

*Original Research*

# Parameter Optimization of the Direct Air Capture (DAC) Process to Achieve Net Zero Emission Targets

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## ABSTRACT

Direct Air Capture (DAC) technology has gained recognition as an effective method for reducing atmospheric carbon dioxide (CO<sub>2</sub>) levels. This study emphasizes the optimization of critical process parameters to improve the efficiency of aqueous hydroxide-based DAC systems while lowering operational costs. Aspen Plus simulations were employed to model the process flow, pinpoint key reaction mechanisms, and evaluate how different operating conditions influence CO<sub>2</sub> capture efficiency. A sensitivity analysis explored the impact of variables such as air contactor parameters, solvent concentration, temperature, pressure, and moisture content on system performance. The results demonstrated that adjusting the Ca (OH)<sub>2</sub> flow rate to 760 t/h achieves a 75% CO<sub>2</sub> capture rate at the air contactor, while maintaining an inlet air pressure of 1.1 atm enhances absorption. The CO<sub>2</sub> capture rate increased gradually with the increase of inlet air temperature. The highest CO<sub>2</sub> capture rate of 92 % is given at 40°C, and 4 % H<sub>2</sub>O content is in the inlet air. However, the impact of the moisture content is negligible. Furthermore, structured packing materials like BX packing outperformed Mellapak 250Y and Mellapak 350Y in efficiency. These insights support the development of economical DAC strategies, advancing technologies for carbon removal to achieve net zero emissions.

## INTRODUCTION

Global climate change is greatly influenced by greenhouse gases, particularly carbon dioxide (CO<sub>2</sub>), which raises sea levels, atmospheric temperatures, and the frequency of extreme weather events (Baker et al. 2018). These impacts have had serious, long-lasting, and irreversible repercussions on ecosystems and human living spaces (Yao et al. 2023). Over the last twenty years, the concern over rising CO<sub>2</sub> emissions has grown significantly due to the rapid expansion of the global economy (Storrs et al. 2023; Han et al. 2023). Anthropogenic carbon emissions have rapidly increased over the decades and reached an atmospheric CO<sub>2</sub> concentration of 410 ppm at an alarming rate (IPCC, 2021). These emissions mostly come from industrial activities and the burning of fossil fuels (M. Pathak et al. 2022).

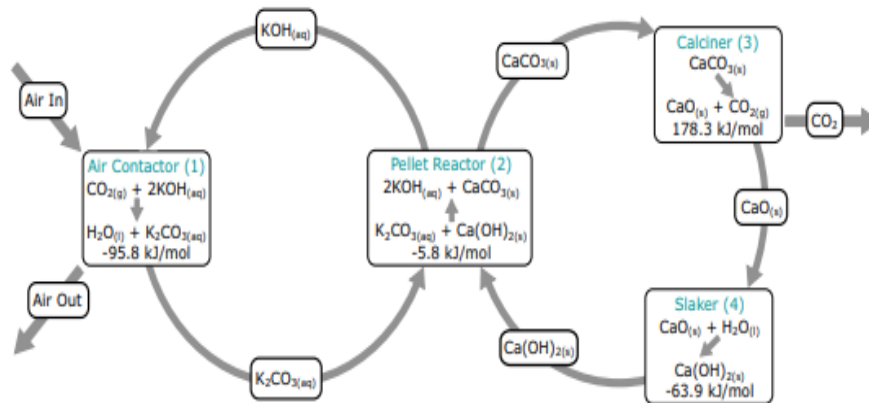
Over a while, multiple ways of CO<sub>2</sub> reduction have been practiced and examined. Out of those technologies, post-combustion carbon capture plays a vital role compared with pre-combustion carbon capture and oxy-fuel combustion (Udara et al. 2020). However, direct air capture (DAC), which captures CO<sub>2</sub> directly from the atmosphere, has been discussed recently due to its economic and technical feasibility over other technologies (Shaik et al. 2021). Comparing post-combustion carbon capture with direct air capture is unrealistic as those technologies address two different CO<sub>2</sub> sources, even though the prime objective is to capture CO<sub>2</sub>.

Multiple technologies are available for DAC comprising absorption with aqueous hydroxide solutions such as potassium hydroxide (KOH), adsorption with solid inorganic bases such as sodium carbonates Na<sub>2</sub>CO<sub>3</sub>, and adsorption with solid-supported amines (SSA) such as silica mesocellular foam (Eloy S. et al. 2016).

Even though there are technical differences between the aqueous hydroxide solution method and solid sorbent method, they operate under the same concept of removal of CO<sub>2</sub> from the atmosphere and by contact with a liquid solution or solid surface followed by desorption process to liberate attached CO<sub>2</sub>. To liberate CO<sub>2</sub>, a high heat temperature will be provided, and a high-purity CO<sub>2</sub> stream will be obtained (Abouelnaga 2022). Once CO<sub>2</sub> is concentrated with the desorption process, this CO<sub>2</sub> can be stored underground, under the ocean, or in un-mineable coal and oil fields, or used for enhanced oil recovery (EOR) to recover additional crude oil once primary and secondary oil recovery is completed (Udara et al. 2019).

