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Ahmed Nazmus Sakib
Dept. of Aerospace and Mechanical Engineering, University of Oklahoma, Norman, OK 73019, USA.

Ahnaf Tahmid Shabab
Dept. of Chemical Engineering and Polymer Science, Shahjalal University of Science and Technology

Firoz Ahmed
Dept. of Chemical Engineering and Polymer Science, Shahjalal University of Science and Technology

Ashiqur Rahman
Center for Midstream Management and Science, Lamar University, Beaumont, TX 77705, USA.

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ORIGINAL STUDY

Optimization of Carbon Capture in Hydrogen Production Via Steam Reforming: A Simulation-based Case Study

Ahmed N. Sakib [a,*], Ahnaf T. Shabab [b], Firoz Ahmed [b,c,**], Ashiqur Rahman [d]

[a] Dept. of Aerospace and Mechanical Engineering, University of Oklahoma, Norman, OK 73019, USA
[b] Dept. of Chemical Engineering and Polymer Science, Shahjalal University of Science and Technology, Bangladesh
[c] Dept. of Chemistry, Wayne State University, 42 W Warren Ave, Detroit, MI 48202, USA
[d] Center for Midstream Management and Science, Lamar University, Beaumont, TX 77705, USA

Abstract

Hydrogen has been considered a future energy carrier for decades and the demand for hydrogen in refineries is always upward due to the revival of new technologies. The steam methane reforming method is frequently employed because of its high hydrogen generation efficiency at a cheap cost and minimal environmental footprint. However, depending on the type of feedstock, one unit of hydrogen generates 9−10 units of CO_2 that need to be treated for environmental sustainability. Therefore, the optimization of hydrogen production and CO_2 capture is critical to address the issue. The simulation research was conducted to anticipate and optimize steam reforming using Aspen HYSYS. A conversion-type reactor was used to develop this simulation-based model. The primary goal of this work is to investigate and optimize hydrogen production efficiency while mitigating CO_2 by varying process parameters. The CO_2 capture efficiency was investigated at the different yields for hydrogen production and a maximum of 98.8 % absorption of the CO_2 was achieved using the carbon capture system proposed in the current study. Later, the Aspen Energy Analyzer tool revealed potential improvements for energy and cost optimization.

Keywords: Aspen HYSYS, SMR, Pinch analysis, PCC, Hydrogen, Carbon capture, MEA-MDEA

1. Introduction

The primary source of electricity generation and greenhouse gas emissions around the globe is fossil fuel-fired power plants. Coal-fired power plants account for 38% of the global electricity generation and 38% of CO_2 production, leading to global warming [1,2]. The recent release of the Intergovernmental Panel on Climate Change (IPCC) in 2022 stated that global warming resulted in widespread shrinkage in cryosphere and ocean warming absorbing more than 90% of excess heat in the climate system. Also, global warming is likely to exceed 1.5 °C between 2030 and 2052 if it continues to increase at the current rate [3]. The ever-surging demand for energy also demands the need for investigations around cost-effective and sustainable energy production to mitigate the climatic crises. This need is critical to industries such as petroleum refineries due to their high energy consumption. In the refinery process, the most energy-consuming processes are crude distillation, followed by the hydrotreater, reforming, and vacuum distillation, emitting more than 1100 million tons of CO_2 per year [4,5]. In addition, transportation and electricity sectors contributed to more than 60 % CO_2 emission reported elsewhere [6]. Therefore, the inclusion of CO_2 capture and storage (CCS) in conventional-fossil fuel-based hydrogen production processes can generate tens of millions of dollars (i.e., a constitute

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* Corresponding author.
** Corresponding author at: Dept. of Chemical Engineering and Polymer Science, Shahjalal University of Science and Technology, Bangladesh.
E-mail addresses: nazmus.sakib@ou.edu (A.N. Sakib), fahmed2@wayne.edu (F. Ahmed).

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for building materials, formation of synthetic fuels) in the long run for refineries [7–9] and serve as a climate change diminution approach.

Due to the highly reactive nature of hydrogen atoms, it instantaneously reacts with other elements [10,11]. Therefore, despite being abundant in nature, hydrogen can never be found in its purest form [12]. So, the chemical compounds containing hydrogen must be decomposed or reformed to get pure hydrogen as gas or liquid. Hydrogen is considered a key raw ingredient for the petroleum and petrochemical industries and a byproduct of numerous petroleum refining and chemical manufacturing processes such as chlorine synthesis, photobiological water splitting, and others [13]. Therefore, substantial measures [14–18] have been being taken not only by international energy agencies [19] but also by different states and industries to establish a hydrogen economy.

Hydrogen is regarded as one of the future's clean energy vectors [5]. It is an excellent alternative to produce lighter, cleaner fuels and reduce our reliance on fossil fuels. The lower heating value or LHV of hydrogen combustion is approximately 143 MJ/kg, which is three times that of petroleum [20]. Hydrogen can be used in fuel cells, devices that convert raw hydrogen into electrical energy to fuel electric automobiles and power plants [21], and thus can serve as a replacement for combustion engines. Currently, in the USA alone, hydrogen production is approximately 14 million tons per year (MT/y), which is enough to power about 3 million cars or about 8 million homes [22].

Among the prominent technologies for hydrogen production are the steam reforming [23] and electrolysis [24,25]. Steam reforming with and without conventional CO_2 capture technologies are termed blue hydrogen and grey hydrogen, respectively. On the other hand, hydrogen produced through water electrolysis using renewable electricity is called green hydrogen [26,27]. Using an electric current, electrolysis separates water into its constituent parts [25]. The production of green hydrogen through electrolysis is an expensive process even after using other renewable energy sources such as wind and solar energy to drive the electrolysis process [28]. Moreover, according to Department of Energy (DOE) reports, the capture of CO2 is an expensive and technologically challenging process costing more than 400 million dollars per unitof the gas captured [28,29]. There are several methods for hydrogen production such as partial oxidation that produces hydrogen and carbon monoxide by combining oxygen with hydrocarbons (such as natural gas, naphtha, petroleum coke, or coal) [31–34] and ammonia decomposition that separates ammonia into its essential components, hydrogen, and nitrogen [35]. Additionally, the emerging technologies for hydrogen production include gasification [36] or pyrolysis [37], or biomass fermentation with microorganisms [38,39], and newly developed photo-electrochemical water splitting [40] and thermochemical processes, such as microbial electrolysis [41] for splitting of water into H_2 and O_2 with lower energy compared to conventional electrolysis [42].

Among all these methods, steam methane reforming is a well-matured technology with an efficiency of over 75–85 % [43–45], the highest of any commercial hydrogen generation process, and runs at or near its maximum capability [46]. Moreover, it is the most often employed technique where natural gas (methane) or other light hydrocarbons such as ethane or propane reacts with steam in the presence of a catalyst. This hydrogen production process is comparatively cheaper than the other methods and is expected to continue to dominate the production platforms in the upcoming decades.

Table 1. Stream data for pinch analysis.

Stream No	Stream Type	Start Temperature (°C)	Target Temperature (°C)	Heat Load **ΔH** (kW)
1	Cold	30	247.7	$5.45*10^8$
2	Hot	222.6	30	$2.85*10^7$
3	Hot	316.7	40	$3.096*10^8$
4	Hot	207.8	99.96	$5.31*10^8$

Table 2. CO_2 removal rate at different reformer yield.

