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Carbon Dioxide Direct Air Capture Using Aqueous Solutions of Potassium Hydroxide and Sodium Hydroxide: Energy Optimization & CO_2 Capture Enhancement

1st Mahmood Bader Alalawi
Department of Chamical Engineering
University of Bahrain
Manama, Bahrain
Alalawi-m@outlook.com

2nd Ali Ahmed Abdunnabbi
Department of Chamical Engineering
University of Bahrain
Manama, Bahrain
Ali3farhan415@gmail.com

3rd Husain Majeed Ali
Department of Chamical Engineering
University of Bahrain
Manama, Bahrain
Alghurifi.2002@gmail.com

4th Kamal M. Sassi
Department of Chamical Engineering
University of Bahrain
Manama, Bahrain
kalmuteer@uob.edu.bh

Abstract
This report investigates the feasibility and efficiency of Direct Air Carbon Capture (DAC) using aqueous sodium hydroxide (NaOH) and potassium hydroxide (KOH) solutions. Through simulations performed in Aspen Plus v.14 software, the study evaluates process performance and energy efficiency. The results demonstrate that KOH outperforms NaOH in carbon dioxide (CO_2) capture efficiency (89.8% vs. 86.4%) due to its higher solubility and ease of regeneration.

A key focus of the study is energy optimization, achieved through pinch analysis, identifying a minimum temperature difference (ΔTmin) of 15°C. This optimization reduced heating and cooling demands to 51 MW and 103 MW, respectively, in the optimal scenario. Additional thermal recovery from the slaker reactor offset 54.7% of heating requirements for KOH systems and 54.4% for NaOH systems, resulting in residual heating demands of 79.282 MW and 80.657 MW, respectively.

The findings underscore the potential of DAC as a viable solution for atmospheric CO_2 removal, especially when paired with energy-efficient designs. Future work will refine process designs, explore alternative absorbents, and integrate renewable energy sources to enhance scalability and sustainability.

I. INTRODUCTION

The need for carbon removal technologies has become more urgent as emissions have continued to increase over the years. Emissions of CO_2 in the world have tripled since 1960, reaching over 35 billion tons a year by 2023, due mainly to fossil fuel combustion and industrial activities. This trend indicates that scalable carbon removal solutions are necessary if climate stability and net-zero targets are to be achieved [1].

In this context, Bahrain faces significant challenges in managing its emissions, which reached 37,960,000 metric tons of carbon dioxide in 2022[2]. According to the ALBA Environmental, Social, and Governance Report 2022 [3], and the Bapco Sustainability Report (2020-2021) [4], the combined contributions from ALBA and Bapco accounted for 15,556,367 tons of these emissions. In response to this pressing issue, the Kingdom of Bahrain has launched a national strategy for climate change, campaigned by His Royal Highness Prime Minister, with the goal of achieving a 30% reduction in greenhouse gas emissions by 2035[5]. The formatter will need to create these components, incorporating the applicable criteria that follow[6].

A. *Aim of The Project*

The project aims to assess the efficiency of capturing carbon dioxide directly from the air using sodium hydroxide (NaOH) and potassium hydroxide (KOH) solutions. This involves evaluating their CO_2 capture potential, energy consumption, and process performance through comprehensive simulations in Aspen Plus software. The goal is to optimize operational parameters and enhance the sustainability and effectiveness of direct air capture systems.

B. *Current State-of-the-Art*

Carbon capture involves the process of capturing carbon dioxide emissions generated from a variety of activities, including fossil fuel combustion in power generation, fossil fuel extraction processes such as natural gas processing, hydrogen production, ammonia synthesis, iron and steel manufacturing, and cement production. There are several methods for capturing CO_2 emissions, either by targeting sources or by directly removing CO_2 from the atmosphere [7].

C. *Constrains*

DAC technology faces several constraints, including energy efficiency, material selection, and operational scalability. Energy consumption is a critical issue, as the system requires substantial heating and cooling, making energy optimization essential to reduce operational costs [8]. Material compatibility and chemical stability of components, such as sorbents (NaOH and KOH), must be ensured to perform effectively under high-temperature and pressure conditions. The process layout also requires precise mass and heat balances, particularly in interconnected sections like the calciner and pellet reactor, which depend on efficient recirculation loops for stability. Additionally, the overall economic feasibility of DAC is limited by high capital and operational costs, presenting significant challenges for widespread

D. *Standerds*

The DAC system design adheres to several engineering standards to ensure safety, reliability, and efficiency.

Thermodynamic modeling follows industry-accepted methodologies, utilizing the Electrolyte-NRTL and Soave-Redlich-Kwong (SRK) equations of state to predict vapor-liquid equilibria and manage complex ionic interactions accurately. Heat exchangers are modeled as "ideal" components with zero pressure drop, ensuring compliance with energy efficiency standards and enabling accurate pinch analysis. The process also integrates rate-based models for mass transfer to align with established engineering practices for absorption columns. Furthermore, operational parameters such as the reactor temperature of 900°C for the calciner and the slaker's operating conditions at 300°C and atmospheric pressure are chosen based on industry norms for chemical and thermal processing equipment [9]. This structure follows industry standards for process simulation, ensuring that all components work smoothly together and are easy to integrate. These engineering standards are crucial for achieving the intended performance, safety, and economic objectives of the DAC plant [10].

