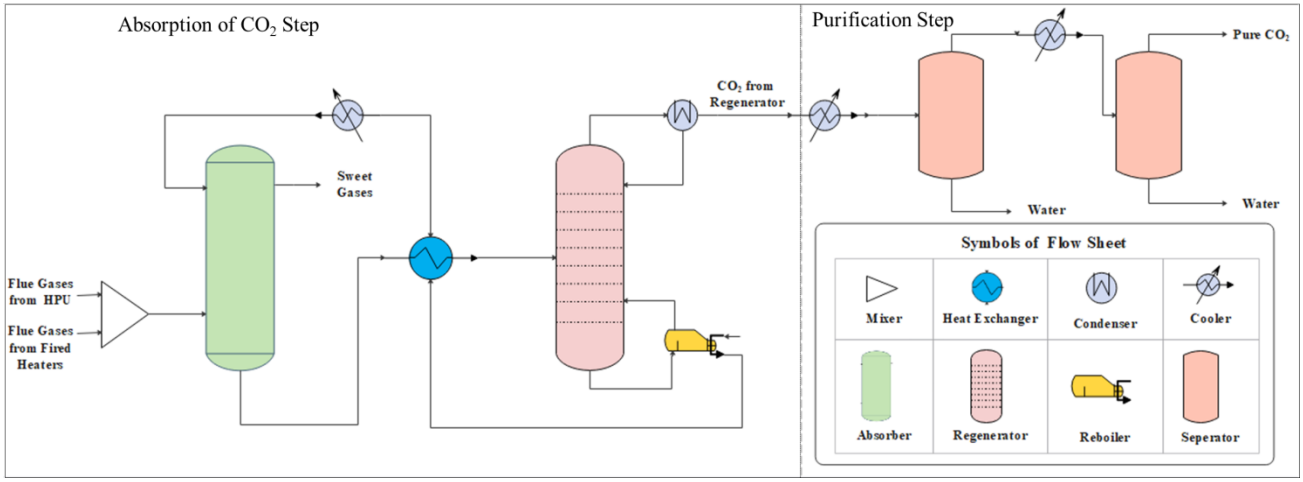


**Figure (1):** simple flow sheet for $CO_2$ capture plant

For absorption process of $CO_2$, MEA is used as a chemical solvent; the process includes two main towers: absorber and regenerator (distillation). For purification process of $CO_2$, the main equipment is separator. The function of the equipment in Figure 1 is explained in Table 4.

**Table 4**
The function of the equipment which used in $CO_2$ capture plant

| Equipment | Function |
|---|---|
| Absorber | Contacting between MEA and flue gas for capturing $CO_2$ from flue gases by MEA. The products are sweet gas from the top and MEA with $CO_2$ from the bottom |
| Heat Exchanger | Heating the bottom stream from absorber by cooling the bottom stream from regenerator. |
| Regenerator | Separation $CO_2$ from MEA for regeneration of MEA to absorber tower. |

### *2.2.2. Process specification and modeling*

Figure (2) describes the modeling process of $CO_2$ capture process. Flue gases from HPU and gases from heaters are mixed by using mixer (MIX-1) for producing stream of total flue gases, then this stream reached specification of entering absorber stream (stream of total flue gases to absorber) by using cooler (Cooler-1). The stream of total flue gases to absorber and stream of lean MEA entered absorber tower for absorbing $CO_2$. In absorber tower, fixed damping is chosen with value of 1. Therefore, absorber tower converged and produced stream of sweet gas from the top and stream of Rich MEA from the bottom. Stream of Rich MEA is pumped (for increasing its pressure to specified pressure of regenerator) by using pump, and then passes through rich/lean heat exchanger (for increasing its temperature to specified temperature of regenerator). In rich/lean heat exchanger, a minimum approach temperature of 10°C is chosen by using adjust (ADJ-1) with stream temperature of rich MEA to regenerator. In regenerator tower, adiabatic damping is selected, and regenerator tower converged when stream of rich MEA to regenerator entered it and produced stream of $CO_2$ from regenerator (which will enter the second step) from the top and stream of lean MEA exited from the bottom of regenerator. Stream of lean MEA from regenerator passes through rich/lean heat exchanger, and then passes through cooler (Cooler-2) for reaching specified temperature steam of lean MEA to makeup. Steam of lean MEA to makeup, water and pure MEA mixed by using mixer (MIX-2), and then pass through valve for reaching specification of lean MEA stream.