Reformer Yield	H_2 Production (kgmole/hr)	Flue Gas Formation (kgmole/hr)	CO_2 Formation (kgmole/hr)	CO_2 Removal (%) in Absorber	Amine Used (kgmole/hr)
80	11,520	8640	2880	100	14,450
70	10,080	9360	2520	100	15,000
60	8640	10,080	2160	99.99	16,200

The well-developed natural gas distribution system in the United States is a major determinant of the overall cost of hydrogen production which makes this particular process most economically feasible over the other production process. However, this process owing to a few constraints and challenges including high carbon products released (~ 7 kg CO_2/ kg H_2 [20]) which is against the goal of the recent CO_2 production [27]. Nowadays, the government, research communities, and industries are more concerned with environmentally benign technologies and CO_2 mitigation, being the primary source of greenhouse gas, which must be captured before release. Moreover, CO_2 is acidic, and as a result, it cannot be sequestrated underwater or in the ocean as it may reduce the pH of the water which would adversely affect the ecohydrology [47]. Furthermore, to achieve environmental sustainability, industries must minimize the CO2 emission to the atmosphere [48]. Therefore, adequate CO2 capture and storage technologies are essential to protect the atmospheric environment from potential CO2 pollution. Carbon capture and storage can be classified as follows-i) carbon-positive, ii) carbon-neutral, and iii) carbon–negative processes [49–51]. Carbon–positive processes continue to release CO2 into the atmosphere, whereas near-carbon-neutral processes do not release any CO2 and carbon–negative processes reduce the amount of CO2 that is already present in the atmosphere [52].

Since the steam methane reforming (SMR) will continue to dominate the production of hydrogen for at least the next decade, it is essential to maximize its production and minimize CO2 emissions from this technology. Numerous studies [20,28,36,53–57] have been done on the production of hydrogen using steam reforming and capturing the emitted CO_2 from SMR. While there are different methods for CO_2 capture, 'Post-Combustion Capture (PCC)' which is one of the three major methods has shown superiority over the other methods since it offers retrofitting without serious alteration to the existing plant design and configuration [57,58]. In addition, PCC has some major advantages including capturing more than 90 % of the CO_2 and ensuring the highest purity in the captured CO_2. Aqueous amine-based technology [30] is a chemical absorption process recognized as the most mature for PCC of CO_2 [59,60]. Studies have shown that amine based CO_2 absorption method can capture up to 100 % of the CO_2 present in the flue gas while maintaining the purity over 99 % [61,62]. Besides this, amine-based solvents are quite inexpensive as well as widely available and thermally stable compared to other methods of CO_2 capture [62]. Aqueous mono-ethanolamine (MEA) and Methyl Diethanolamine (MDEA) are considered fundamental solvents for PCC technology because of their high separation selectivity for CO_2 and rapid rate of reaction [59,60,63]. The major barriers faced at the implementation of CCS is the high cost for carbon capture and the post carbon capture procedure [8,9,61,64]. A properly integrated heat exchanger network system will reduce this cost [61,64]. High purity of carbon dioxide will lead to the reduction in production cost of the processes where CO_2 is necessary [8,9,61]. In this study, Pinch Analysis (PA) has been done in a couple of the most energy demanding streams to optimize the heat integration. This also serves to debottleneck operations, optimize utility use, and improve the energy efficiency of overall systems [65]. The multi-stage compression is performed in several phases to maintain thermal equilibrium [57]. The CO_2 capture technologies which are long been discussed are applicable for steam reforming hydrogen plants, however, only a few studies are available on removing CO_2 from flue gas though interest in the technology is growing. While several carbon capture and hydrogen production methods and strategies have been developed, this comprehensive review carefully investigates the gap in this field and describes a simulation-based method that could be a game-changer. The goal of this work is two-fold- i) to present a unique approach and set a baseline for simultaneously increasing the production of hydrogen and, ii) improving the removal of CO_2 from the SMR system.

2. Model development and process simulation

2.1. System description

The process flow diagram for the steam methane reforming considered in this study is depicted in Fig. 1. This work thoroughly investigates hydrogen production via steam reforming and the CO_2 capture that evolves during the process. The reforming reaction of methane and steam is a highly endothermic reaction. Therefore, this reaction is usually carried out at higher temperatures of 800–1000 °C and at a pressure of about 14–20 atm which are the set operating conditions. The reaction between methane and steam produces H_2 and CO in the reactor-1 with a molar ratio $CH_4 : H_2O$ of 1:3 based on the following reaction (1):

$$CH_4 + H_2O \rightarrow 3H_2 + CO \ \Delta H = 206 \text{ kJ/mol} \quad (1)$$

For fast reforming reactions, a catalyst bed reactor is usually used [66]. The catalytic reactor

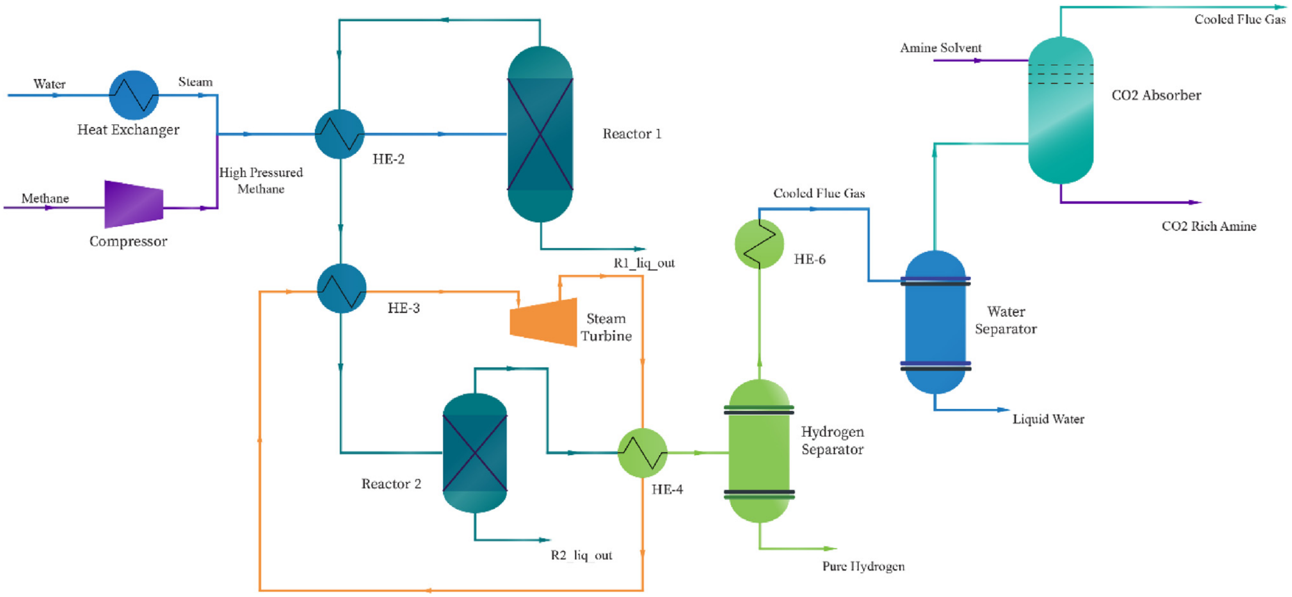

Fig. 1. Process flow diagram of the proposed steam methane reforming process.

concept has been explored for steam reforming of tars in the producer gas and to promote the water-gas shift reaction to maximize hydrogen production [66]. Also, research has been carried out to introduce a combined catalyst/sorbent system to replace three catalytic reactors. Following this reforming process, the Water Gas Shift (WGS) takes place in reactor-2 to reduce the carbon monoxide content at the outlet of reactor-1 where the SMR reaction took place. Thus, the flue gas is then fed into the reactor-2 for WGS reaction to remove the CO produced in reaction (1) and increase the hydrogen production. The WGS reaction is moderately exothermic, therefore, occurs at lower temperatures (300–400 °C) than the reaction (1) [36]. The reaction (2) follows as,

$$CO + H_2O \rightarrow H_2 + CO_2 \ \Delta H = \text{-}41 \ kJ / mol \tag{2}$$

Figure 1 along with reaction 1 and reaction 2 can be schemed in a block diagram in Fig. 2.