II. THEORETICAL BACKGROUND & LITERATURE REVIEW

A. Thermodynamic models

The accuracy of software calculations in simulations depends on the proper selection of thermodynamic models as all unit operations require property calculations. While flash and enthalpy calculations mainly require mass and heat balances, additional thermodynamic properties must also be considered. Interaction occurs between gas phase streams and aqueous phase streams in the air contactor and the absorber units, where CO_2 is removed from gas mixtures [11]. To model the Vapor-Liquid Equilibrium (VLE) in these components, the following thermodynamic models are applied: the Electrolyte NRTL for the liquid phase and the SRK EOS for the gas phase [12],[13],[14].

B. Mass transfer model

The process of mass transfer between the gas phase and liquid phase is fundamental in absorption columns and air contactors. These phenomena form the theoretical basis in order to understand the interactions within this equipment. As stated earlier, the formation of ionic species mainly involves the liquid phase while molecular species contribute to vapor-liquid equilibrium. Two primary models explain mass transfer and kinetics in absorption columns [15]:

- Equilibrium-Based Stage Efficiency Model: This model assumes equilibrium between vapor and liquid phases at each stage of the column, but this assumption is unrealistic in real practice and to address this problem, a stage efficiency factor is introduced. Despite this adjustment, the results accuracy is low compared to the results of the rate-based model.

- Rate-Based Model: The rate-based approach overcomes the limitations of the equilibrium-based model. It applied the two-film theory segmenting films into different sections on each stage. This method provides a comprehensive analysis of energy balance, kinetics, heat transfer, mass transfer and system properties. The separation process is driven by mass transfer between phases with phase equilibrium achieved solely at the vapor-liquid interface at each stage. The Two-Film Theory, proposed by Lewis and Whitman in 1924 [16] is an integral to the rate-based model. It focuses on mass transfer analysis at the liquid-vapor interface, it assumes steady state conditions with mass transfer resistance concentrated in two finite-thickness films near the gas-liquid interface. Convective mixing is excluded in these films, emphasizing diffusion as the primary mechanism. The resulting solute concentration is nearly uniform except near the films, which function as diffusional resistances in series. The mass transfer coefficient (k_c), crucial in the rate-based model, is expressed as a function of CO2 diffusivity and film thickness (δ). It can be mathematically represented as [17]:

$$k_c = \frac{D_{co_2}}{\delta} \tag{2.7}$$

C. Literature Review

1) Process Modelling of a Direct Air Capture (DAC) System Based on The Kraft Process

This paper presents a detailed modeling and simulation of a Direct Air Capture (DAC) system inspired by the Kraft process, aiming to evaluate its energy performance and overall feasibility for capturing CO_2 from the atmosphere. Using Aspen Plus software, the DAC system was methodically divided into sections aligned with the primary chemical reactions in each stage. While a complete techno-economic assessment was not possible due to data limitations, the technical findings were validated against existing literature, providing a solid foundation for future research [18].

The DAC plant model serves as a crucial starting point for exploring energy efficiency and operational dynamics. The energy analysis highlighted the importance of thermal integration, employing pinch analysis to demonstrate that approximately 90% of thermal energy could be internally recovered, highlighting the system's efficiency. The study also identified that the minimum heat supply required is 51.82 MW, which can be provided by the same natural gas used to power the calciner and the combined cycle power island. Notably, the system’s electricity demands are entirely met by gas and steam turbines.

Overall, these results affirm the technical feasibility of the DAC system and offer valuable insights into the potential of DAC technologies for reducing atmospheric CO_2 levels. This research lays a solid foundation for further advancements and underscores the promise of innovative approaches to tackling climate change. [18].

2) Simulation of Carbon Dioxide Direct Air Capture Plant Using Potassium Hydroxide

The paper presents the design and optimization of a direct air capture (DAC) plant utilizing potassium hydroxide (KOH) as the absorbent, with an emphasis on enhancing energy efficiency and CO2 purity. The DAC process was simulated using Aspen Plus software, employing various thermodynamic models and databases to accurately represent the different components of the system. Key reactions involved in the DAC process were specified, along with the parameters used to calculate the equilibrium constants. Additionally, pinch analysis was employed to optimize energy recovery and minimize energy consumption by identifying the pinch point and designing the heat exchanger network accordingly [19].

The findings indicate that while DAC technology is a promising solution for combating climate change, the current costs remain high, necessitating further advancements to reduce both expenses and energy consumption. The designed system has the capacity to capture 1.1 Mt of CO2 per year, with the captured CO2 potentially being sold to partially offset operational costs. Optimization efforts, including the implementation of pinch analysis and thermal integration, resulted in significant improvements in energy efficiency, achieving a 21.1% increase in heat recovery and reductions of 34.85% and 84.7% in hot and cold utility consumption, respectively. The paper also suggests several avenues for future research, including techno-economic assessments, environmental impact analyses, and the integration of DAC technology with other processes [19].