The prime chemical used in the present study was aqueous hydroxides with multiple inter-circular material recovery stages. The main idea behind replenishing liquid chemicals is to overcome the damage to the CO<sub>2</sub> absorption capability with heat degradation. Air contactor is the core of the process which is used to capture the CO<sub>2</sub> by contacting aqueous solution with the atmospheric air effectively.

The simplified process flow diagram is given in Fig. 1.



**Fig. 1** :Process Chemistry and Thermodynamics (Keith et al. 2018)

The main four-unit operations are given in boxes named Air contactor, Causticizer (pellet reactor), Calciner, and Slaker. The main reaction of CO<sub>2</sub> absorption proceeds in the Air contactor unit, where those are converted to potassium carbonate (K<sub>2</sub>CO<sub>3</sub>) and water (H<sub>2</sub>O). Followed by air contactor, the causticizer unit operation plays another important role in converting K<sub>2</sub>CO<sub>3</sub> into KOH by reacting with calcium hydroxide (Ca(OH)<sub>2</sub>) by creating a by-product of KOH and Calcium carbonate (CaCO<sub>3</sub>). KOH can be recycled back to the air contactor unit, while CaCO<sub>3</sub> will transfer to the Calciner unit, where it is heated up to a higher temperature to produce calcium Oxide (CaO) and CO<sub>2</sub>. The CO<sub>2</sub> generated at this stage will be recovered as the main output, which will be considered for sequestration. CaO will follow the Slaker unit to react with H<sub>2</sub>O to produce Ca(OH)<sub>2</sub>, which will then be transferred to the causticizer unit again or next cycle (Keith et al. 2018; Terlouw et al. 2021).

### 1.1. Advantages and Disadvantages of DAC

Plenty of advantages are associated with the aqueous DAC capturing system, which is summarized for further consideration for the optimization process and given in Table 1 (Natonal Academies, 2018; Keith et al. 2006; Royal Society 2018).

Table 1: Advantages and disadvantages of the DAC process for carbon removal

Advantages	Disadvantages
The higher cumulative removal capacity compared to the other carbon dioxide removal technologies (CDR)	Higher Capital cost
The lower area of land required to install and operate the DAC system and unproductive land can also be used.	Higher Operational cost

The amount of water required is considerably lower than the bioenergy carbon capture and storage (BECCS) mechanism.	Energy requirement to operate the process is significantly larger.
Captured CO <sub>2</sub> can be stored permanently for much longer without any issues.	
According to energy availability, the plant can be located as it does not require any further support or geographical considerations.	
Even with the lower concentration of CO <sub>2</sub> , plants will operate to capture the maximum amount of available CO <sub>2</sub> .	

The main reason behind the higher operational cost is that the atmospheric concentration of CO<sub>2</sub> is around 0.04 % compared to the CO<sub>2</sub> percentages in flue gases such as 13 % for coal-fired power plants, 4-5 % for gas-fired power plants, and 15-30 % for cement industry flue gas (Udara et al. 2019; David et al. 2018). The parameter optimization to minimize the required energy for operational process of DAC is important. Therefore, DAC process was developed in Aspen Plus and conducted simulations to identify the optimum parameters such as inlet air pressure, moisture content of the air, inlet air temperature, liquid solvent temperature, and the packing material used in the reactor.

## 2. MATERIALS AND METHODS

The overall process model is designed with the main chemical reactions involving the four major sections: Air Contactor, Pellet unit, which is also called Causticizer, Calciner unit, and Slaker unit. The process flow diagram with important chemical reactions is given in Fig.2.

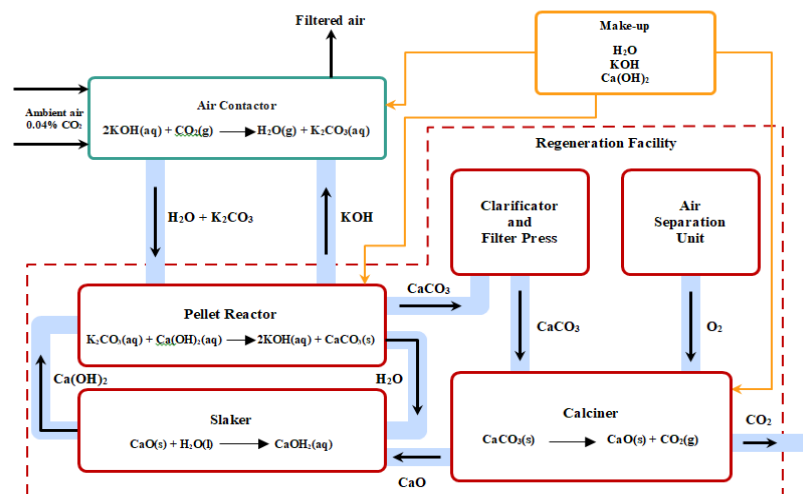
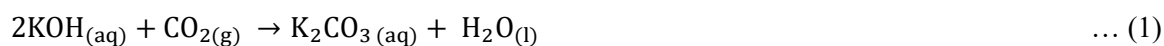


Fig. 2: The process flow diagram with important chemical reactions

## 2.1. Process Modeling

The DAC plant was developed in Aspen Plus V11 with the available literature data and support from Aspen Plus data banks. The most important chemical reactions of the four major sections are given in Equation 1 to 4.