For purification of $CO_2$ as a second step of process, stream of $CO_2$ from Regenerator enters cooler (Cooler-3) for reducing temperature and enhancing separation in separator (Sepeator-1). Adjust (ADJ-3) was used to minimize amount of water in stream of Vap-1. Then, stream of Vap-1 passed through cooler (Cooler-4) for the same function mentioned before. Adjust (ADJ-4) was used to maximize amount of $CO_2$ in a stream of Vap-2 (approximately pure $CO_2$). Stream of Liq. 1 from bottom of Sepeator-1 and Stream of Liq. 2 from bottom of Sepeator-2 were mixed by using mixer (MIX-3) to produce stream of Total liq. Water.

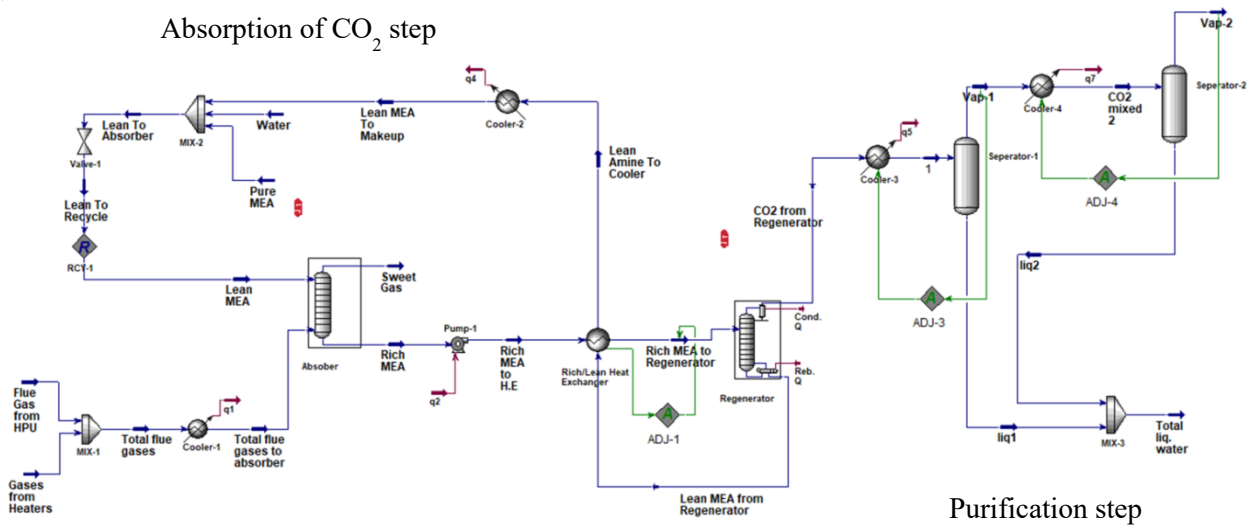


**Figure (2):** modeling of $CO_2$ capture plant on Aspen HYSYS

**Table 5**
The specifications of different stream.in $CO_2$ capture plant

| Specifications (unit) | Total flue gases stream | Lean MEA stream | Lean MEA To makeup stream | Water stream | Amine stream |
|---|---|---|---|---|---|
| Temperature(˚C) | 315.9 | 41.4 | 30 | 60 | 59.5 |
| Pressure (KPa) | 101.3 | 100 | 150 | 120 | 120 |
| Molar flow rate (Kgmole/h) | 26122 | 214100 | 162360 | 75800 | 30 |
| MEA (mole%) | 0 | 0.1595 | 0.2337 | 0 | 1 |
| $CO_2$ (mole%) | 0.1341 | 0 | 0.0015 | 0 | 0 |
| $H_2O$ (mole%) | 0.1757 | 0.8395 | 0.7649 | 1 | 0 |
| $N_2$ (mole%) | 0.6649 | 0.001 | 0 | 0 | 0 |
| Argon (mole%) | 0.0027 | 0 | 0 | 0 | 0 |
| $O_2$ (mole%) | 0.0226 | 0 | 0 | 0 | 0 |
| Total mole fraction | 1 | 1 | 1 | 1 | 1 |

**Table 6**
The specifications of main equipment in $CO_2$ capture plant

| Specifications (unit) | Absorber | Regenerator | Heat Exchanger | Cooler-3 |
|---|---|---|---|---|
| Temperature(˚C) | 40 | 97.01 | - | -64.37 |
| Pressure (KPa) | 100 | 150 | - | 101 |
| Number of stages | 20 | 10 | - | - |
| Reflux ratio | - | 500 | - | - |
| Reboiler Temperature (˚C) | - | 120 | - | - |
| $\Delta T_{min}$ (˚C) | - | - | 10 | - |
| $\Delta T$ (˚C) | - | - | - | - |

It must be mentioned that in absorber and regenerator tower, HYSIM Inside-Out solver is selected for convergence. All pumps were selected with adiabatic efficiency of 75%. Tables 5 and 6 describe the specifications of the different streams and the main equipment, respectively.