Afterward, the produced hydrogen is separated from the flue gas using a separator, and the rest of the flue gas is sent to a cooler to reduce the temperature followed by a water separator. About 99.72 % of the water and 1.13 % CO_2 is separated as the bottom cut of the water separator. The remaining products leave the separator as the top stream. This top stream then goes into the CO_2 absorber column where an amine solvent solution is added from the top of the column. This amine solution absorbs the CO_2 present in the flue gas and leaves the column from the bottom as the CO_2 rich solution and the clean flue gas leaves the column as the top product of the carbon capture column.

2.2. Model assumptions

Some of the key assumptions used in this process modeling are:

- All components possess adiabatic boundaries.
- Kinetic exergy and potential exergy overlooked for all the system components.
- Usage of catalyst is considered.
- Formation of coke is overlooked due to negligible concentration.
- The outlet stream temperature of the reactors is considered as reactor's temperature.
- Tray efficiency in absorption column is assumed to be 100 %.

Fig. 2. Input and output scheme of the SMR process.

2.3. Model description

Typically, a steam reforming process involves two successive shift reactors for hydrogen generation followed by hydrogen and carbon dioxide separators [66]. The production of hydrogen via steam methane reforming process, and simultaneous capture of CO_2 using an amine solution were investigated. The simulation-based steady-state model as shown in Fig. 1 was developed using Aspen HYSYS V12.1 and Fig. 2 illustrates the general outcome of the steam methane reforming process. Peng Robinson equations of state and Acid Gas- Chemical solvent fluid packages were used to estimate the thermodynamic properties of the components and the mixtures in the streams.

Water is heated for steam generation and a multistage compressor mechanism is employed (Fig. 1) to increase the pressure of the natural gas. The mole fraction of natural gas was considered 1 for methane. So, the gas is compressed in the first compressor and an inter-cooler is employed for cooling down the high-temperature gas. This process is repeated at least twice to ensure reproducibility. Then, methane and steam were mixed and heated in HE-2 before entering the conversion-type steam reforming reactor (reactor- 1). Conversion type reactors are the simplest type of reactor in HYSYS. Because of its simplicity it is extremely useful for designing complex reactors [67,68]. The primary focus of the study was optimization of carbon capture during steam reforming. Due to this, a simple yet configurable reactor type, such as conversion type reactors, was utilized in developing the model. The SMR is a well-established procedure, so the conversion rate was presumed based on previous research [42–44].

Here, a counter-current shell and tube configuration is assumed for all the heat exchangers. Natural gas and steam are heated-up to produce syngas $(CO + H_2)$ according to the endothermic steam methane reforming reaction-1. The water gas shift (WGS) reaction for high CO conversion is favored at lower temperatures. Therefore, the overhead product of reactor-1 was cooled using HE-2 and HE-3 and fed into the WGS reactor (reactor-2). After that, the overhead product goes into the shell side of HE-4 for cooling before going into the hydrogen splitter. Hence, a cooling stream loop was introduced around the WGS reactor.

The remaining flue gases from the Hydrogen splitter (S-1), which is not good for the environment is fed into the carbon capture and storage system (CCS). Before that the stream is cooled down and then most of the water is separated from the stream using a separator (S2) to achieve a better carbon dioxide capture. Natural and refinery gases contain acid gases like hydrogen sulfide (H_2S) and carbon dioxide (CO_2). A refinery usually consumes 1.5 %–8 % of feed as fuel depending on the complexity of operation. A refinery having capacity of 300,000 bbl per day is usually accountable for CO_2 emission of 0.8–4.2 million tons per year [69]. Natural gas can contain up to 28%hydrogen sulfide gas (H_2S), which may be considered as air pollutant near petroleum refineries and in oil and gas extraction areas [70]. Because of the corrosivity of acid gases in the presence of water, the toxicity of H_2S, and the lack of heating value of (CO_2), the gases must be purified prior to use with the aid of aqueous solutions of alkanolamines. They react reversibly with acid gases and therefore are generally used to remove them [21]. Chemical reaction processes remove the H_2S and/or CO_2 from the gas stream by chemical reaction with a material in the solvent solution [70]. Clause process [71] is one of the most popular methods for removing large quantities of H_2S where one third of the H_2S to be removed, is burnt to form sulphur dioxide. The reaction is an exothermic one. Then the produced SO_2 reacts with the unreacted H_2S to form high quality sulphur (purity >99.9%) [71].

$$2H_2S + O_2 \rightarrow SO_2 + 2H_2O\ \Delta H = \text{-}519\ kJ / mol \tag{3}$$

$$2H_2S + SO_2 \rightarrow \frac{3}{8}S_8 + 2H_2O\ \Delta H = \text{-}146\ kJ / mol \tag{4}$$

In this simulation, MEA and MDEA are used as aqueous solvents according to the industrial case. Likewise, amines and polyamines have been employed as low-cost and effective CO_2 capture support materials [72]. They offer several benefits over other CO_2 capture systems, including a reduced regeneration energy penalty when compared to aqueous amine solutions and a higher moisture tolerance when compared to some of their physi-sorbent equivalents, such as metal organic frameworks (MOFs) [67,68]. The gas-sweetening facility has twenty identical amine trains and a suitable pressure gradient across the column for an efficient CO_2 removal.

2.4. Fluid packages

2.4.1. Peng–Robinson

The Peng–Robinson equation of state (Peng and Robinson, 1976) is satisfactory for predicting the gas phase properties of CO_2 and can be used to determine the enthalpy and entropy of a fluid or fluid mixture as a function of temperature and pressure [69]. This law does not work if the gas pressure is below the triple point due to the discontinuity of physical and chemical characteristics of gases. For instance, there is no latent heat of fusion found for gases beyond the triple point. However, the enthalpy estimation of a specific gas relative to a selected state is possible by using the Peng–Robinson equation of state unless the fluid is not obeying the ideal gas law [70]. Additional terms including reduced temperature, compressibility factor and acentric factors are included in the enthalpy and entropy function where fluid does not obey ideal law [73,74]. Due to its well-developed model, accurate representation of non-ideal behavior, versatility, phase equilibria, exhaustive database, and widespread acceptance, the Peng–Robinson equation of state is frequently used as a property package in Aspen. Therefore, Peng Robinson fluid package was selected as the primary property package [74].

2.4.2. Acid gas – chemical solvent

The Acid Gas – Chemical Solvent package in Acid Gas technology supports is used to prepare the solvents including Methyl Diethanolamine (MDEA), Diethanolamine (DEA), Mono Ethanolamine (MEA), Diglycolamine (DGA), Diisopropanolamine (DIPA), Piperazine (PZ), and Triethanolamine (TEA). Additional supports are provided for multiple (>2 types) solvent blends including Sulfolane + DIPA, Sulfolane + MDEA, Sulfolane + MDEA + PZ, MDEA + MEA + DEA and any two chemicals solvent blend. The Acid Gas - Chemical Solvents package is developed with the Peng–Robinson equation of state for vapor phase and electrolyte nonrandom two-liquid (eNRTL) for electrolyte thermodynamics [73,74].

2.5. Pinch analysis

Pinch analysis is a method used to reduce the energy consumption of the process by optimizing the energy recovery methods [75,76]. It examines potential heat exchanges between cold (requiring heat) and hot (emitting heat) streams to reduce irreversibility. The process data is represented as an array of energy flows or streams as a function of heat load (or enthalpy) vs. temperature. These data are integrated for all of the plant's streams to generate composite curves, one for all “hot streams” (streams that release heat) and one for all “cold streams” (requiring heat). The point of closest approach between the hot and cold composite curves is the pinch temperature (pinch point or plain pinch), and it is the point where design is most limited [75,76]. Consequently, the energy objectives may be met by utilizing heat exchangers to recover heat between hot and cold streams by identifying this location and beginning the design process there. In fact, cross-pinch heat transfers between streams with temperatures above and below the pinch are frequently seen during the pinch study. By eliminating these exchanges through alternate pairing, the process reaches its energy goal [77].