Air Contactor:



Pellet Reactor:



Calciner:



Slaker:



As the property method for calculations in Aspen Plus, ENRTL-RK is used with the Redlich – Kwong equation of state (RK-SOAVE) and Henry's law for vapor phase properties. Atmospheric air composition and flow rates, as well as the other operating conditions of the DAC model, are given in Table 2. The two-film theory considers the rate-based model, which considers mass transfer analysis at the liquid–vapor interface. Other than the four major chemical reactions, multiple equilibrium reactions, salt formation, and dissociation reactions are happening in the DAC system (Table 3).

**Table 2:** Operating Conditions and basic parameters of the rate-based model (An, K et al. 2022).

Unit: Air Contactor	
Property Method	ENRTL-RK
Model	Mixer
Operating Temperature	21°C
Pressure	1 bar
Unit: Pellet Reactor	
Property Method	ENRTL-RK
Model	Crystallizer
Operating Temperature	21°C
Pressure	1 bar
Unit: Calciner	
Property Method	PENG-ROB
Model	RStoic
Operating Temperature	900°C
Pressure	1 bar

	Unit: Slaker Unit	
Property Method		PENG-ROB
Model		RStoic
Operating Temperature		300°C
Pressure		1 bar

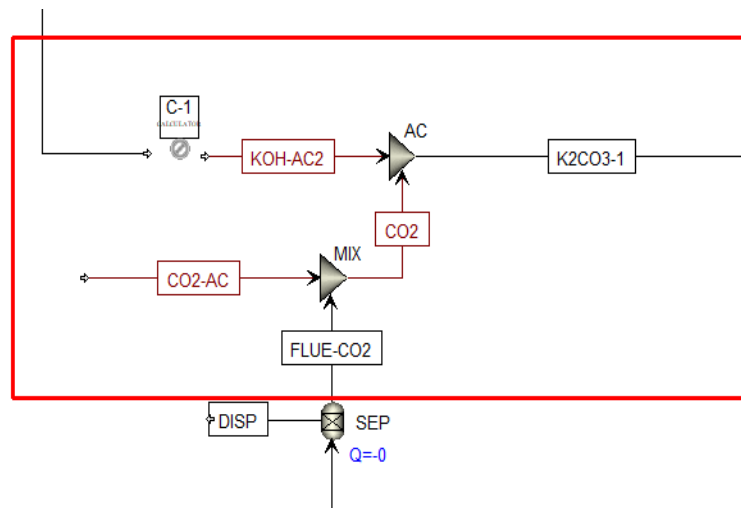
The following equilibrium reactions (Table 3), salt formation, and dissociation reactions were considered for the process modeling for the DAC system (An, K et al. 2022). At the same time, natural gas (NG) combustion is also included in the calcination process.

**Table 3:** Multiple equilibrium reactions

Air Contactor
$CO_2 + OH^- \rightarrow HCO_3^-$
$HCO_3^- + OH^- \rightarrow CO_3^{2-} + H_2O$
$2H_2O \rightarrow H_3O^+ + OH^-$
Pellet Reactor
$Ca^{2+} + CO_3^{2-} \rightarrow CaCO_3$
Calciner
$CH_4 + O_2 \rightarrow CO_2 + H_2O$
$CaCO_3 \rightarrow CaO + CO_2$
$2C_2H_6 + 7O_2 \rightarrow 4CO_2 + 6H_2O$
$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$
Slaker
$CaO + H_2O \rightarrow Ca(OH)_2$

## 2.2. Process Layout

The key sections of the process comprise four major parts, including the Air contactor, Pellet Reactor, Calciner, and Slaker. The air contactor was designed with the Mixer unit and separator block to represent the carbon absorption process to liquid solvent stream (Fig. 3). As the air contactor of the DAC process is an innovative component of the real process, Aspen Plus does not provide a specific unit operation model for process implementation.



**Fig. 3:** Air Contactor section

AC block: Air Contactor Unit

MIX: Mixer for ambient air and flue gas

KOH: Potassium Hydroxide flowrate

To model the air contactor without complex calculations, three different Aspen blocks, a separator, and two mixer units were used to separate  $\text{CO}_2$  from atmospheric air. MIX block is used to mix the ambient air with flue gas  $\text{CO}_2$ , which comes from the gas turbine exhausts once they have isolated the  $\text{CO}_2$ . After that, at the AC block,  $\text{CO}_2$  will absorb into the liquid solvent, aqueous KOH (lean solvent), composed of 2.0M  $\text{K}^+$ , 1.10 M  $\text{OH}^-$ , and 0.45 M  $\text{CO}_3^{2-}$ . Based on previous studies by Keith et al. (2018), liquid solvent flow rate and atmospheric air flow were extracted for the base-case simulation (Keith et al. 2018). Even though liquid solvent flow is introduced for the air contactor unit, in the real plant, it will come from the pellet unit as a product of the reaction with  $\text{Ca}(\text{OH})_2$ . An open-loop process simulation has been developed to minimize convergence issues and reduce the complexity of the simulation process. The required solvent and air flow rates were taken from previous studies (Keith et al. 2018).