3) Direct Air Capture as Carbon Removal Solution

This paper explores how existing Direct Air Capture (DAC) methods could be scaled up and made more affordable by applying principles from technological change theory. The findings reveal that by 2050, solid sorbent DAC methods could lower costs to a range of \$100 to \$400 per ton of CO_2, while liquid solvent methods might achieve costs between \$100 and \$220 per ton. The study draws these estimates from a detailed review of existing literature and comparisons with similar technologies to uncover potential pathways for cost reduction and scalability.

By analyzing common DAC methods alongside analogous technologies, the research identifies strategies for accelerating progress and reducing costs. These include leveraging economies of scale, optimizing early design choices, and fostering innovation. The paper also outlines actionable opportunities for key stakeholders such as: Policymakers: Can play a vital role by establishing standards for measurement, reporting, and verification (MRV) to ensure the credibility of carbon dioxide removal efforts. Ultimately, this study highlights the collaborative effort required to make DAC an effective tool for combating climate change, emphasizing the need for innovation, policy support, and market engagement to unlock its full potential [20].

III. DESIGN & IMPLEMENTATION

In this chapter, a full description of the entire process simulation is presented, outlining the assumptions made for each stream and component, along with the tools employed to achieve the desired outcomes.

The facility is divided into six main sections, each thoughtfully defined to simplify the development of a clear and accurate model of the entire system. This approach was essential to manage the complex material flows interacting between various parts of the plant. By clearly identifying these sections, the design ensures a better understanding of how each part contributes to the overall operation. The sections are named as follows:

1. Air Contactor and Absorber
2. Pellet Reactor
3. Steam Slaker
4. Calciner
5. CO2 Compression
6. Power Island

The simulation was conducted using Aspen Plus® (version 14), a product of Sentech®, an American company.

The model utilizes the "electrolyte template" available on Aspen Plus®, which is useful for simulating chemical reactions between electrolytes. All the reactions can be specified in the Property section of the software, and in its Simulation section, it can simulate a reaction even when two streams are simply mixed. In other words, the reactions occur outside of specific reactors, which was extremely helpful for managing the numerous reactions throughout the plant.

A. AIR CONTRACTOR

The hierarchy model aims to replicate the functions of the air contactor section. The air contactor is a new part of the real plant, so the Aspen Plus® software does not have a specific block for direct use in the model. As a result, additional blocks were needed to accurately describe how the block functions. The air contactor has been modeled using three different Aspen blocks: MIXER-1, MIXER-2, and SEP-1. These blocks conduct the necessary functions for separating CO2 from atmospheric air.

MIXER-1 combines the ambient air (stream 1) with the gas turbine exhausts after they have been stripped of about 90% of the initial CO2 content in the ABSORBER block (stream 74). Stream 2 is then mixed with stream 3, which consists of the liquid solution.

Once the CO2 has reacted in stream 4 with the liquid solution in stream 3 to produce potassium and potassium carbonate, the SEP-1 block performs a simple gas-liquid separation, separating gaseous compounds in stream 5 and allowing liquid substances to continue to the PUMP-1 block. Additionally, Stream 5 represents the ambient air exiting the air contactor and has a much lower CO2 content compared to the ambient air entering the first MIXER-1 (stream 1).

MIXER-3 combines the remaining liquid solution from the air contactor with the liquid solution exiting the ABSORBER block. The same liquid solvent solution is used in both the air contactor and the absorber, recovered from the pellet reactor in a closed loop. To simplify and avoid convergence issues, the streams containing the solution have been modeled with an open loop, using two different streams (stream 3 and stream 8).

Stream 10 is heated in the first heat exchanger of the plant, named HX, without any pressure drop. All heat exchangers of the plant have been modeled as "ideal" heat exchangers, characterized by zero pressure drop.

The absorber block, filled with structured packing material provided by BERL Ceramic and with a column size of 12 x 7.5 m (height x diameter) as indicated in the reference paper [18], is one of the most critical components of the simulation due to the high number of required performance parameters. A rate-based model calculation has been applied to the column, which has been divided into 16 stages. The flow model and film characterization have been considered as established by the theory.

The reaction condition factor, film discretization ratio, liquid film discretization points, and interfacial area factor have been taken from the literature [18]. The correlations used for the absorber simulation are the ones suggested in the literature [18].

B. PELLET REACTOR

The pellet reactor serves to eliminate carbonate ions (CO32-) formed in the air contactor. The reactor facilitates a slightly exothermic crystallization reaction. While the actual plant will utilize a fluidized bed reactor, the existing 'FLUIDBED' component in Aspen Plus® necessitated extensive parameters and details not available in the reference publication.

literature on this particular block has been challenging to procure. In light of the reaction's nature (CaCO3 crystallization), the decision has been made to model this component using the software's crystallizer block (PELLET block). This necessitates temperature and pressure specifications (25°C, 1 bar) and the "saturation calculation method" for compound crystallization.

Stream 10 comprises the solvent from the air contactor hierarchy, while stream 11 primarily consists of Ca(OH)2, essential for the crystallization reaction. Although stream 11 has been modeled as an "open" stream, it should correspond to stream 72, modeled in the subsequent section (Steam slaker hierarchy). This was done to prevent potential convergence issues between the two sections during the simulation.