3. Results and discussion

3.1. Effects of change in process parameters

This section discusses the outcome of the modeling and the effects of process parameters on carbon capture and H_2 production. The process optimization for efficient system functioning is described in depth. In addition, the model was used to assess the impact of modifying the most critical parameters. Some critical parameters considered include Steam to Carbon ratio (S/C), molar flow, temperature, and mole fraction. The higher the steam to carbon ratio, the lower the residual methane will be for a given reformer outlet temperature. Hence, less fuel energy is required in the furnace. Fig. 3 shows the change in the molar flow of the hydrogen produced at the splitter with the change of the S/C (at different methane flowrates).

The S/C ratio was considered from 1 to 10 and change in hydrogen production was observed. With increasing S/C ratio the production also increased. However, after reaching an equilibrium point at S/C ratio of 2 the production of hydrogen remained the same even with the increasing ratio. Thus, when the S/C ratio reached 10, there was no significant effect on the hydrogen production. The reactors used in the simulation are conversion-type reactors as

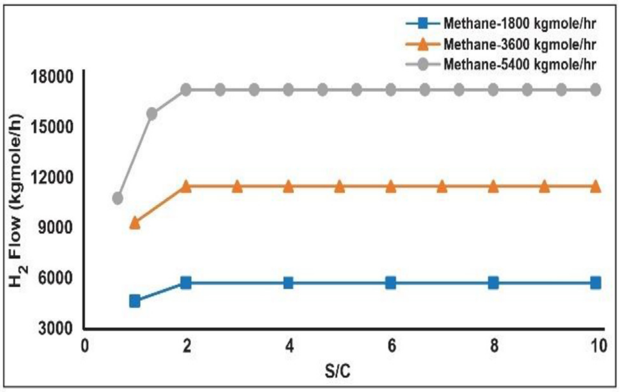

Fig. 3. Hydrogen production vs S/C.

mentioned earlier. In conversion-type reaction, the percent of conversion remains constant throughout the process. Therefore, the production did not vary after reaching an equilibrium point. The increasing S/C ratio will have a negative effect on the CCS in the later part of the production as the increasing S/C will lead to the increase in the production of flue gas and water formation. However, an optimum S/C ratio of 3 [78] was maintained for the cost-minimization of the production process.

Fig. 4 shows the variation in flow rates of liquid water and the flue gas with the variation of S/C ratio at the outlet-stream of water separator (S-2). As observed from the graph, the flow rate of liquid water increases drastically with increasing S/C. With the variation of the S/C ratio from 1 to 10, the flow rate varies between 0 and 30,420 kgmole/h. However, with the increase of S/C, the formation of flue gas did not vary that much. It reached a peak of 3605 kgmole/h at S/C of 2 and then decreased to 3419 kgmole/h. Thus, the effect of increasing S/C resulted in no significant change in the flue gas flow rate but a drastic increase in the liquid water flow rate is observed. On the other hand, the pure hydrogen production was 9360 kgmole/h at S/C of 1 as displayed in Fig. 4. The maximum conversion rate which was 11,520 kgmole/h reported when S/C ratio was 2 and remained constant after reaching this equilibrium point. This result indicates that the production of hydrogen did not vary with increasing S/C ratio. Thus, it only increases the cost of the process. Increasing S/C also has an adverse effect on the separator as the separator needs to remove more water before the flue gas is transferred to the carbon dioxide separator.

Fig. 5 shows the change in mole fraction for methane and carbon monoxide in reactor 1 with the change of the S/C. The S/C ratio was considered from 1 to 10, and the mole fraction of CO and methane gas varied from 0.22 to 0.06 and 0.05 to 0.01, respectively. The lowest point was attained when the S/C was 10.

Fig. 6 demonstrates the change in the overall UA of the heat exchangers 2 and 3 to S/C ratio, the values considered for the S/C ratio were from 1 to 10. For heat exchanger (HE)-2, the resultant UA varied from 0.1 to 2.7 kJ/C-h, respectively. The graph shows that in the initial stages, the overall UA would barely have an effect; however, with the increase in the S/C ratio from 6, the heat exchanger UA starts increasing. However, the UA was significantly affected when the S/C ratio exceeded 7, demonstrating that when S/C > 5,discernible results

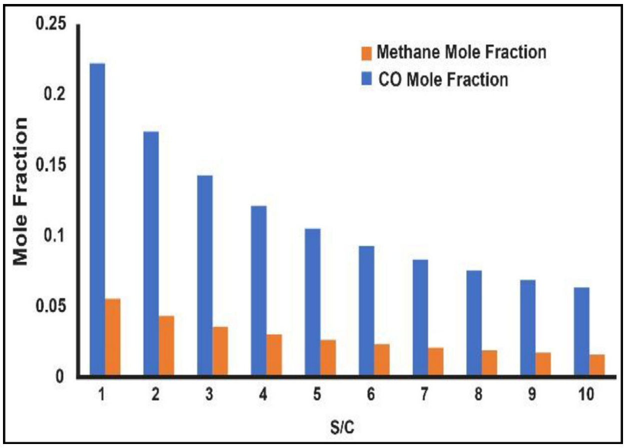

Fig. 5. Mole fraction of methane and CO in reactor 1 vs S/C ratio.

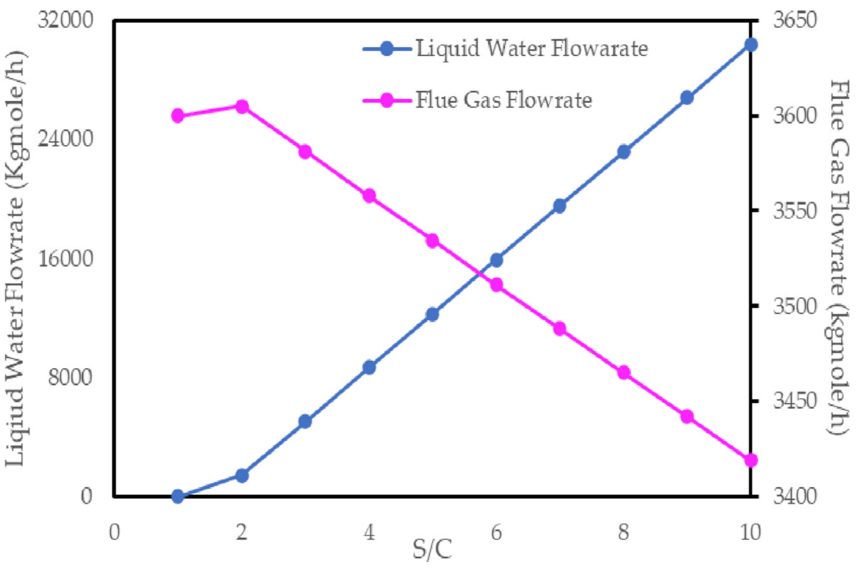

Fig. 4. Hydrogen, liquid water, and flue gas flowrate of S-2 vs S/C.

