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Design and simulate an amine-based CO_2 capture process for a steam methane reforming hydrogen production plant

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Abstract. Steam methane reforming (SMR) is a common technique for hydrogen production, however CO_2, which is created as a by-product, needs to be captured. Chemical absorption utilizing amine solvents is the most economically practical method of CO_2 capturing. Amines are a class of organic compounds that are commonly used as chemical solvents for carbon capture. The effectiveness of a particular amine as a carbon capture solvent depends on its chemical structure and properties. Some commonly used amines for carbon capture include monoethanolamine (MEA), diethanolamine (DEA), and methyldiethanolamine (MDEA). This study aims to simulate SMR hydrogen production plant utilizing amine-based carbon dioxide capture system using Aspen HYSYS V11 software and figure out the efficiency of different chemical solvents in capturing carbon dioxide. The results of this study show that MEA has high efficiency to capture CO_2 due to its high reactivity and ability to form a strong chemical bond with CO_2. However, it is also highly corrosive and can be costly to regenerate.

1. Introduction

Hydrogen has the ability to provide answers to problems associated with rising global energy demand, such as global warming, that are economically practical, financially rewarding, socially favourable, and energetically efficient [1]. Hydrogen is an important element with a wide range of applications and potential benefits. Hydrogen has a variety of commercial applications, such as the production of ammonia for fertilisers, the refining of petroleum, the production of chemicals and materials, and the production of fertilisers without using fossil fuels in agriculture. Hydrogen can also be used as a clean and sustainable energy source for power generation and transportation. It can also be used as a medium for storing renewable energy.

SMR is one of the most often used technique for generating blue hydrogen from natural gas. The majority of hydrogen (H_2) produced globally comes from natural gas steam reforming, which is regarded as a cost-effective process in terms of product yield and energy usage. Figure 1 depicts the SMR with the capture and storage of carbon process flow diagram. From the figure below, it is obvious that in order to absorb and store this carbon, carbon capture and storage (CCS) is needed. Syngas, a mixture of CO and H_2, is produced in the reforming reactor by the high-pressure reaction between natural gas and steam. The process employs nickel-based catalysts to generate syngas with high quantities of H_2 and CO. Prior to entering water gas shift reactors, the syngas is cooled. In these reactors, the steam-added

CO is converted to CO_2 and H_2. The generated hydrogen is cleaned up in the amine plant (Purification unit). Then, it is compressed and maintained in storage tanks. CO_2 emissions from the purifying facility are compressed and transmitted to a cavern below earth [2-3].

An amine plant steam reformer with two subsequent shift reactors are common components of industrial natural gas steam reforming systems, which first create hydrogen gas in a reaction zone before capturing CO_2 and CO in a purification zone. Almost all of the CO_2 and H_2S from the incoming gas stream is removed using an amine plant. CO_2 is removed from gases through the process of amine scrubbing, which is also known as amine gas treatment, gas sweetening, or acid gas removal. "Sour gas" meaning it contains high levels of H_2S or CO_2, enters the process and is transformed into "sweet gas”. Figure 2 shows the overall reaction structure of the CO_2-amines technology [4,5].

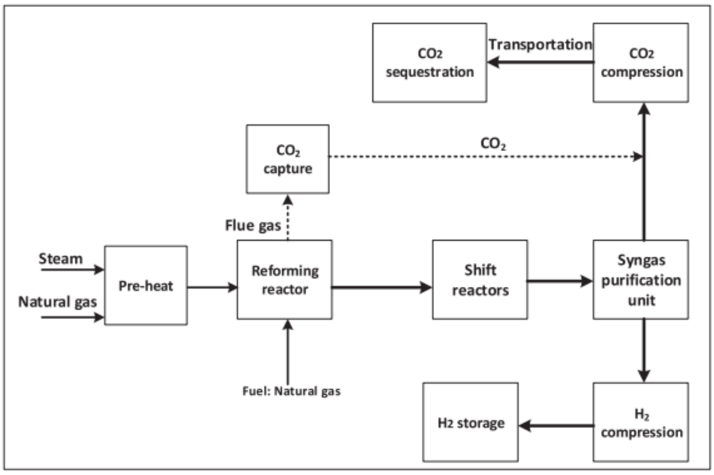

Figure 1. Steam methane reforming with carbon extraction and retention process flow diagram [3].

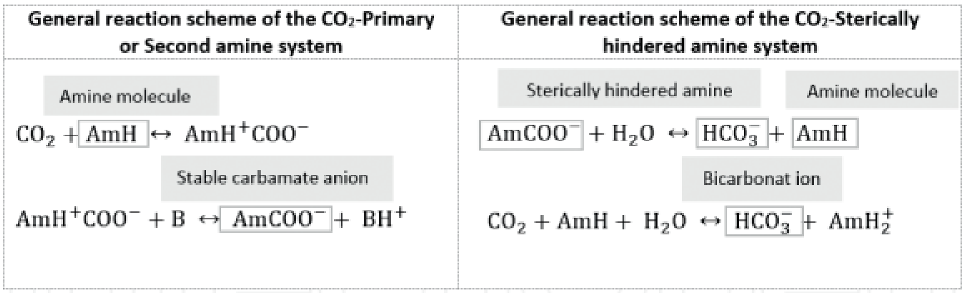

Figure 2. CO_2 capturing in the Amine plant [5].