One crucial factor in this section is the amount of calcium retained. When modeling the two recirculation loops connected to the pellet reactor (upper and lower recirculation loops), it is important to consider this factor. To address this, we introduced block SEP-2. The issue is that the lower loop recirculates more liquid solution, where there should be less solid calcium carbonate. To solve this, a simple separator (block SEP-2) was used to collect only the solid CaCO3 formed in the reactor and send it to the upper recirculation loop.

To respect the mass balances on the pellet reactor given by Keith et al.[31], the block SPLIT-1 was modeled to split 99.9% of liquid stream 14 to stream 16, and only 0.1% to the upper stream 15.

Moving on to the upper recirculation loop, once the solid CaCO3 flow (stream 13) is mixed in MIXER-4 with the liquid stream 15, the resulting stream 20 is sent to MIXER-5. This is necessary because the pellet reactor needs a 'makeup' of solid calcium carbonate to sustain the reaction. Stream 21 is composed of CaCO3 only and, in addition to streams 20 and 21, stream 75 is mixed with the other two in the mixer. Stream 75 is constituted by a fraction of solid CaCO3 filtered in the lower loop (by FILTER-1 and FILTER-2) and then recirculated to the upper loop. Consequently, stream 22 is a mixed stream, composed of liquid solution and solid CaCO3 pellets. This final stream is filtered in the subsequent FILTER-3 (a solid separator), where almost all solid calcium carbonate is filtered and sent to the Steam slaker section (stream 24), while the liquid separated in the block is recirculated to the pellet reactor again (stream 23).

As mentioned earlier, stream 16 is almost all liquid but still contains a small amount of solid calcite (CaCO3) that must be removed before being sent back to the reactor. For this purpose, in the lower recirculation loop, FILTER-1 and FILTER-2 are used to separate the remaining quantity of CaCO3. Both blocks have been modeled as standard "solid separators." FILTER-1 can separate a certain amount of solid CaCO3, with a certain pressure drop inside established by the data of the reference publication [18]. Therefore, the liquid stream that exits FILTER-1 (stream 18) is pumped through PUMP-2 before being sent back to the Pellet reactor. After the first filtration step, a second filter, FILTER-2, is used to remove all the solid CaCO3 from liquid stream 17. Once the solid fraction has been removed in stream 25, also in this case, as done in the air contactor section, stream 26 has been modeled as an "open stream". It should be connected to the blocks that represent the air contactor and the absorber column, but for reasons of convergence of the simulation and to implement the design specification in the air contactor section more easily, it has been decided to model it as an open flow. However, this is an acceptable approximation, especially because the high flow rates indicated by the reference paper in this part of the plant give greater freedom during the modeling phase, ensuring not to overestimation the solvent flow rate [18]. Finally, the solid CaCO3 flow (stream 25) is split into three streams (27, 28, and 75). Stream 75 has already been discussed, while stream 27 could be sent to the calciner block and stream 28 is made of CaCO3 to be disposed of.

C. STEAM SLAKER

The slaker acts as a fluidized bed reactor that hydrates quicklime (CaO) from the calciner and preheats CaCO3 pellets from the pellet reactor (stream 24). However, since Aspen Plus® does not have a component that matches the real reactor, this section is modeled to replicate its functions. After passing through FILTER-3 in the pellet reactor, solid CaCO3 is washed in the WASHER block using water (stream 46), which is sourced externally as described in the CO2 compression section. This washing process aims to separate the solid CaCO3 from the liquid hydroxide solution.

Consequently, the liquid exits the washer in stream 30, while the calcite in stream 29 is dried and heated to 300°C using heaters HE-1 and HE-6. To facilitate this process, two heat exchangers are employed. Specifically, HE-1 heats the CaCO3 and associated water without superheating (set to 0°C), while HE-6 raises the CaCO3 temperature to 300°C, thereby simulating the slaker's function.

Stream 31 (at 300°C) goes through a separator, SEP-4, which uses a 0/1 logic to fully remove water from the solid. This setup removes all vapor-phase compounds, directing them to the slaker (stream 33-A) for the slaking reaction. The solid CaCO3 left over is sent to the calciner for thermal decomposition (stream 33-B). Since Aspen Plus® does not have a reactor block that can heat a stream without changing its properties (like the real reactor) heaters HE-1 and HE-6 are fictional components used to simulate the heating of CaCO3. Stream 33-A, containing only water, enters the slaker. If CaCO3 were allowed in, it would increase the vapor content. Although the real plant uses a fluidized bed reactor, a different component is modeled here for simplicity, as the RStoic block in Aspen Plus® effectively manages the slaking reactions. This block needs just a few key details:

- operating temperature.
- operating pressure.
- reactions involved.
- fractional conversion of reactants.

The software's required conversion of reactants matched the 85% CaO conversion found in the reference paper [18]. The steam slaker operates at 300°C and atmospheric pressure, with the only reaction being between quicklime (CaO) and water. The SLAKER block is fed by water stream 33-A, stream 62, stream 64, and recycled CaO from stream 68. Stream 62, coming from the calciner, contains only calcium oxide, which is crucial for the slaking reaction. Stream 64, connected to stream 58, models a 42-bar steam line at 253°C that heats the slaker in the real plant. While slakers usually use water, they can also be heated with steam to 300°C. The advantage of steam slaking over regular water slaking (used in the Kraft process) is that it releases heat at higher temperatures.