The main objective of this study was to identify optimum parameters to minimize the operational cost of the DAC process. To achieve that, optimization of the Air Contactor unit, specifically considered as the amount of  $\text{CO}_2$  absorbed by the unit, will increase overall efficiency and reduce the operational cost. Based on the literature (Keith et al. 2018), the total air inflow is 251,000 t/h with 0.06 %  $\text{CO}_2$  content at 21 °C atmospheric pressure (total  $\text{CO}_2$  content in the air inflow as 150.6 t/h).

There are key points to consider for process optimization.

- A:  $\text{Ca}(\text{OH})_2$  flowrate and parameters to enhance the Pellet reactor operation

- B: Natural Gas ( $\text{CH}_4$ ) flowrate and parameters to enhance the Calciner unit operation
- C: Natural gas (NG) flowrate and parameters to enhance the Slaker process
- D: Atmospheric air flowrate and parameters
- E: KOH solvent flowrate and parameters to enhance Air contactor unit and Pellet reactor
- F:  $\text{H}_2\text{O}$  flowrate and parameters to enhance the Slaker Process and  $\text{CO}_2$  purification process

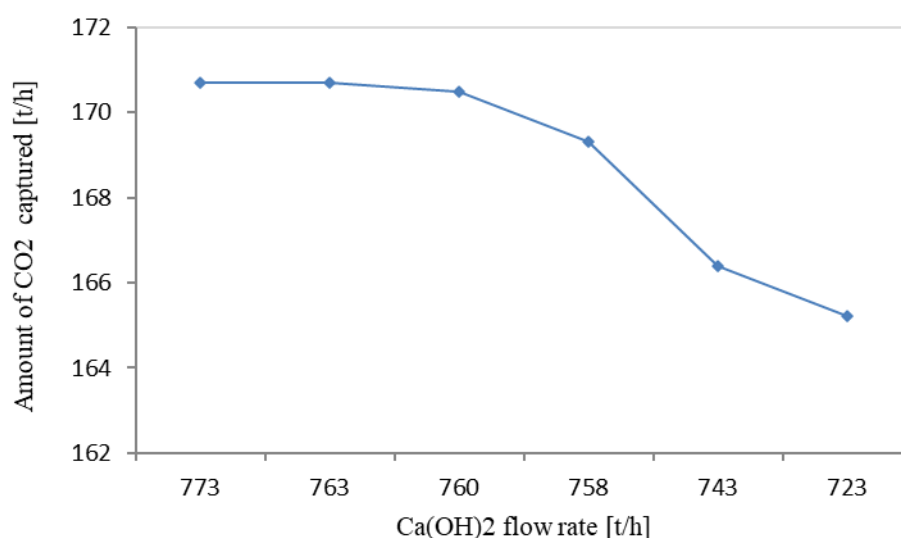
Even though water is generated during reaction 1 (air contactor unit), it will not be fully secured for reaction 4 (Slaker unit) due to evaporation and other losses during the operation. Therefore, water must be supplied to the Slaker unit as steam and cold water and to the  $\text{CO}_2$  purification process at the final stage of the DAC process.

### 2.3. Sensitivity Analysis – DAC overall industrial scale plant

The abovementioned A-F, six potential key points for the process optimization, were considered to implement the DAC as a viable option for achieving net zero emission standards.

Optimization of  $\text{Ca}(\text{OH})_2$  flow rate and parameter optimization, such as the temperature and pressure, as well as the composition of the stream, were considered. With the changes in those parameters, the amount of  $\text{CO}_2$  captured at the final stage after the Calciner was analyzed.

As the base case value 229.753 t/h flowrate of  $\text{Ca}(\text{OH})_2$ , which 773 t/h of total  $\text{Ca}(\text{OH})_2$  stream flowrate is considered as that will be the theoretical flowrate required to react with potassium carbonate ( $\text{K}_2\text{CO}_3$ ) and produce  $\text{CaCO}_3$  and  $\text{CO}_2$  with 75 % capture rate at the air contactor.