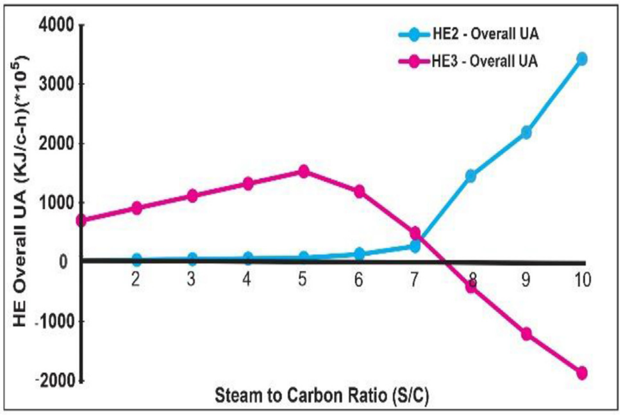

Fig. 6. HE-2 and 3 overall UA variation with S/C ratio.

were observed. At S/C ratio of 8, an abrupt peak was observed where change in the UA was recorded from 6.00E+06 to 1.50E+07 kJ/C-h. Nevertheless, the peak values of the UA were retained at 2.7E+07 kJ/C-h when S/C was set at 10. In contrast, the recorded UA values for HE-3 ranged from 8.00E+05 to −8.00E+05kJ/C-h, The UA of the heat exchanger increases with the increase in S/C up to 5.5. However, when the S/C ratio is approaching 6, a dramatic downward slope of UA was recorded with a minimum value of -2000×10^5 kJ/C-h. Here, higher overall heat transfer coefficient signifies better heat transfer between the fluids and works better where higher heat transfer is required. On the other hand, lower heat transfer suggests that the medium is better for insulation purpose [79]. The negative value of UA indicates the reverse direction of heat transfer inside the heat exchanger.

Fig. 7 demonstrate the percentage of separated liquid water in the separator S-2 with varying cooled flue temperature. The value considered for the temperature was in the range of 30–240 °C. The highest separation was almost 99.8 % which was recorded at 30 °C. Afterward, the amount of water that had been isolated began to decrease gradually. Eventually, at 190 °C, the percent of liquid water separated in S-2 became 0 (zero) and remained the same for the rest of the study. Unless the water is removed earlier before entering the absorber, this water would create barrier in the column while separating the CO_2 from the flue gas. Thus, this separation of water makes the CCS more efficient.

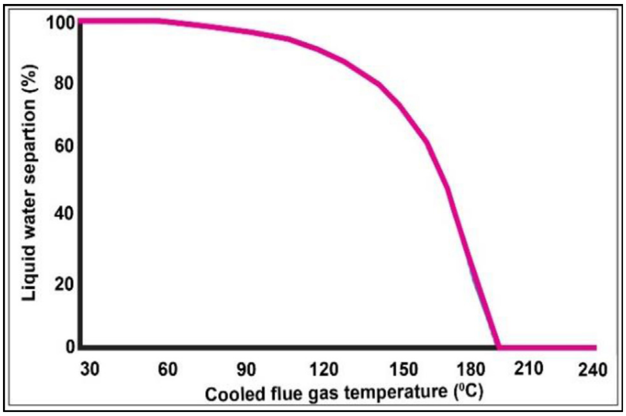

Fig. 7. Liquid water separation (%) vs Cooled flue gas temperature.

Fig. 8 indicates the significance of using a cooler beforehand the flue gas enters the Separator-2 and CO_2 absorber. As observed from the graph, with an increase in the flue gas temperature the absorption capability of the absorption column decreases. It can be observed that at lower temperatures the column performs the best, having an efficiency of capturing 100 % of CO_2 in the flue gas. The effect of flue gas's temperature on liquid water removal is already described in Fig. 6. However, it can be observed that the temperature not only affects the removal of water in separator 2 but also the CO_2 concentration in the flue gas. At lower temperature, about 2 % of CO_2 goes with water which decreases as the temperature increases.

3.2. Pinch analysis

For the system, four streams are considered for pinch analysis:

Stream 1, from the initial water to the mixer.

Stream 2, from the output of compressor 1 to the input of compressor 2.

Stream 3, from the output of the hydrogen splitter to the input of the water separator.

Stream 4, from the output steam turbine in the Rankine cycle subsystem to the water pump.

The streams are described numerically in the Table 1:

Figs. 9 and 10 present the current model's composite and grand composite curves. It should be noted that this analysis is done independently of the current heat exchanger system, using the information related to the reactors and separators. This way, the analysis can be used to either validate or improve the heat exchanger network. The pinch analysis assumes that the minimum temperature difference between the hot and cold streams is 10 °C to find a theoretical minimum for the modeled system. Heating and cooling utilities would be required outside of process exchange sections. It was revealed that there is a requirement for an additional heat exchanger for this optimized heat integration network which is the major contributor to the increase in the overall cost. This leaves room for further optimization of the overall process.

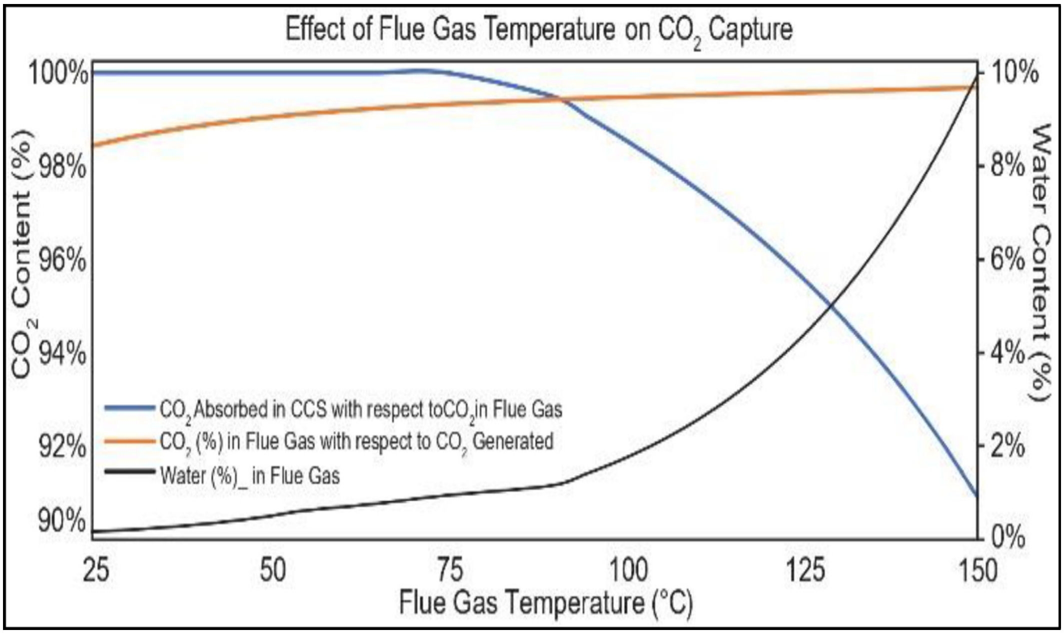

Fig. 8. Effect of flue gas temperature on CO_2 capture and water separation.

According to the pinch analysis findings, this system's theoretical minimum hot utility requirement is 245 kW. However, after the heat exchanger network design, the requirement for the hot utility was reduced to 0 kW. Therefore, it can be demonstrated that the current heat exchanger network is adequate to save the hit energy possibly through heat exchange. As for the requirement for cooling utility, it theoretically required about 90 MW which was optimized by 0.3 % requiring 99.7 % of the required cooling utility. If the system has not yet been constructed and is still in the design phase, it may be recommended to use the alternative network to save money on the heat exchanger network.