To model the steam line's contribution, the simulation uses SPLIT, NOZZLE, and heaters HE-8 and HE-25. The SPLIT block divides the incoming 42-bar steam into two streams, with one (stream 60) expanded to 1 bar via the NOZZLE, simulating steam expansion into the reactor. Although it cools, its temperature remains high enough to heat the reactor. In the real plant, steam not injected into the slaker passes through and heats up, reaching thermal equilibrium with the reactor at 253.3°C. This is modeled with two heaters (HE-8 and HE-25) to simplify pinch analysis, heating the steam to 300°C with no pressure drop.

Steam from stream 61-B is sent to the calciner, where it passes through the SUPH heat exchanger and is heated to 415°C in the superheater. It then enters the steam turbine (stream 65), generating additional power for the plant. The turbine data is provided in. After expansion with stream 54 (from the HRSG), the steam is cooled to 50°C using three coolers (HE-5, HE-20, HE-21) for pinch analysis. It exits the turbine (stream 55), is pumped back to 42 bars by PUMP-3, and recirculated to the slaker. Streams 58-BIS and 58 were modeled separately for convergence, but their flow rate and composition are identical.

The recirculation loop of the steam slaker manages the leftover 15% of unreacted CaO. Stream 63 carries the quicklime, which is first separated by CYCLONE (simulating the primary cyclone) and any remaining CaO is removed by DUST-COL (simulating a dust collector). The loop also includes a lime cooler (LIME) and MIXER-7, which recovers heat from hydrated lime and combines Ca(OH)2 with liquid from the WASHER. The mixed stream (72) will be sent to the pellet reactor for the lime to react with potassium carbonate.

D. CALCINER

The calciner reactor plays a significant role in this process. In this reactor, the calcination of CaCO3 occurs, which is crucial for recycling the solvent and producing concentrated CO2 simultaneously. Calciners are large steel vessels where the fluidizing gas is supplied at the bottom of the reactor. The reactor operates at ambient pressure and 900°C. The fluidized bed reactor has been modeled using a simple stoichiometric reactor provided by Aspen Plus® (RStoic block). This choice aligns well with the reactor's operating conditions and the CaCO3-to-CaO conversion efficiency provided by the reference source [18], which has been set to 98%. The calciner receives CaCO3 pellets from the steam slaker hierarchy at a temperature of 300°C (stream 33-B). Before entering the reactor, solid calcite passes through two heat recovery cyclones arranged in a counterflow configuration with the outgoing gas stream. These two cyclones have been modeled with simple counterflow heat exchangers (HE-2 and HE-3) to align with the data provided by Keith et al. Once the gaseous stream 41 produced by the calciner has been cooled by HE-3 and HE-2, it is sent towards the superheater (block SUPH) to preheat the water vapor (stream 44) for its successive expansion in the steam turbine.

The stoichiometric reactor chosen in the software can receive more than one incoming flow but generates only one product stream. The reactor is fed by solid CaCO3 contained in stream 35 (almost completely converted), almost pure oxygen from the Air Separation Unit (ASU, not modeled here) in stream 37, and natural gas in stream 38. The software does not use a Gibbs reactor (RGibbs) but instead requires the manual input of the thermal decomposition reaction of CaCO3 and the combustion reactions of natural gas. The product stream will contain both a solid and a gaseous fraction. Therefore, the block SEP-3 has been used to model a solid-gas separator. The calcium carbonate produced by the calciner at about 900°C is separated in stream 40 and sent to the heat exchanger HE-4, where it is cooled to 674°C in a single cyclone and preheats the incoming oxygen (stream 36) to the same temperature of CaO (674°C) before sending it to the steam slaker.

E. CARBON DIOXIDE COMPRESSION

The CO2 gas stream (stream 44) from the calciner reactor contains a high concentration of CO2 but it requires further processing. Firstly, the gas is cleaned in a water knockout system which involves cooling the gas by mixing it with water (stream 45) and this will condense the water vapor from the gas in SEP-5. The exiting stream (stream 47) has a higher CO2 concentration compared to stream44. The water, including the injected water and the condensed water from stream 44, exits separately as stream 46.

After separation, stream 47 is compressed from atmospheric pressure to 150 bar using a four-stage compressor system (CMP1, CMP2, CMP3, CMP4), each with a pressure ratio of 3.5. These compressors are modeled as isentropic which means that they operate without adding or removing heat and each has the same efficiency. To reduce compression work and prevent overheating, interstage cooling is between stages, maintaining a constant temperature of 45°C between each compression stage. Interstage cooling helps to prevent elevated temperatures that could damage materials, also interstage cooling helps to reduce the energy required for compression.

F. POWER ISLAND

This is the final hierarchy of the simulation it is designed to account for the internal power demand of the plant. The power system includes a combined cycle: a natural gas turbine followed by a heat recovery steam generator (HRSG). The steam from the HRSG is used to produce power while the gas turbine exhaust is processed to help in removing CO2 in the gas-liquid column in the air contactor unit.