### *2.3. Simulation of methanol production plant*

For overall process simulations, Aspen HYSYS V.12 is used as simulation program software. Fluid packages "Peng-Robinson" is used as a fluid package in Aspen HYSYS program for methanol production plant. Feed stream of $CO_2$ come from Vap-2 and stream of $H_2$ come from HPU (used as black hydrogen).

#### *2.3.1. Process description*

Two main steps in methanol production plant: conversion of $CO_2$ to methanol, and then purification of methanol, shown in Figure (3). For conversion of $CO_2$ process, the process includes two main reactors for enhancing conversion of $CO_2$ to methanol. For purification of methanol, the main equipment is distillation towers as explained in Table 7.

**Table 7**
The specifications of main equipment in methanol production plant

| Equipment | Function |
|---|---|
| Mixer | Mixing stream of $H_2$ with steam of Vap-2 (total $CO_2$ captured)<br>Mixing stream of outlet gases for purging.<br>Mixing streams of methanol liquid for purification. |
| Reactor | Partially converting reactants to methanol.<br>Enhancing converting of the remaining vapor reactants for increasing methanol production. |
| Cooler | Decreasing temperature of stream for separating methanol as a liquid. |
| Separator | Separating vapors from methanol liquid. |
| Distillation tower | Separating of methanol solution (methanol with water) from gases.<br>Purification methanol from water and other impurities for obtaining pure methanol. |