**Fig. 4:** Effect of  $\text{Ca}(\text{OH})_2$  flow rate on  $\text{CO}_2$  capture efficiency



It can be noticed that the amount of  $\text{CO}_2$  captured decreased with the increase of  $\text{Ca}(\text{OH})_2$  flow rate (Fig. 4). The main reason for that is the number of reactants required for the pellet reactor decreasing, and it will not produce enough  $\text{CaCO}_3$ . Here, the total  $\text{Ca}(\text{OH})_2$  flow rate is evaluated in the pellet reactor. The total amount of  $\text{CO}_2$  at the final stage of purification after the Calciner unit is given in Fig. 4. It can be concluded that the  $\text{Ca}(\text{OH})_2$  minimum flow rate should be 760 t/h to capture 75 % of  $\text{CO}_2$  (112.6 t/h) at the air contactor. However, the temperature and pressure of the  $\text{Ca}(\text{OH})_2$  do not impact the  $\text{CO}_2$  capture, varying from 1-2 bars and 21- 45 °C.

KOH flow rate, as well as natural gas flow rate, can be reduced to minimize the cost of operation. However, a reduction of KOH will reduce the amount of  $\text{CO}_2$  captured at the air contactor and pellet reactor, and a reduction of natural gas flow reduces the heat supply to the Calciner unit to recover captured  $\text{CO}_2$ . Therefore, both are at optimized values, such as 35000 t/h KOH flowrate to the air contactor unit and 12.6 t/h Natural gas flowrate to the Calciner unit.

#### 2.4. Sensitivity analysis – Kinetic Behavior of the Air contactor

The impact of atmospheric air temperature on the  $\text{CO}_2$  removal process was analyzed to identify the effect of climate conditions on the DAC process. Atmospheric air temperature varied from 0 °C to 40 °C, and pressure varied from 1.1 – 2 atm to identify the behavior of the air contactor unit as the amount of  $\text{O}_2$  removal. The base case values for the rate-based model are absorbed from An, K et al. 2022 and Sabatino et al., 2021 (An, K et al. 2022; Sabatino et al. 2021). The most important parameters of the inlet air stream and solvent stream are given in Table 4.

**Table 4:** Operating conditions of rate-based air contactor unit

Most important parameters for air contactor unit	
Inlet air flowrate [t/h]	150.6
Inlet solvent flow rate (lean solvent flowrate) [th]	19.08
KOH concentration in the lean solvent [mol/litre]	1.1
$\text{K}_2\text{CO}_3$ concentration in the lean solvent [mol/litre]	0.45
Number of air contactor units	6
Reaction condition factor	0.9
Film discretization points	5
Interfacial area factor	1.2
Liquid film discretization points	5
Parameters of packing bed for base case model development	
Packing type	Sulzer 250Y
Packing bed depth [m]	1.28
Packing bed diameter [m]	5.64
Range of Inlet air operating conditions	

Inlet air temperature [°C]	0-40
Inlet air pressure [bar]	1-2
Lean solvent temperature [°C]	0-40
Lean solvent pressure [bar]	1-6
Moisture content [%]	1-4

Based on the case, an Air contactor unit was developed in Aspen Plus to identify the atmospheric temperature, moisture content of the atmosphere (relative humidity), solvent temperature, and pressure of the inlet air and solvent stream. Moreover, three different packing materials compared with slight diameter and depth ratio changes. For each case, the CO<sub>2</sub> capture rate was calculated to compare the impact of the parameters and select the optimum values for better efficiency; the CO<sub>2</sub> capture rate can be calculated by the difference between rates of CO<sub>2</sub> entering the column and the rate of CO<sub>2</sub> leaving the system, which is given in equation 5.

$$\text{CO}_2 \text{ capture rate} = (\dot{m}_{\text{CO}_2-\text{IN}} - \dot{m}_{\text{CO}_2-\text{OUT}}) / \dot{m}_{\text{CO}_2-\text{IN}} \quad \dots (5)$$

The reaction kinetics was taken from Table 2 with the literature values for the rate of reaction parameters (Stefano 2018; Pinsent et al. 1956).

## 2.5. Chemical reactions and Kinetics

The mass transfer phenomenon between the liquid and vapor phases can be simplified in the following section. Those explanations are vital as they constitute the theoretical basis of the liquid and gaseous phase reaction process in the air contactor unit. The mass transfer mechanism can be explained using equilibrium-based stage efficiency and rate-based models.

The chemical kinetics of the main chemical reactions are listed in Tables 5 and 6, along with the equilibrium and kinetic data used for the Aspen Plus model development. For the equilibrium reactions (7-10), the equilibrium constant can be found using the equation 6:

$$\ln K_j = A_j + \frac{B_j}{T} + C_j \ln T + D_j T \quad \dots (6)$$

Equilibrium Reactions



**Table 5:** Constant values of equilibrium constant equations

Parameter	Reaction 7	Reaction 8	Reaction 9	Reaction 10
A <sub>j</sub>	132.899	216.049	214.582	-9.742
B <sub>j</sub>	-13445.9	-12431.7	-12995.4	-8585.47
C <sub>j</sub>	-22.4773	-35.4819	-33.5471	0
D <sub>j</sub>	0	0	0	0

Kinetic reactions are listed below, with the kinetic data in reaction numbers 11 and 12. The kinetic Equation used for mathematical calculations is defined in Aspen Plus and given in Equation (13).