The block CMPR represents the compressor of the gas turbine section which compresses air from an atmospheric pressure to a pressure of 10 bar. It is modeled with an isentropic efficiency of 85% and a mechanical efficiency of 90% [18]. The combustor of the real gas turbine is modeled using the block AIR-COMB, which is a Gibbs reactor in Aspen Plus®. This automatically determines the product composition based on the input components (considers all components present in the “Property” section of the software as possible products). In this case, the two input streams are compressed air (stream 49) and natural gas (stream 50), Natural gas enters at 25°C and 10 bar, while air enters at 10 bar and 315°C. AIR-COMB operates at about 1000°C and 10 bar.

The products from the combustion process are sent to the gas turbine (TURB-GAS), which expands the gases to atmospheric pressure. The gas turbine is modeled with a discharge pressure of 1 bar. The exhaust is then sent to the HRSG block, which is simplified in the model as a heat exchanger, with steam exiting at 415°C (stream 54) which is same temperature as stream 65. Both are entering the steam turbine (block ST-TURB).

IV. RESULTS & DISCUSSION

This chapter analyzes the outcomes obtained by the simulation. Through looking at the mass flow of CO2 captured along with the solution recovery for both solutions (KOH& NaOH) in the model of the plant, utilizing pinch analysis to evaluate the energy performance of the model. The results obtained through the simulation stand out with low deviation from the literature results [18], in terms of mass flow rate. Table 4-1 presents the percentage deviation for Certain streams from each section of the simulation in difference from the values obtained from the literature.

Table IV-1 Percentage Deviation

Section	Stream	Mass flow rate (tonne/hr)		%Deviation
		Simulation	Literature	
Air Contactor	**9**	**189.749**	**191.8**	**1%**
Calciner	**44**	**162.43**	**163**	**0.2%**
Slaker	**61**	**63**	**63.2**	**0.3%**
CO_2 Compressors	**CO2**	**162.432**	**144.2**	**12.6%**

Table 4.1 reveals that the simulation mass flow rates are close to the literature values. There are some results that show a slight deviation from the literature due to the reason that the literature uses design specifications tool provided by Aspen Plus in certain blocks inside the simulation. These tools let the simulation outcome establish a certain value that is set by the user. For example, In the literature a design specification is used to vary the mass flow rate of the solvent (stream 3) to achieve a CO2 capture of about 75% in the SEP-1 block. In this simulation results were converged without using design specification tool.

A. CARBON CAPTURE

The main objective of the Direct air capture method is to reduce the amount of carbon dioxide in the air, for this reason, capture percentage is evaluated. Tabel 4-2 shows the percentage carbon dioxide capture for each solution in comparison with literature.

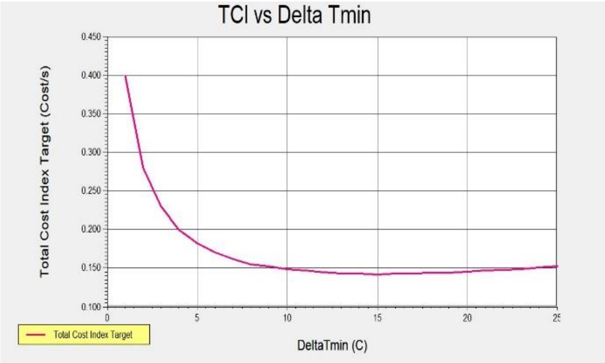

Figure IV-1 Total Cost Index VS. ΔTmin.

Table IV-2 Capture Percentage

	KOH	***NaOH***
Stream 2 (tonne/hr) CO_2	***157.22***	***157.22***
Stream 5 (tonne/hr) CO_2	***15.94***	***21.2834***
Carbon capture	***%89.8***	***%86.4***
Enhancement percentage	***%15.2***	***%12.25***

Table 4.2 summarizes two important observations of the DAC simulation. One is that, at the same process conditions, CO_2 capture efficiency is higher with KOH than with NaOH. This is simply because has a higher KOH solubility in water compared to NaOH, since it forms stable potassium carbonate (K_2CO_3). Consequently, KOH is more efficient in CO_2 capture, and its regeneration is easier, which makes it cost-effective even at big scales. On the other hand, NaOH gives rise to the less stable sodium carbonate, Na_2CO_3, which will be harder to regenerate and, therefore, would require more energy input for regeneration. That scenario increases its operating cost and furthers more environmental problems in terms of waste generation.

Both NaOH and KOH are caustic and hence need to be overseen with care. However, in most DAC systems, KOH is preferred since the by-products are relatively easy to manage besides having less environmental impact. The simulation results show an excellent possibility of enhancing CO_2 capture efficiency much larger than that reported in the literature.

B. ENERGY ANALYSIS

Energy efficiency is important to improve the performance and sustainability of Direct Air Capture (DAC) systems. This section focuses on utilizing pinch analysis to optimize the Heat Exchanger Network (HEN) of a DAC system that uses potassium hydroxide (KOH) and sodium hydroxide (NaOH) solutions as absorbents. The analysis aims to reduce energy demands, operational costs, and the total cost index by improving heat recovery within the system. Using Aspen Energy Analyzer (V14), the hot and cold streams within the DAC system were analyzed to identify the optimal ΔT_{min}, calculate energy recovery potential and propose the most energy-efficient HEN configuration for the process.