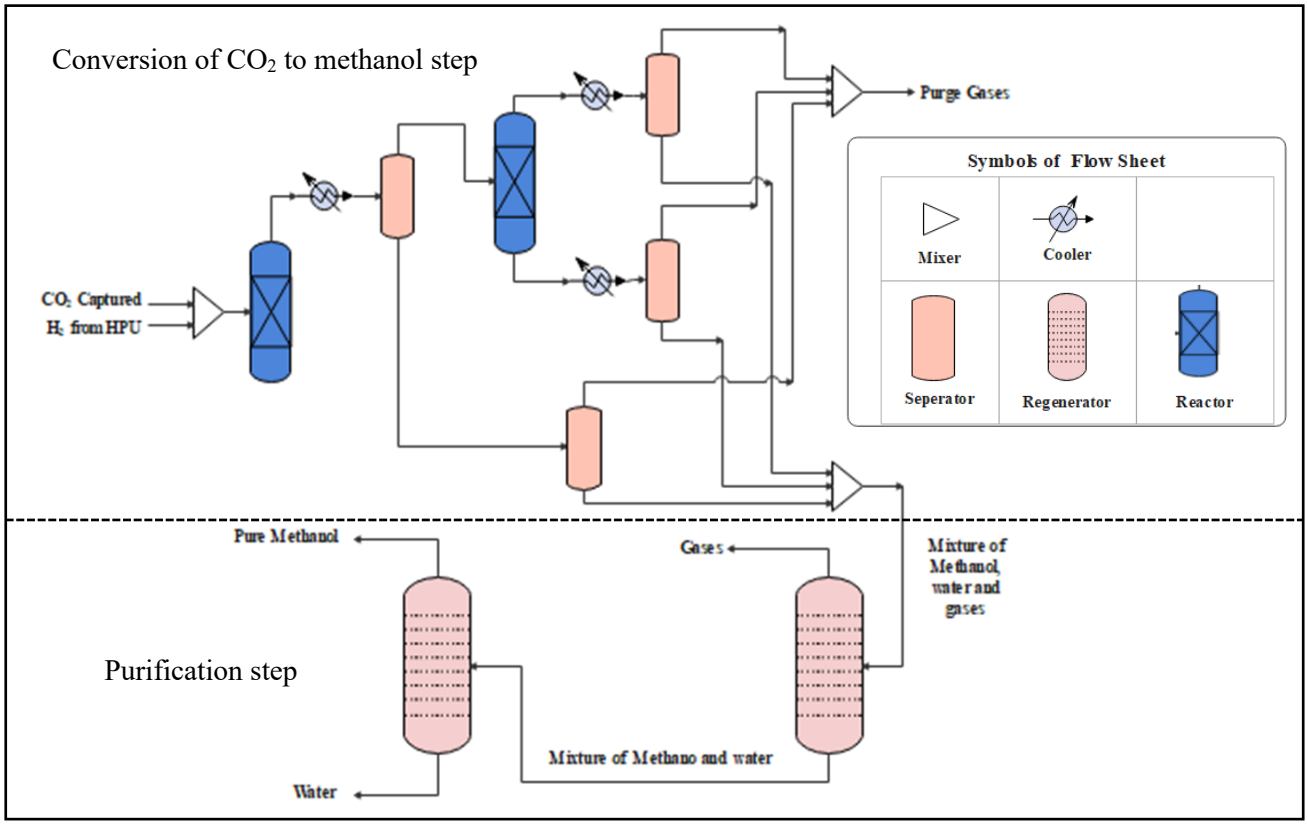

**Figure (3):** simple flow sheet of methanol production plant.

### *2.3.2. Process specification and modeling*

Figure (4) describe the simulation of methanol production plant on Aspen HYSYS. The feed of carbon dioxide at 40°C and 20 bar was mixed with the hydrogen at 25°C and 20 bar (mole ratio of $H_2/CO_2$ is 3/1). The mixture passed through compressor then heater to reach the specification of entering steam to reactor-1 (stream 4-4). In reactors, $CO_2$ converted to methanol. All the products from reactor-1 are vapor and passed through cooler and then separator-3 for separating methanol as a liquid from the bottom and unreacted gases ($CO_2$ and $H_2$) from the top to enter the second reactor (reactor-2). The top stream of separator-3 passed through compressor-3 to reach the specification of entering steam to reactor-2. The bottom stream of separator-3 passed through valve and then separator-4 for separating methanol as a liquid from the bottom and unreacted gases from the top. In reactor-2, the amount of methanol production was increased, the products from the top and bottom of reactor passed through cooler and then separator (seperaot-5 and separator-6) for improving the separation of methanol from unreacted gases.