Kinetic Reactions



$$r_j = k_j \left( \frac{T}{T_0} \right)^{n_j} \exp \left[ -\frac{E_j}{R} \left( \frac{1}{T} - \frac{1}{T_0} \right) \right] \quad \dots (13)$$

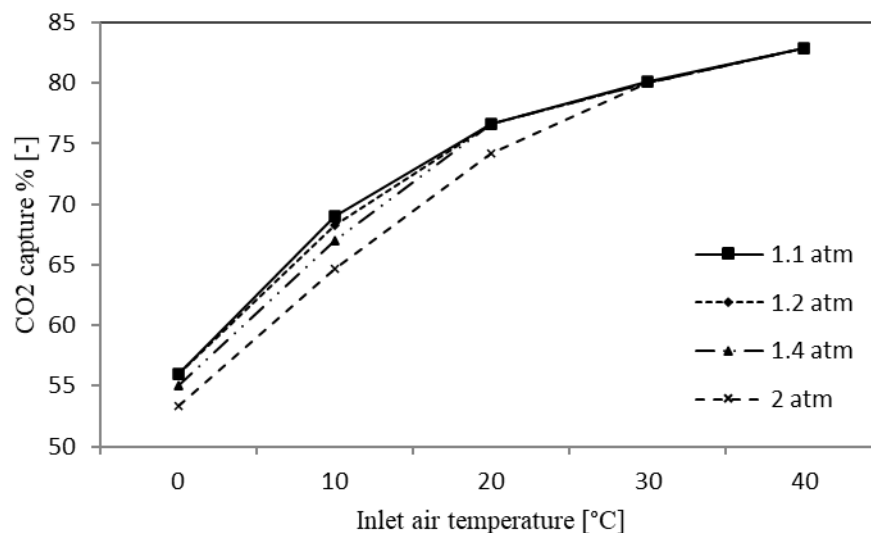
**Table 6:** Rate constant values

Parameter	Reaction 11	Reaction 12
k <sub>j</sub>	4.32e+13	2.38e+17
n <sub>j</sub>	0	0
E <sub>j</sub> (J/mol)	55470913.2	123305447
T <sub>0</sub> (K)	298	298

### 3. RESULTS AND DISCUSSIONS

#### 3.1. Effect of the inlet air temperature and pressure

The CO<sub>2</sub> capture percentage was calculated with the variation of inlet air temperature and pressure while maintaining flow rate and composition at the constant value (1 % H<sub>2</sub>O). The temperature of the stream was changed from 0 – 40 °C while pressure changed from 1.1 – 2 atm. CO<sub>2</sub> capture at the air contactor unit is shown in Fig. 5. Moreover, the lean solvent temperature is always maintained, like the inlet air temperature during every simulation. Based on the simulation CO<sub>2</sub> capture rate increased gradually with the increase of inlet air temperature. The outcome has been aligned with the previously reported analysis which is given in Keith et al. 2018 which is 21 °C temperature, and 1 bar pressure given 75% removal efficiency.

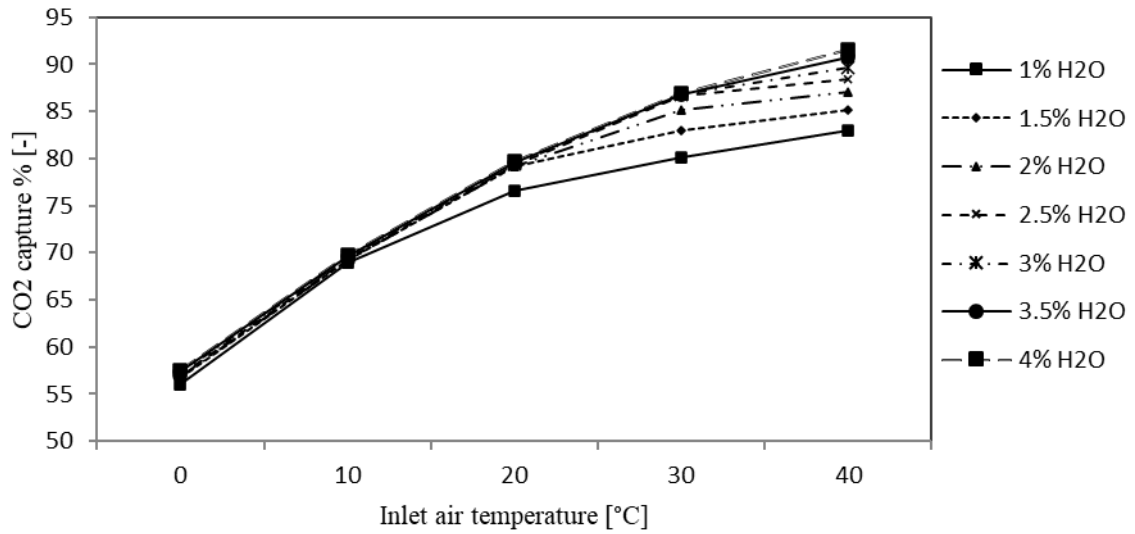


**Fig. 5:** Effect of inlet air temperature on CO<sub>2</sub> capture efficiency at different pressures

However, the air pressure has no significant impact on CO<sub>2</sub> capture. The main reason is that the rate of chemical reaction is only dependent on the temperature. However, the CO<sub>2</sub> removal percentage decreased with increased pressure at lower temperatures. The main reason for this is that with high pressure, the percentage of air contacting with the liquid sorbent will reduce due to higher pressure. Therefore, some air will not have enough contact time with the solvent for the reaction.