1) *Minimum Temperature Difference*

A key parameter influencing system design and performance is the minimum temperature difference (ΔTmin) in the heat exchangers. Figure 4-2 shows the relationship between ΔTmin and the cost index, where the optimal ΔTmin is identified =15 C. The optimal ΔTmin represents a balance between energy recovery and capital costs, minimizing the total cost index. For the current systems, the identified optimal ΔTmin aligns with an optimized energy performance.

2) *Composite Curves*

As shown in figure 4-2 the composite curves, for both systems, derived from the simulation, are identical due to consistent operational and thermal integration assumptions. The theoretical minimum energy requirements from the composite curves are as follows:

- Minimum Heating Demand: 23 MW
- Minimum Cooling Demand: 98 MW

These values represent the lowest achievable heating and cooling energy demands under perfect heat integration scenarios.

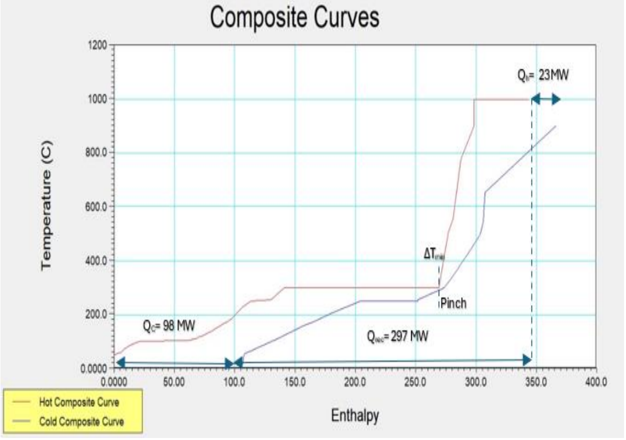

Figure IV-2 Composite Curves.

3) *Grand Composite Curve*

In the GCC as shown in figure 4-3, the pinch temperature is found where the curve touches the temperature axis, it is 299 C. In addition, GCC represents minimum heating and cooling utility duty, are 23 MW and 98 MW, respectively, while a pocket represents the region of process-to-process heat transfer. Furthermore, the negative slop of the curve shown below the pinch point indicates that the process in this region acts as a heat source, while the positive slop shown above the pinch point means that the process in that region acts as a heat sink [23].

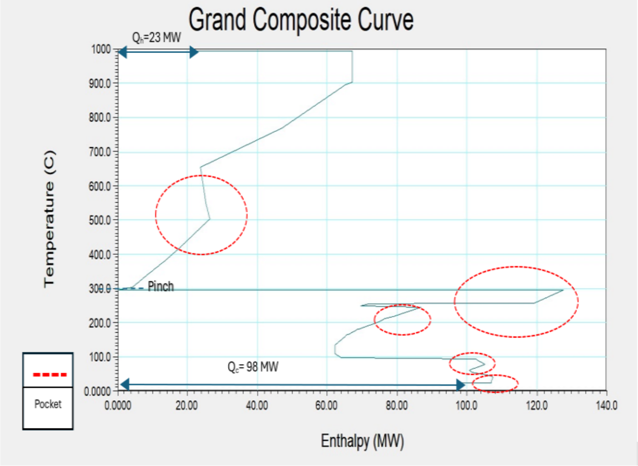

Figure IV-3 Grand Composite Curve

4) *Optimal Scenario*

Based on the above analysis, the software has redesigned the base model and obtained 10 different scenarios, trying to find the optimal case which results in highest energy and cost saving. All the 10 scenarios were infeasible. After retrofitting them, all except one becomes unfeasible. That unfeasible design becomes infeasible because it violates the second law of thermodynamics. From the table, it is obvious that the fifth design is the optimal one, by looking at the total capital index and the other crucial factors. Beyond that, a comparison between the optimal case and the base case was conducted as shown in table 4-3 below. This balance highlights the potential for significant energy savings through proper selection of ΔTmin, ensuring efficient thermal integration without excessive equipment costs.

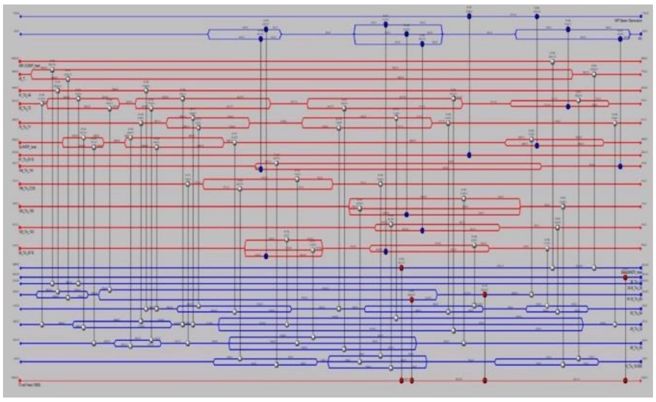

Figure IV-4 Optimal Scenario

Table IV-3 Comparison Between the Optimal Case and the Base Case

	Base Case	**Optimal Case**	**Saving Percentage**
Total Cost index ($/s)	**0.7173**	**0.2298**	**%67.96**
Heating (MW)	**174.972**	**51**	**%70.85**
Cooling (MW)	**246.611**	**103.3**	**%58.1**