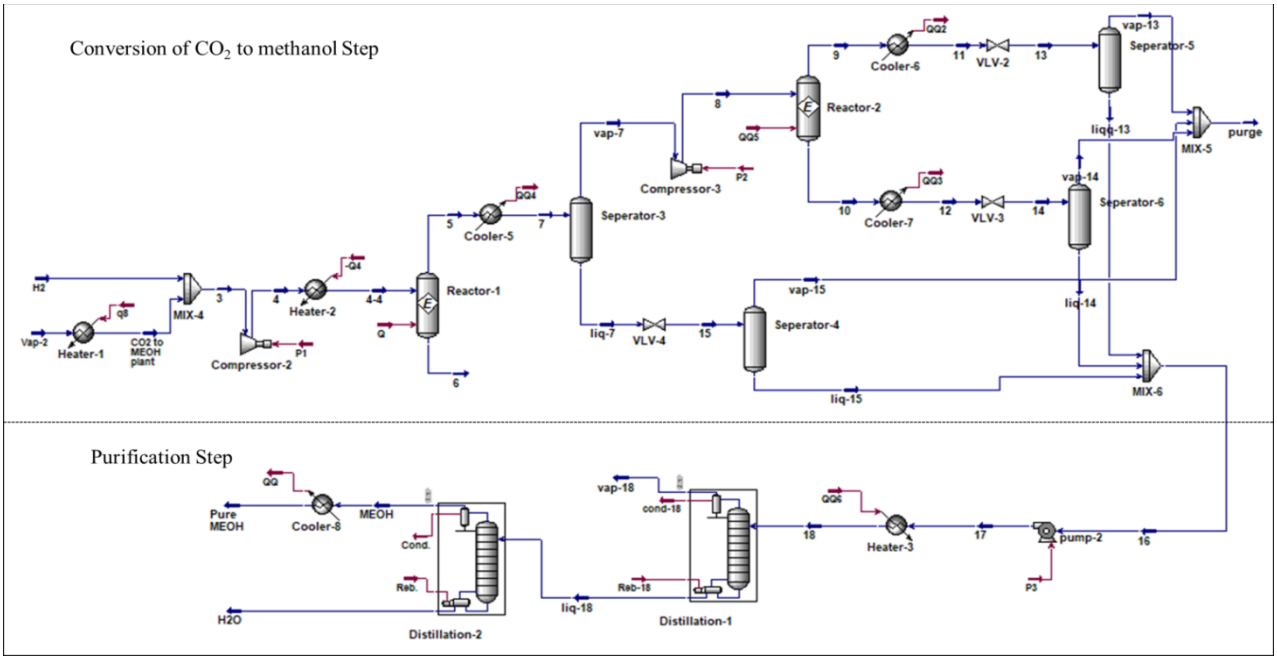


**Figure (4):** modelling methanol production plant on Aspen HYSYS

The top steams of sepearor-4, seperaot-5 and separator-6 are unreacted gases; therefore they collected in mixer-5 for purging. The bottom steams of sepearor-4, seperaot-5 and separator-6 are impure methanol, they collected in mixer-4 for purification step.

For purification step, the mixture of liquid methanol is pumped and heated to reach the specification of entering steam to distillation-1. In the first distillation tower, light compounds separated from the top (Vap-18) and methanol with water separated from the bottom. The bottom product from first distillation tower entered to the second distillation tower for producing pure methanol as a vapor from the top. The top stream temperature of distillation-2 was reduced for obtaining methanol as a liquid product by using cooler-8. The bottom stream of distillation-2 is separated water. In process modeling, all pumps and compressors were selected

with adiabatic efficiency of 75%. Table 8 and Table 9 describe specifications of different streams and the main equipment in methanol production plant, respectively.

**Table 8**
The specifications of streams in methanol production Plant

| Specifications (unit) | $H_2$ stream | 4-4 stream | 7 stream | 8 stream | 13 stream | 14 stream | 18 stream |
|---|---|---|---|---|---|---|---|
| Temperature(°C) | 25 | 183.6 | 10 | 130.9 | -38.95 | -26.19 | 57.8 |
| Pressure (KPa) | 2000 | 5780 | 5780 | 16210 | 8000 | 8000 | 400 |

**Table 9**
The specifications of main equipment in methanol production Plant

| Specifications (unit) | Reactor-1 | Reactor-2 | Distillation Tower-1 | Distillation Tower-2 |
|---|---|---|---|---|
| Temperature(°C) | 183.6 | 130.9 | 51.8 | 51.8 |
| Pressure (KPa) | 5780 | 16210 | - | - |
| Condenser pressure (KPa) | - | - | 400 | 500 |
| Reboiler pressure (KPa) | - | - | 400 | 320 |
| Number of stages | - | - | 10 | 20 |
| Reflux ratio | - | - | 0.5 | - |

## 3. Methodology of environmental analysis

### 3.1. Environmental analysis of $CO_2$ capture plant

After simulation of $CO_2$ capture plant on Aspen HYSYS, environmental analysis can be estimated by using the following estimated amount of $CO_2$:

Estimated amount of $CO_2$ in stream of sweet gas by HYSYS, symbolized by letter A.

Estimated amount of $CO_2$ in stream of Vap-2 by HYSYS, symbolized by letter B.

Estimated amount of $CO_2$ in stream of total flue gas by calculation mentioned in section 2.1, symbolized by letter C.

Amount of $CO_2$ in stream of sweet gas is considered emissions of $CO_2$ after capturing process (symbolized by A). Amount of $CO_2$ in stream of Vap-2 which is considered total amount of $CO_2$ captured from simulation plant, is taken as a feed for simulation of methanol production plant (symbolized by B). Amount of $CO_2$ in stream of total flue gas is considered emissions of $CO_2$ before capturing process (symbolized by C). It must be mentioned that all estimated amount used by unit of ton/y

For calculating percent of $CO_2$ emissions after capturing process, the following formula is used:

$$CO_2 \text{ emissions after capturing process } \% = \frac{A}{C} * 100 \quad (1)$$

### 3.2. Environmental analysis of methanol production

After simulation of methanol production plant on Aspen HYSYS, environmental analysis can be estimated by using the following:

Estimated amount of $CO_2$ in stream of sweet gas by HYSYS, symbolized by letter A.

Estimated amount of $CO_2$ in stream of total flue gas by calculation mentioned in section 2.1, symbolized by letter C.