3.3. Reformer 1 yield variation

Conversion type reactors are the simplest type of the reactor in Aspen HYSYS [80,81]. Due to their simplicity the yield needs to be defined at the beginning of the designing process leaving less

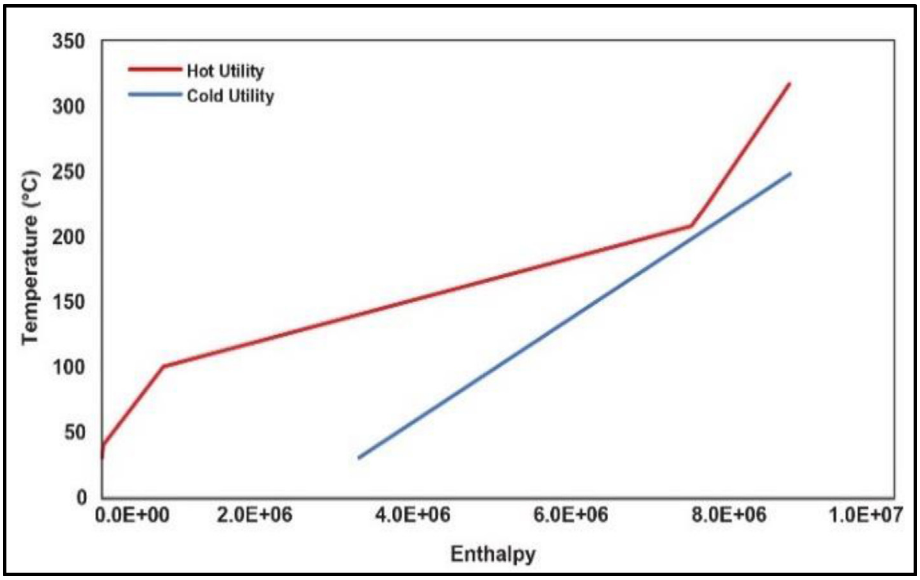

Fig. 9. Composite curve of hot utility and cold ulity comparision where enthalpy is placed as a function of temperature.

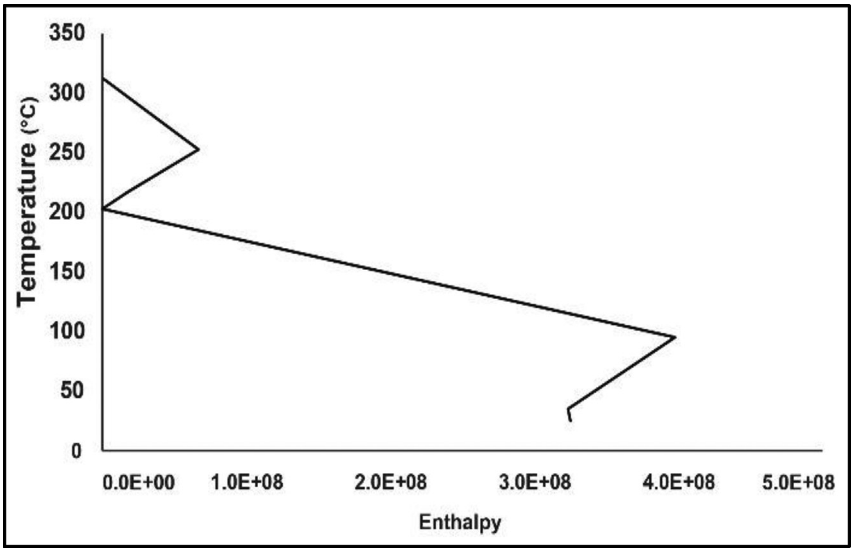

Fig. 10. Graphical representation of grand composite curve.

room for investigating the effect of the change of process parameters on the final product. However, the steam methane reforming process is a well matured process, and the overall conversion efficiency is about 65–85 % [45]. Therefore, the yield of the reformer 1 was varied within an acceptable conversion yield of the reforming process and the H2 production, flue gas formation and CO2 capture process were investigated and mentioned at Table 2.

3.3.1. Multi-stage compression

Initially, methane was compressed before mixing with water and feeding into the reactor. The compression of methane was done in multiple stages because compression generates heat. Therefore, the compressed gas needs to be cooled before sending into the next compressor, making the compression less adiabatic, but more isothermal.

The effect of compressing methane in a multi-stage process to single-stage compression is shown in Fig. 11. As observed from the graph, the rise in temperature of the gas in the three-stage compression is not higher than single stage compression. The usage of interstage cooling also has a significant effect on compression. This phenomenon resulted in a less adiabatic and more isothermal condition because there is no significant increase in temperature.

3.4. Carbon capture system (CCS)

Different absorbents (MDEA, MEA, Propylene carbonate) are simulated to determine the most efficient solvent for the current carbon capture system. Upon reviewing a wide range of research work [58–63,72,82–88], rate of CO_2 capture depends on the temperature of the solvent. However, absorption

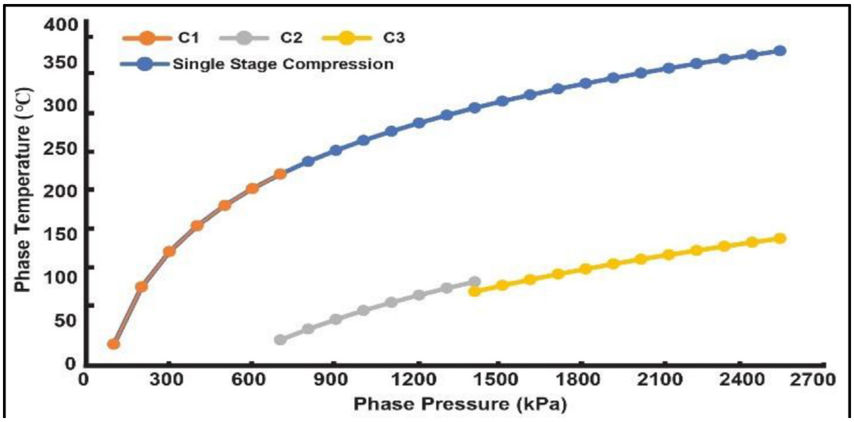

Fig. 11. Multistage vs single stage compression (temperature effect).

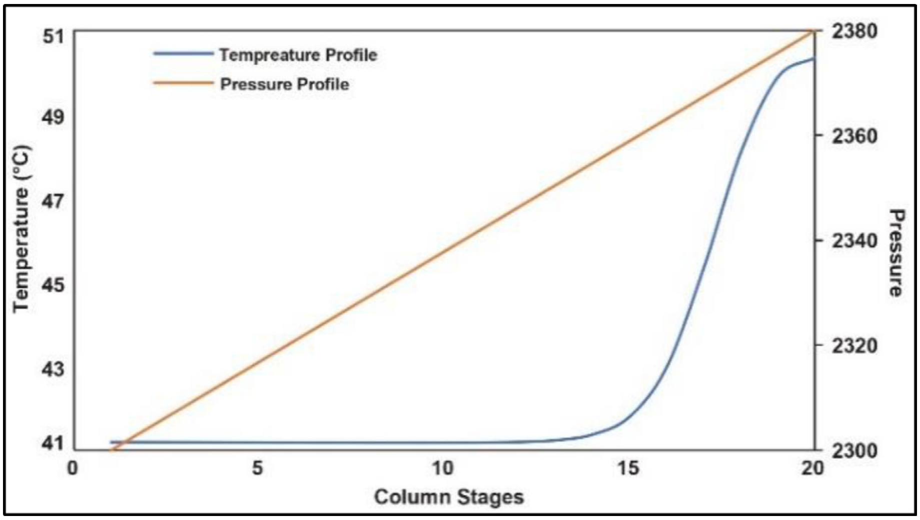

Fig. 12. Temperature and pressure profile of the absorption column.

increases with increasing temperature and decreases once a certain temperature is reached. Several studies have been conducted to find out the optimum temperature for both solvent and flue gas to achieve the maximum CO_2 capture [58,82]. Therefore, the flue gas, which was released at a higher temperature, needed to be cooled down for efficient absorption. Absorption of CO_2 varies depending on the characteristics of the solvents. Therefore, a suitable solvent selection is important to ensure the highest efficiency of CO_2 absorption. Two of the most used amines in large scale industrial production are MEA, and MDEA which have shown higher percentage of CO_2 absorption [84]. Consequently, these two as well as Propylene Carbonate, which is also used as a solvent, were considered for further case study in order to select the most suitable amine.