#### 3.2. Effect of the moisture content of the air

The CO<sub>2</sub> capture percentage was calculated with the moisture content of the inlet air. Moisture content varied from 1 % to 4 %, and the impact was analyzed by changing the air temperature from 0 to 40 °C as shown in Fig. 6.

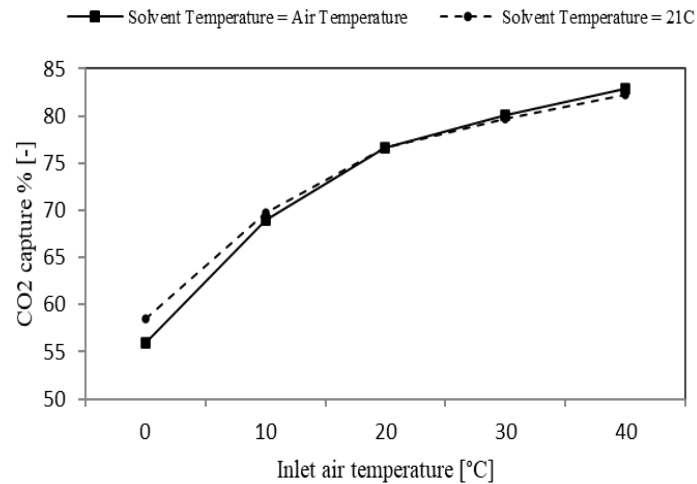


**Fig. 6:** Impact of Inlet Air Temperature on CO<sub>2</sub> Capture Efficiency Across Different Moisture Levels

According to Fig. 6, it can be seen that the moisture content of the air has a positive correlation with the CO<sub>2</sub> capture percentage. The highest CO<sub>2</sub> capture rate of 92 % is given at 40°C, and 4 % H<sub>2</sub>O content is in the inlet air. At the same time, the CO<sub>2</sub> capture rate gradually increased with the temperature increase for every case. However, there is no significant variation in the CO<sub>2</sub> capture rate with the moisture percentage in the inlet air for a given temperature. Based on the analysis, it is obvious that the CO<sub>2</sub> capture rate will drastically drop during the winter period. However, this analysis assumes that liquid solvents will always keep at the same atmospheric air temperature. The water in the solvent leads to water dissociation, forming more carbonate and bicarbonate at higher temperatures. The formation of more OH<sup>-</sup> ions eventually increases the molarity, increasing the CO<sub>2</sub> capture rates. The results are aligned with the previous experiments which have been published and identified relative humidity is less significant for DAC process (An, K et al. 2022).

### 3.3. Effect of the liquid solvent temperature

However, carbon capture rate variation has been analyzed with the assumption of maintaining the solvent temperature at 21 °C for the entire period. Even though atmospheric air temperature drops to 0 °C, liquid solvent supply to the air contactor unit will maintain 21 °C. Fig. 7 represents the variation of the CO<sub>2</sub> capture rate with the air temperature when solvent temperature is maintained at 21 °C.



**Fig. 7:** Impact of Inlet Air Temperature on CO<sub>2</sub> Capture Efficiency at constant solvent temperature

When the atmospheric temperature is 0-10 °C, there is a slight increment in the CO<sub>2</sub> capture rate as the solvent temperature is higher than the air temperature. However, maintaining solvent temperature at a much higher value than atmospheric temperature will eventually increase energy consumption. Therefore, the percentage of increase in CO<sub>2</sub> capture rate is not significant enough compared to the energy cost. The results are aligned with the previously published results by Keith et al. 2018, which was considered 21 °C as the solvent temperature for multiple changes of other parameters in DAC process.