Estimated amount of $CO_2$ in stream of purge by HYSYS, symbolized by letter D.

Estimated amount of $CO_2$ in stream of Vap-18 by HYSYS, symbolized by letter E.

Estimated amount of methanol in stream of Liq-18 by HYSYS, symbolized by letter F.

Estimated amount of methanol in stream of pure methanol by HYSYS, symbolized by letter G.

Estimated flow rate of Liq-18 stream, symbolized by letter H.

Estimated flow rate of pure methanol stream, symbolized by letter I.

Amount of $CO_2$ in stream of sweet (symbolized by A) and amount of $CO_2$ in stream of total flue (symbolized by C) are explained in section 3.1. Amount of $CO_2$ in stream of purge is considered

emissions of $CO_2$ after methanol production (symbolized by D). Amount of $CO_2$ in stream of Vap-18 is considered emissions of $CO_2$ after first stage of methanol purification (symbolized by E). Amount of methanol in stream of Liq-18 is considered total amount of methanol solution (methanol mixed with water) produced after first stage of methanol purification (symbolized by F). Amount of methanol in stream of pure methanol is considered total amount of pure methanol produced from all over process (symbolized by G). Flow rate of Liq-18 stream is considered total flow rate quantity of stream of Liq-18 (symbolized by H). Flow rate of pure methanol stream is considered total flow rate quantity of stream of pure methanol (symbolized by I). It must be mentioned that all estimated amount used by unit of ton/y

For calculating percent of $CO_2$ emissions after only methanol production plant, the following formula is used:

$$CO_2 \text{ emissions after methanol plant } \% = \frac{(D+E)}{C} * 100 \quad (2)$$

For calculating percent of reduction of $CO_2$ emissions after methanol production plant (environmental efficiency of overall process), the following formula is used:

$$\text{Reduction of } CO_2 \text{ emissions after all over process of methanol production } \% = \frac{C-(A+D+E)}{C} * 100 \quad (3)$$

For calculating ratio of $CO_2$ tones/one tone methanol, the following formula is used:

$$CO_2 \text{ tones/one tone methanol} = \frac{(A+D+E)}{I} \quad (4)$$

For calculating purity of methanol in Liq-18 stream, the following formula is used:

$$\text{Purity of methanol in Liq-18 stream } \% = \frac{F}{H} * 100 \quad (5)$$

For calculating purity of methanol in pure methanol stream, the following formula is used:

$$\text{Purity of methanol in pure methanol stream } \% = \frac{G}{I} * 100 \quad (6)$$

## 4. Results and discussions

### *4.1. Target amount of $CO_2$ capture*

After calculation of $CO_2$ emissions from previous mentioned refinery plant (see section 2.1), it is found that estimated amount of $CO_2$ in stream of total flue gas, symbolized by letter C, is approximately 1233617 ton/y.

### *4.2. Amount of $CO_2$ captured*

According to process modeling of $CO_2$ capture plant by using Aspen HYSYS V.12 as simulation program software and previous specification (see section 2.2.2). It must be mentioned that recovery of $CO_2$ in absorber is 0.9999 mole fractions, and using regenerator achieved 0.9985 mole fractions of $CO_2$ removal. Table 10 shows the specifications of outlet vapour stream from $CO_2$ capture plant (sweat gas and Vap-2). It was found that the estimated amount of $CO_2$ in stream of Vap-2 by HYSYS, symbolized by letter B, is approximately 1217424 ton/y. Therefore, the results of overall process modeling showed that approximately 99% $CO_2$ emissions were captured ($CO_2$ removal efficiency from all over $CO_2$ capture process).

**Table 10**
The specifications of outlet vapour stream from $CO_2$ capture plant.

| Specifications | Sweat gas stream | Vap-2 stream |
|---|---|---|
| Temperature(°C) | 39.97 | -98.28 |
| Pressure (KPa) | 100 | 101 |
| Mass flow rate (Kg/h) | 528993.795 | 152224.323 |
| $CO_2$ (mass%) | 0 | 0.9997 |
| $H_2O$ (mass%) | 0.0391 | 0 |
| MEA (mass%) | 0.0003 | 0 |
| $N_2$ (mass%) | 0.9197 | 0.0003 |
| Argon (mass%) | 0.0052 | 0 |
| $H_2S$ (mass%) | 0 | 0 |
| $O_2$ (mass%) | 0.0357 | 0 |
| $H_2$ (mass%) | 0 | 0 |
| Total mass fraction | 1 | 1 |

### *4.3. Production of methanol*

According to process modeling of methanol production plant by using Aspen HYSYS V.12 as simulation program software and previous specification (see section 2.3.2). Table 11 shows the specifications of streams (Purge, Vap-18, Liq-18 and Pure MEOH) from methanol production plant.