Fig. 12 indicates the variation of absorption column temperature and pressure profile. As observed from the graph, the temperature of the column started rising around stage 13. On the other hand, the pressure profile throughout the column remained linear. Fig. 12 provides information on the concentration of CO_2 at different stages of the absorption column. The graph revealed that there was no CO_2 present above stage 12 and the concentration raised rapidly towards the bottom stages of the column. It showed that the maximum amount of CO_2 was in the bottom stage of the column indicating that the amine was absorbing the CO_2 in the flue gas.

Fig. 13 compares the percentage of CO_2 absorbed in the solvent along with the change in concentration of different solvents (using single amine only). Each of the solvents was studied under the same

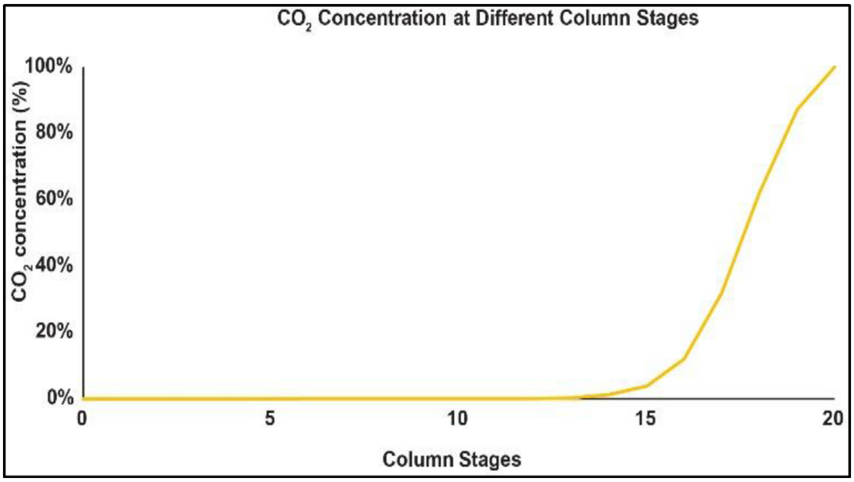

Fig. 13. Concentration of CO_2 (%) at different absorption column stages.

condition to find out the most suitable solvent for absorption. The mole fraction of amine solvents to H_2S was varied between 0.1 and 0.8 and thus, the absorption of CO_2 were studied. The CO_2 absorption varied from the minimum value of 75.02 % to maximum of 95.60 % for different solvents. Based on the study, the highest CO_2 capture is achieved while using MEA and at a molar fraction of 0.1005 to H_2S. Thus, it was selected for highest efficiency to CO_2 capture.

Fig. 14 indicates the change in the molar flow of the CO_2 in CCS with respect to the change of solvent_in flow rate. Solvent flowrate from 11,500 to 15,000 kgmole/h is considered as long as the column converged successfully. However, the increase of absorption of CO_2 became less significant with respect to the increase of molar flow of the CCS solvent as the curve became flatter. That is why an acceptable value was chosen.

Fig. 15 indicates the highest overall CO_2 removal from the flue gas that enters the absorption column using different amines at different concentration (using single amine or multiple amines mixed). Fig.-17 compares the maximum CO_2 capture using single amine and amine blend (mixture of MEA and MDEA). Here, when single amine was used, the molar concentration was with H_2S. The graph indicates that the maximum absorption of 98.87 % of

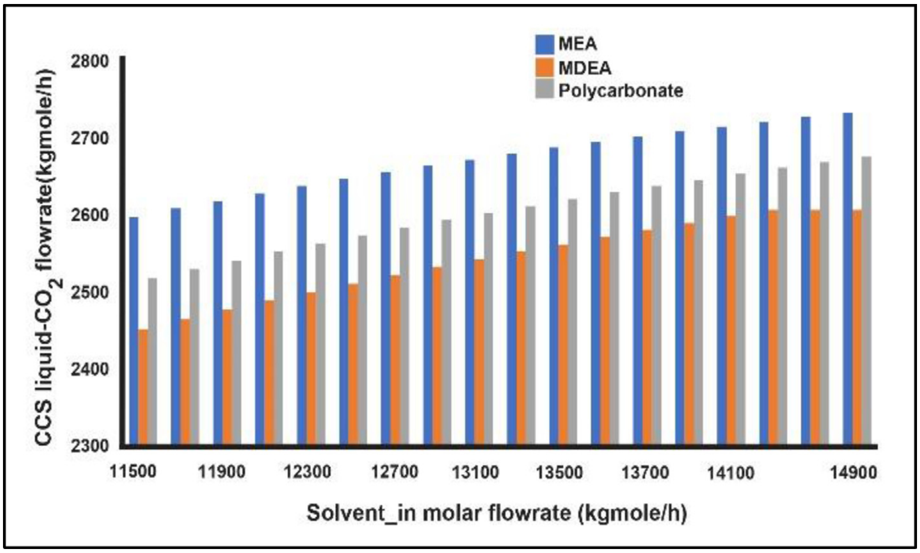

Fig. 14. Molar flow of the CCS Liquid vs the molar flow of Solvent.

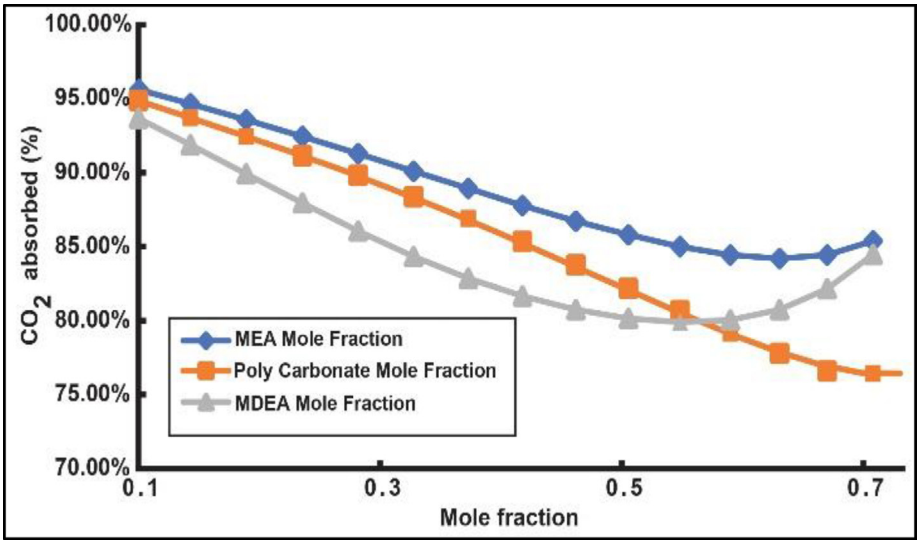

Fig. 15. Amine molar concentrationin solvents vs CO_2 Absorbed (%).

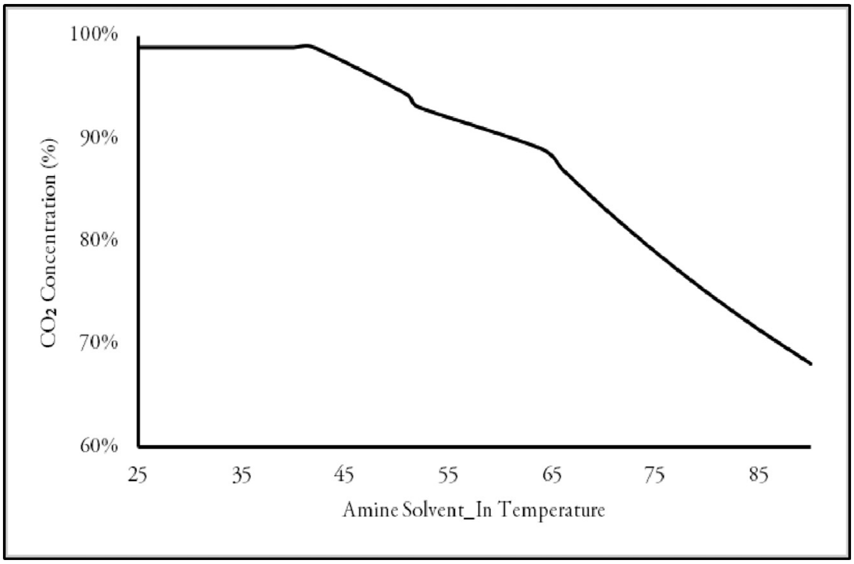

Fig. 16. CO_2 absorption in CCS liquid variation vs Amine solvent_ in temperature.