### 3.4. Effect of the packing material

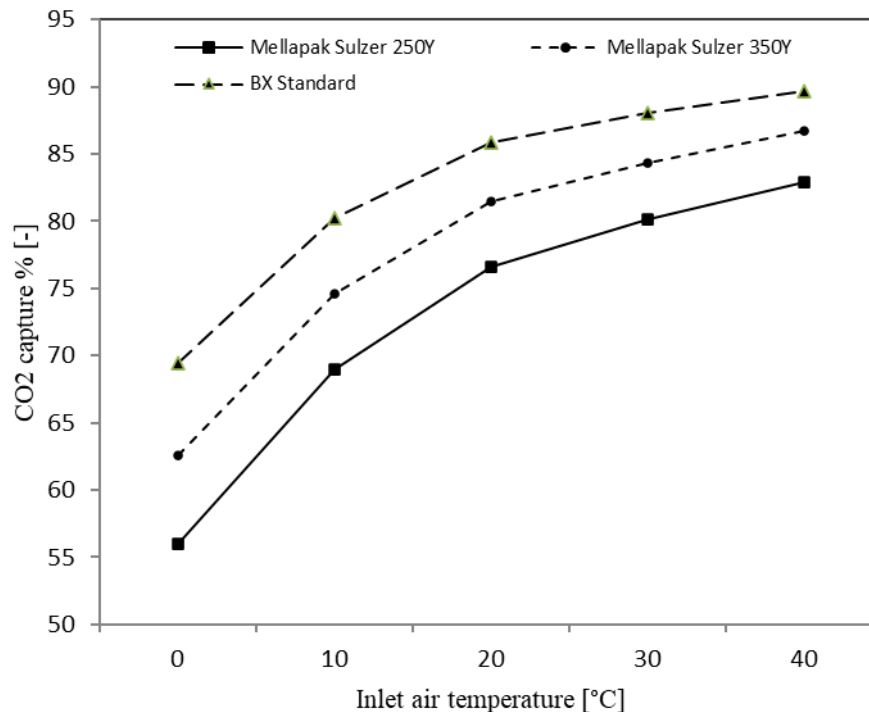
The packing section in the absorption column plays a vital role in CO<sub>2</sub> absorption by providing a surface area for gas and liquid phases to come into contact with the chemical reactions. Structured packing is considered for the simulation due to the higher mass transfer coefficient than the random packing. The most important parameters for selecting packing materials are void fraction and surface area for the reaction. Aspen Plus uses the Stichlmair Correlation for pressure drop calculations, which consists of three Stichlmair coefficients (Stichlmair et al. 1989). For the mass transfer calculations, information was taken from Bravo et al. 1985 during the simulation (Bravo et al. 1985).

Mellapak 250Y, Mellapak 350Y, and BX standard packing were considered for the analysis. During the simulations, base case values of air intake and solvent were maintained with the 1 % moisture content in the atmospheric air. The CO<sub>2</sub> removal efficiency was calculated for each case with the five different temperature values. Information about the packing materials is given in Table 7.

**Table 7:** Information about the packing materials

Packing Type	Size	Area (m <sup>2</sup> /m <sup>3</sup> )	Voids (%)	C1	C2	C3	Vendor	Reference
Mellapak	250Y	250	98	1	1	0.32	Sulzer	(Stichlmair et al. 1989)
Mellapak	350Y	350	98	1	1	0.32	Sulzer	(Stichlmair et al. 1989)
BX	-	450	86	15	2	0.35	Sulzer	(Stichlmair et al. 1989)

CO<sub>2</sub> capture variation with temperature is given in Fig. 8. According to the figure, BX packing shows the highest CO<sub>2</sub> removal efficiency, followed by Mellapak 350Y and Mellapak 250Y. The main reason is that the higher surface area of the packing material dominates the absorption process. When the surface area is high, the available contacting area for gas–liquid reaction is higher. With the temperature increase, CO<sub>2</sub> removal efficiency increased for all packing materials. The CO<sub>2</sub> removal efficiency is around 12 % higher for the process with Mellapak 350Y and 24 % higher for the process with BX packing than the Mellapak 250Y process.

**Fig. 8:** CO<sub>2</sub> capture variation with temperature

However, the cost of the packing material should also be considered for the techno-economic evaluation as that will have a significant role in capital cost calculation. Therefore, packing material cost is also considered to identify the optimum packing material for the air contactor unit.

Moreover, packing dimensions are also considered for the process optimization, as the gas absorption process is the key component of the DAC operation. The height of the two theoretical stages, as well as the diameter of the packing bed, was considered for the simulations. However, the packing diameter impact on CO<sub>2</sub> capture is not significant enough to overcome the cost of the packing material.

#### 4. CONCLUSION

This research highlights the critical role of optimizing key parameters in DAC systems to enhance CO<sub>2</sub> capture efficiency. The results reveal that maintaining a Ca(OH)<sub>2</sub> flow rate of 760 t/h, an inlet air pressure of 1.1 atm, and utilizing packing materials with high surface area significantly boost performance. With the temperature increase, CO<sub>2</sub> removal efficiency increased for all packing materials. The CO<sub>2</sub> removal efficiency is changed with different packing material and around 12 % higher for the process with Mellapak 350Y and 24 % higher for the process with BX packing than the Mellapak 250Y process. Although increased moisture content improves CO<sub>2</sub> absorption, careful consideration is required to manage the energy demands of maintaining solvent temperatures. The operational cost, capital cost and energy requirement for the DAC process must be analyzed with the experimental setup and validated with the simulation results. Future studies should prioritize techno-economic analyses, the integration of renewable energy sources, and strategies for scaling up to identify cost-effective approaches for large-scale DAC implementation.

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