**Table 11**
The specifications of streams of methanol production plant.

| Specifications | Purge Stream | Vap-18 Stream | Liq-18 Stream | Pure MEOH Steam |
|---|---|---|---|---|
| Temperature(°C) | -37.52 | -4.93 | 122.9 | 40 |
| Pressure (KPa) | 800 | 400 | 400 | 320 |
| Mass flow rate (Kg/h) | 22222.4 | 5197 | 145724.55 | 93088 |
| $CO_2$ (mass%) | 0.8279 | 0.9957 | 0 | 0 |
| $H_2O$ (mass%) | 0 | 0 | 0.3612 | 0 |
| $N_2$ (mass%) | 0.002 | 0 | 0 | 0 |
| Argon (mass%) | 0 | 0 | 0 | 0 |
| $H_2S$ (mass%) | 0 | 0 | 0 | 0 |
| $O_2$ (mass%) | 0.0001 | 0 | 0 | 0 |
| $H_2$ (mass%) | 0.1492 | 0.0001 | 0 | 0 |
| CO (mass%) | 0.0204 | 0 | 0 | 0 |
| Methanol (mass%) | 0.0004 | 0.0042 | 0.6388 | 1 |
| Total mass fraction | 1 | 1 | 1 | 1 |

It is found that the estimated amount of methanol in stream of Liq-18 (symbolized by letter F), and Estimated amount of methanol in stream of pure methanol (symbolized by letter G) are nearly the same (equal to 744654 ton/y). However, the purity of each stream, calculated by formula (5) and formula (6), are 64%, 99.99%, and respectively.

### *4.4. Comparison the obtained results with previous work*

Figure (5) shows comparison $CO_2$ removal efficiency obtained from our simulation of $CO_2$ capture with that from previous work. The result proved that our methodology achieved higher removal efficiency than results of previous works which used the same technology of capturing.

Figure (6) shows comparison amount of $CO_2$ and $H_2$ of feed and methanol produced from our simulation of methanol production plant with previous work that applied the same technology.it is found that amount of methanol produced depend on amount of $CO_2$ entering. As amount of $CO_2$ entering the feed increased, amount of methanol produced increased. Therefore, our methodology achieved great result.

Figure (7) show comparison purity of methanol obtained from our simulation with that from mentioned previous work. The result proved that our methodology achieved higher methanol purity than results of mentioned previous works.

### *4.5. Environmental analysis*

#### *4.5.1. $CO_2$ emissions results from $CO_2$ capture plant*

For calculation of $CO_2$ emissions results from $CO_2$ capture plant, formula (1), illustrated in section 3.1, is used. Therefore, the percent of $CO_2$ emissions after capturing process is only 0.0002%.

#### *4.5.2. $CO_2$ emissions results from methanol production plant*

For calculating the $CO_2$ emissions from only methanol production plant, formula (2), illustrated in section 3.2, is used. Therefore, the percent of $CO_2$ emissions from only methanol production plant is only 15.287%.

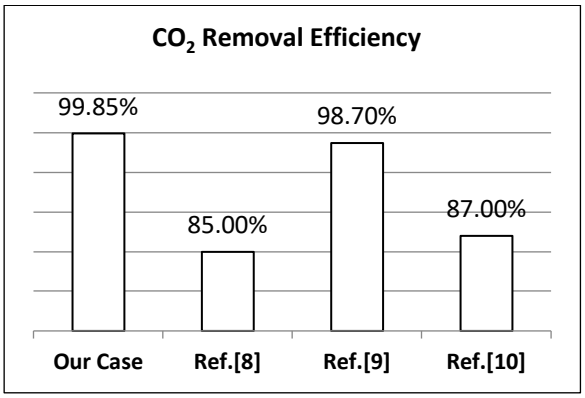


**Figure (5):** comparison $CO_2$ removal efficiency obtained from our simulation of $CO_2$ capture with that from previous work.