the produced CO_2 in the flue gas was absorbed in the CO_2 absorber and goes out of the column as the bottom stream that previously was about only 0.37 % (before the model optimization), achieved when a mixture of MEA and MDEA amines were used. It also revealed that a maximum of about 94.51 % absorption was achieved with MEA, 93.78 % with poly carbonate, and the lowest absorption of 92.6 % among these three was achieved while using MDEA. Additionally, the mixture of MEA and MDEA can absorb the maximum of 100 % of the CO_2 present in the flue gas entering the CO_2 capture absorption column as some of the CO_2 leaves the flue gas stream with liquid water at water separator. Other similar case studies have shown CO_2 capture from flue gas efficiency ranging from 80 % to 97.27%at maximum [61,89–91].

Fig. 16 compares the (%) of molar concentration of the major absorbed CO_2 in the CCS liquid with the variation of the solvent (amine blend) inlet temperature. The graph indicates that the maximum of 98.87 % of the produced CO_2 in steam reforming process was absorbed only at certain temperatures. When the solvent's temperature exceeded that certain temperature, the CO_2 absorption efficiency decreased and continued decreasing with increasing solvent's inlet temperature. Case studies revealed that when the inlet temperature of the solvent was

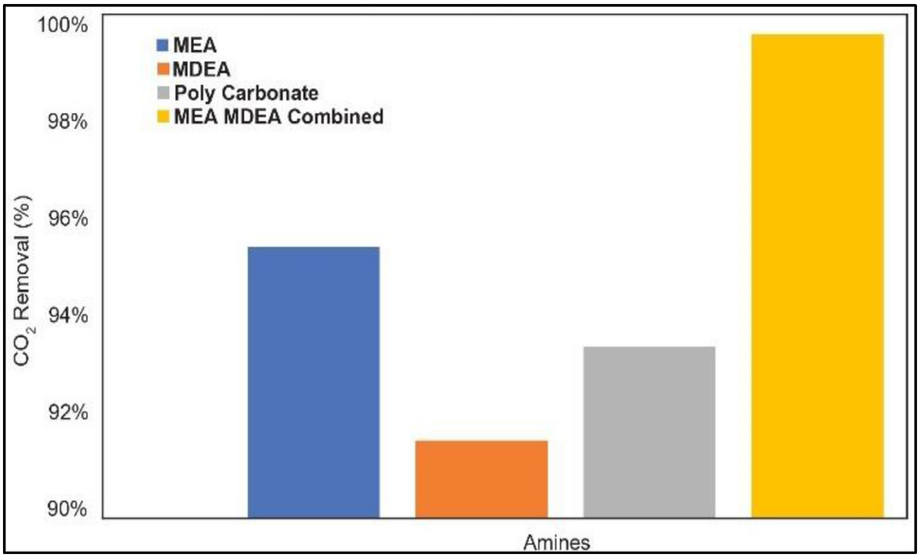

Fig. 17. CO_2 capture from the flue gas entering the absorption column using different amines.

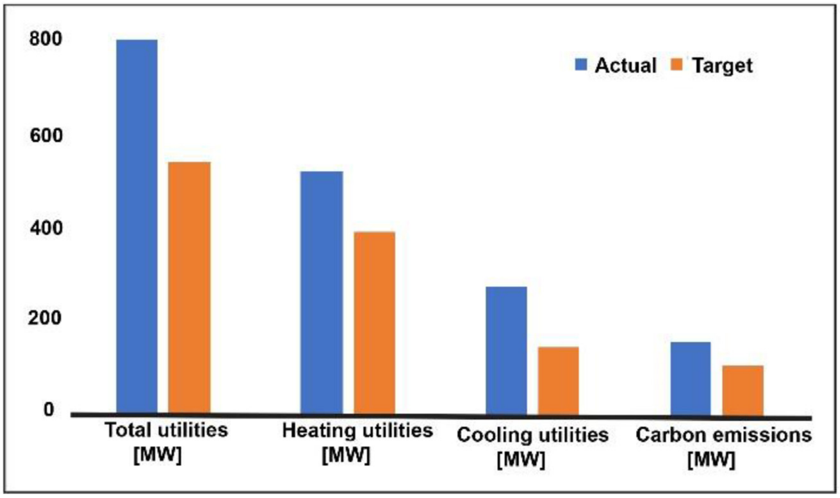

Fig. 18. Scope of utility optimization using aspen energy analyzer.

less than 50 °C, the solvent absorbed the CO_2 with maximum efficiency. However, as the temperature increased, the absorption efficiency decreased gradually, with 89.02 % at 64 °C, to finally 68.18 % of total CO_2 produced at 90 °C.

3.5. ASPEN energy analyzer

ASPEN Energy Analyzer tool uses pinch technology in all the utility to optimize the process. Fig. 18 gives information about the possible scope optimization.

The figure shows that the total utility used is about 784 MW, in which hot utility is about 511.4 MW and cold utility is about 272.5 MW. It can be optimized to save about 24.9 % for hot utility and 46.6 % for cold utility which will be a savings of 32.43 % in gross. Fig. 13 also displayed that carbon emissions could be reduced from 157.7 tons/h to 106.6 tons/h which will be ~32.44 % saving in total. In addition, this process is a high energy demanding as reported in the graphical representation in Fig. 13. Therefore, it is essential to optimize the process to reduce the overall production cost.

4. Conclusion

In this study, a comprehensive investigation was performed on the performance of the hydrogen production by varying various design parameters. The study revealed that the S/C ratio significantly impacts flue gas formation and the carbon capture system. Due to the simple nature of the conversion-type reactors, the hydrogen production did not vary after reaching an equilibrium point. Moreover, the flue gas formation and CO_2 capture largely depend on the yield of reactor 1 which was revealed in a case study. Another important finding of this simulation-based investigation is how the change in process parameters affects the CCS which shows that an effective CCS depends not only on the temperature and pressure but also on the solvent itself, molar flow, and mole fraction. Case studies revealed that the temperature of the flue gas and the separation of the liquid water from the flue gas increased the overall performance of the CCS. Before the process optimization, only 0.37 % of the produced CO_2 was separated from the absorber column as the bottom stream. Moreover, only 8.29 % of the amine left the column as the bottom stream whereas it should have been 100 % of the amine leaving with the absorbed CO_2. Again, the temperature of the flue gas also contributes to the water content removal from the flue gas. It was also found that the high-water content in the flue gas contributes to the inefficiency of the absorber column. Therefore, to make this process efficient, the flue gas needed to be cooled down (40 °C) to ensure that the water is separated before it enters the absorption column. The temperature (41 °C) and molar concentration (MDEA: MEA = 0.4: 0.6) of the amine solvent are also vital in an efficient CCS. The effect of using a mixture of two amines enhanced the overall carbon capture process. The pinch analysis and Aspen energy analyzer revealed that the process can be optimized and thus the overall cost can be reduced.

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Appendix A Nomenclature

SMR	Steam Methane Reforming
LHV	Lower Heating Value

MDEA	Methyl Diethanolamine
DEA	Diethanolamine
MEA	Mono Ethanolamine
CCS	Carbon Capture and Storage
PCC	Post Combustion Capture
PA	Pinch Analysis
WGS	Water Gas Shift
COP	Climate Change Conference of Parties
DGA	Diglycolamine
DIPA	Di-isopropanolamine
PZ	Piperazine
TEA	Triethanolamine

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