5) *Heat Demand After Energy Analysis and Thermal Recovery*

After applying the pinch analysis, additional potential heat sources within the plant were evaluated. The slaker, being a highly exothermic process, enables the recovery of thermal energy. For the KOH-based system, assuming a 75% efficiency in directly utilizing the generated thermal energy, the heat recovered from the reactor is calculated as -95.69 MW. Consequently, the residual heat demand that cannot be met by the plant's heat recovery system is 79.282 MW, which must be supplied by natural gas. In the case of the NaOH-based system, due to differences in reaction energetics and process efficiency, the recovered heat is calculated as -96.27 MW under the same 75% efficiency assumption. The remaining heat demand for this system is slightly higher, at 80.657 MW, also requiring supplementation by natural gas.

These results highlight the relative energy demands and recovery efficiencies of the two solutions. While the KOH-based system demonstrates marginally lower heating requirements compared to the NaOH system, the differences are minimal, reflecting the similar thermodynamic properties of the two solutions under the given operating conditions. A detailed summary of these findings is presented in Table 4-4

Table IV-4 Final Heat Demand After Energy Analysis and Thermal Recovery

	Heat Demand /Availability	
	NaOH (MW)	**KOH (MW)**
From energy analysis	**176.972**	**174.972**
Slaker reactor	**-96.27**	**-95.69**
Total	**80.657**	**79.282**

6) The energy performance of Direct Air Capture (DAC) technology

The energy performance of Direct Air Capture (DAC) technology has been analyzed in relation to other studies. Table 4-5 summarizes the electricity and heat demands based on existing literature. The heat demand necessary for the system, primarily supplied by natural gas in the calciner and combustion tower units, ranges from 1420 to 2250 kWh per ton of CO_2. The electricity demand for DAC is estimated to be between 2366 and 2790 kWh per ton of CO_2, primarily generated by compressors, air blowers, and CO_2 compression. In this simulation it is found out that the heat demand reached 1060 kWh per ton of CO_2 and the electricity demand reached 179 kWh per ton of CO_2 for KOH solution Whereas, for NaOH solution it is found out that the heat demand reached 1114 kWh per ton of CO_2 and the electricity demand reached 186 kWh per ton of CO_2. Moreover, in 2018, Carbon Engineering reported a system powered entirely by electricity, requiring a total of 1500 kWh per ton of CO_2 for both electricity and heating. Additionally, research by Keith et al. highlights significant advancements in meeting the energy needs of DAC and presents three scenarios. In the first scenario, thermal energy and electricity are supplied by natural gas, steam turbines, and gas turbines, requiring 8.81 GJ of natural gas or 2450 kWh per ton of CO_2. The second scenario removes the gas turbine and relies on grid electricity, resulting in energy consumption of 5.25 GJ of natural gas and 366 kWh of electricity. The third scenario assumes that the CO_2 compression unit is eliminated, meaning the produced CO_2 is readily available, thus avoiding costs associated with the compressor and its electricity demand.

Table IV-5 The energy required for the HT DAC system.

Aqueous solution	***Energy Demand***		***References***
	Electricity (kWh/t-CO_2)	***Heat (kWh/t-CO_2)***	
NaOH	***440***	***1678***	*[25]*
NaOH	***764***	***1420***	*[26]*
NaOH	***1199***	***2461***	*[27]*
NaOH	***494***	***2250***	*[28]*
NaOH	***2790***	***-***	*[29]*
KOH	***1500***	***-***	*[30]*
KOH	***-***	***2450***	*[31]*
KOH	***366***	***1458***	*[31]*
KOH	***77***	***1458***	*[31]*
KOH	***179.588***	***1060.16***	***This Simulation***
NaOH	***186.655***	***1114.523***	***This Simulation***

V. CONCLUSION &FUTURE WORK

This study explored the design and performance of Direct Air Carbon Capture (DAC) systems using sodium hydroxide (NaOH) and potassium hydroxide (KOH) solutions as absorbents. Through detailed simulations in Aspen Plus, the research assessed the energy demands and CO_2 capture performance of these systems.

The findings indicate that KOH offers superior CO_2 capture efficiency (89.8%) compared to NaOH (86.4%), primarily due to its higher solubility and ease of regeneration. Energy optimization was achieved through pinch analysis, reducing heating and cooling demands to 51 MW and 103 MW, respectively, in the optimal design. Thermal recovery from the slaker reactor contributed significantly to overall energy savings, offsetting 54.7% of heating demands in the KOH-based system and 54.4% in the NaOH-based system, resulting in residual demands of 79.282 MW and 80.657 MW, respectively.

These results underscore the viability of DAC systems for atmospheric CO_2 removal, particularly when optimized for energy efficiency and integrated with advanced thermal recovery mechanisms. While KOH-based systems demonstrate better performance, both systems highlight the importance of balancing capture efficiency and energy requirements to ensure sustainability.

Future work should focus on addressing remaining challenges, including improving scalability and integrating renewable energy sources to further enhance the feasibility of DAC technology. The results of this study provide a solid foundation for advancing DAC systems as a critical tool for mitigating climate change.

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