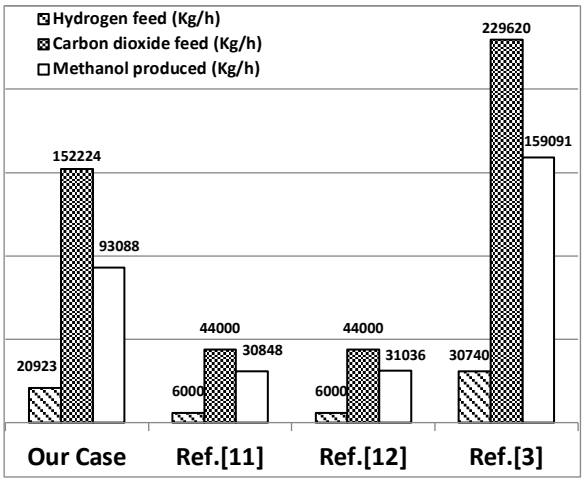


**Figure (6):** comparison $CO_2$ feed, $H_2$ feed and methanol produced from our simulation of methanol production plant with previous work.

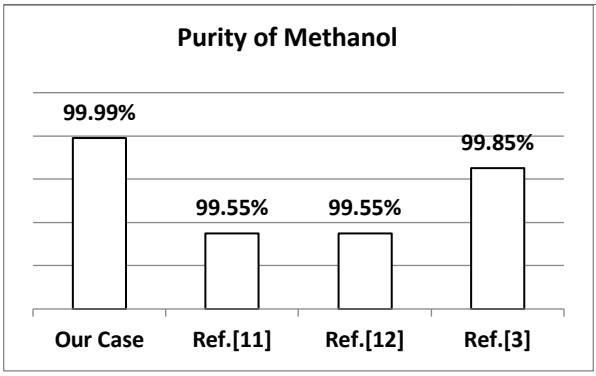


**Figure (7):** comparison purity of methanol obtained from our simulation with that from previous work.

#### *4.5.3. $CO_2$ emissions results from all over process of methanol production*

The sources of $CO_2$ emissions after all over process of methanol production came from $CO_2$ emissions in streams of sweet gas (symbolized by A), purge (symbolized by D) and vap-18 (symbolized by E). Therefore, amount of $CO_2$ emissions after all over process of methanol production is calculated by summation (A+D+E). The results show that total amount of $CO_2$ emissions, which resulted from overall process, calculated to be 188582.3 ton/y.

For calculating percent of reduction of $CO_2$ emissions after all over process of methanol production (environmental efficiency of overall process), formula (3), illustrated in section 3.2, is used. The results show 84.7 % reduction of $CO_2$ emissions. These support environmental aspects.

#### *4.5.4 Comparison $CO_2$ tones/one tone methanol of our work with previous work*

For calculating ratio of $CO_2$ tones/one tone methanol, formula (4), illustrated in section 3.2, is used. Therefore, ratio of $CO_2$ tones/one tone methanol is calculated to be 0.26. Table 12 shows comparison between $co_2$ tones/one tone methanol of our work and reference [3].

**Table 12**
Comparison between $CO_2$ tones/one tone methanol of our work and previous work

| Cases | $CO_2$ tones/one tone methanol |
|---|---|
| Our Case | 0.26 |
| Reference [3] | 1.467 |

The results proved that total $CO_2$ emissions produced from our simulation plant for one tone of methanol production is lower than that of reference [3] by 82.3%.

## 5. Conclusion

$CO_2$ emissions are considered a great catastrophe in the world. This paper presented actual solution for reduction $CO_2$ emissions of refining plant in Egypt, which produced huge amount of $CO_2$ emissions. The results showed that more than 99.99% of these $CO_2$ emissions were reduced by applying our methodology of $CO_2$ capture. Additionally, our methodology of methanol production achieved approximately 744654 ton methanol/year with 99.99% purity. Also, environmental analysis of all over process result shows that there is 84.7 % reduction of $CO_2$ emissions before $CO_2$ capturing. As well as, comparisons proved that total CO2 emissions produced from our simulation plants for one tone methanol is 82.3% lower than that of reference [3].

**Conflicts of interest**

There are no conflicts to declare.

**Formatting of funding sources**

This research didn't receive any fund from any organization.

**Table of abbreviation**

| | |
|---|---|
| DMFC | Direct methanol fuel cell |
| MEA | Monoethanolamine |
| HPU | Hydrogen production unit |
| $\Delta T_{min}$ | Minimum approach temperature |
| $\Delta T$ | Delta temperature |

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