To reduce CO_2 emissions, several technologies have been employed, including oxyfuel combustion, chemical looping, and pre- and post-combustion. At ambient conditions, chemical absorption is the most common method of CO_2 removal. The application of an amine-based solvent for CO_2 capture post combustion may directly extract CO_2 from flue gas, which is a sensible technique that is reasonably affordable and easily adaptable to modern power plants. This approach is superior to other CO_2 capture technologies [6-7]. Figure 3 shows the streams that contain carbon dioxide in the SMR process. CO_2 emissions to the atmosphere can be reduced by capturing CO_2 from any of the three streams that contain carbon dioxide (tail gas, flue gas, and shifted gas). As much as 99% of CO_2 may be removed from steam methane reforming streams at spot 1 (shifted gas), 90% at position 2 (tail gas), and 70% at position 3 (flue gas), depending on the removal location [8].

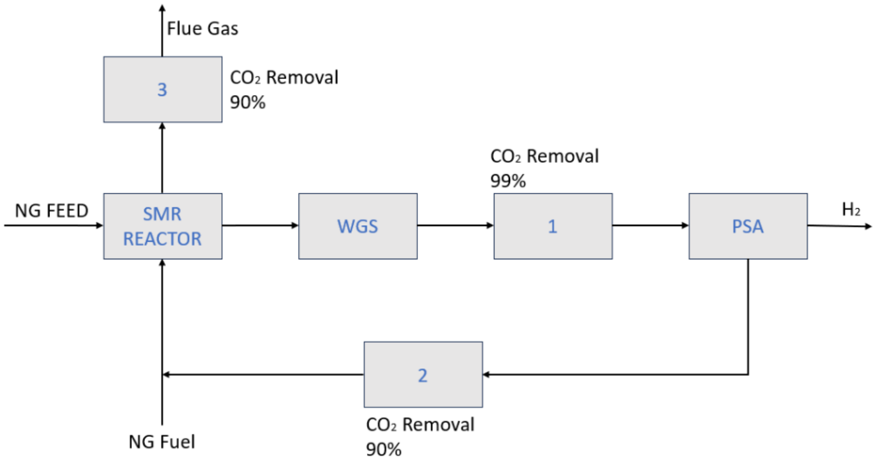

Figure 3. SMR CO_2 containing streams [8].

2. Methodology

Figure 4 presents a simulation model of an industrial natural gas SMR process using amine plant as a carbon capture and storage system created by ASPEN HYSYS.

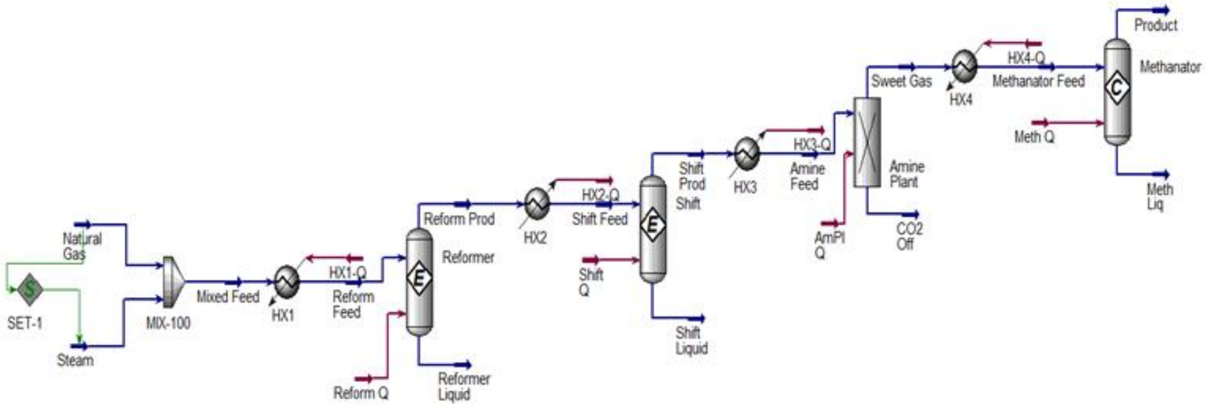

Figure 4. Industrial natural gas SMR process simulation.

As shown in the figure above, prior to being fed into a reforming reactor, natural gas and steam were combined and heated at heater 1 (HX1). Conventional reforming reactors employ catalysts made of nickel. The reformer's overhead stream was then cooled in cooler 1 (HX2) before being sent to a high-temperature shift reactor (HTS). The HTS's overhead stream was then cooled in cooler 2 (HX3) before being fed into the Amine plant to capture CO_2 and the stream is then further purified in a Methanator to remove any leftover CO in order to fulfil market product requirements.

2.1 Fluid package and thermodynamic variable optimization

The modelling process in the reformer and water gas shift reactors was optimised using the Peng Robinson fluid package. This fluid package could estimate the pressure and temperature (thermodynamic data) of light gases such as (CO_2, H_2, CO, CH_4….C_nH_m) [4,9].

Additionally, Aspen HYSYS was used to simulate the reaction's product yield and reactant consumption by deriving the equilibrium constant of the reaction from an alteration in free energy at a given temperature as shown in the equation below [10].

$$\ln(K_{eq}) = -\frac{\Delta G_{reaction}}{RT} \tag{1}$$

Where K_{eq}, ΔG, R, and T are stand for equilibrium constants, free energy changes, gas constants, and temperatures, respectively.

The proportion of steam to carbon (S/C), pressure and temperature in the generation zone were optimised after the fluid packages and practical reactors were selected for the steady state model. In addition, the HYSYS simulator computed the heat duty needed to run at optimum performance.

First, the pressure and temperature of the reformer were adjusted. The reason for changing the reformer pressure initially come from its intended use of promoting the primary steam reforming reactions. The reformer inlet temperature was another crucial element that needed to be changed. Since methane concentration is higher at this reactor's entrance, the non-uniform temperature distribution may cause carbon to deposit there. The catalyst becomes fouled and becomes inactive as a result of this carbon deposition. Experience has shown, however, that a typical input temperature of between 450 and 550 °C maintains coke formation at a low-level. This is why more than 500 °C inlet temperature was selected. To ensure natural gas circulation in the process, the initial natural gas stream may be given to the heater at any pressure greater than 7 atm. Steam and natural gas methane are present in the feed stream. The stream was heated to 730 ˚C using a heater (HX1) before entering the reformer [9-11]. Table 1 shows the summary of models and utilities used in the simulation.

Table 1. Simulation models and specifications [9-11].

Code	Equipment	Specifications
HX-01	Heat exchanger (Heating)	Cold stream outflow T: 730 ˚C
HX-02	Heat exchanger (Cooling)	Cold stream outflow T: 420 ˚C
HX-03	Heat exchanger (Cooling)	Cold stream outflow T: 38 ˚C
HX-04	Heat exchanger (Heating)	Methanator feed T: 260 ˚C
Reformer	Reformer equilibrium reactor	Operating temperature: 730 ˚C
Shift	Water gas shift reactor	Operating temperature: 430 ˚C
Amine plant	Component Splitter	Overhead stream pressure: 297 KPa

3. Results and discussion

Using Aspen HYSYS software, with the use of numerous amine solvents including monoethanolamine (MEA), diethanolamine (DEA), and methyldiethanolamine (MDEA), hydrogen production by steam methane reforming is simulated. Table 2 shows the results of using different amines on carbon capture efficiency. From the figure below, it's clear that the effectiveness of a particular amine as a carbon capture solvent depends on its chemical structure and properties. The amount of CO_2 that can be captured by a particular amine solvent depends on several variables, such as the solvent concentration, the temperature and pressure of the system, and CO_2 concentration in the feed gas stream. In general, amines with higher reactivity and stronger affinity for CO_2 will capture more CO_2.

MEA is one of the most commonly used amines for carbon capture due to its high reactivity and ability to form a strong chemical bond with CO_2. However, it is also highly corrosive and can be costly to regenerate. DEA and MDEA are also commonly used for carbon capture and have lower corrosivity and lower energy requirements for regeneration than MEA. However, they may not capture as much CO_2 as MEA due to their lower reactivity.

It is essential to keep in mind that a specific amine's ability to capture CO_2 can be affected by several variables, including pressure, temperature, and gas composition, and that the amine selected for a given application will depend on a number of variables, including cost, availability, and the unique requirements of the carbon capture system.

Table 2. Comparison of some of commonly used amines for carbon capture based on their CO_2 capture efficiencies and properties.

Amine	Chemical structure	CO_2 capture performance	Regeneration energy requirement
Monoethanolamine (MEA)	$HOCH_2CH_2NH_2$	High reactivity	High energy requirement
Diethanolamine (DEA)	$HOCH_2CH_2NHCH_2CH_2OH$	Lower reactivity than MEA, lower corrosivity	Lower energy requirement than MEA
Methyldiethanolamine (MDEA)	$CH_3OCH_2CH_2NHCH_2CH_2OH$	Lower reactivity than MEA, lower corrosivity	Lower energy requirement than MEA

4. Conclusion

Steam reforming natural gas (SMR) is considered one of the most common blue hydrogen production processes. Although hydrogen is produced, carbon dioxide is a by-product. In order to absorb and store this carbon, carbon capture and storage (CCS) is needed. Chemical absorption utilising amine solvents is the most commercially facility to capture CO_2. Because of its high reactivity and capacity to form a strong bond with CO_2, MEA can be the best option for carbon capturing. However, it is also highly corrosive and can be costly to regenerate.

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