CENG 124B CO_2 Capture Final Report

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Abstract

This project addresses the challenge of designing a scalable Direct Air Capture (DAC) system capable of removing 1 MMt CO_2/year from ambient air using potassium carbonate sorbent technology. The design integrated four primary unit operations: an air contactor achieving 74.5% CO_2 conversion, a pellet reactor with 90% calcium retention, a calciner operating at 900°C with 98% $CaCO_3$ decomposition, and a slaker with 85% CaO hydration, supported by heat exchangers and CO_2 compression. Process optimization through pinch analysis eliminated external heating requirements and reduced utility costs from \$33.07 M/yr to \$4.13 M/yr, while air contactor optimization using a packed bed reactor increased CO_2 conversion to 89.2% and eliminated spray nozzle complexity. The final design achieves the 1.17 MMt CO_2/year target (147.3 t/hr), resulting in CO_2 removal of 58.2 t/hr (509,832 t/yr). However, economic analysis revealed significant challenges with an NPV of -\$2.02 trillion over 25 years, primarily driven by unreasonably high methane combustion and electricity costs, indicating that future work must should correct errors in optimization and focus on proper energy integration, alternative heating sources, heat recovery, and simplifying the process to achieve commercial viability for large-scale carbon removal applications.

Contents

1 Introduction

This project focuses on the design of a scalable Direct Air Capture (DAC) system capable of removing 1,000 metric tons of CO_2 annually from the atmosphere. The system employs a potassium carbonate-based sorbent that reacts with CO_2 in ambient air to form potassium bicarbonate, which is then processed through a series of regeneration steps to recover CO_2 and recycle the sorbent. The full process includes an air contactor, slaker, crystallizer, calciner, and CO_2 compression stage. Each unit operation must be optimized to meet performance, and energy targets, while ensuring the system can be deployed at commercial scale in diverse geographic and infrastructural contexts.

Market demand for DAC technologies is accelerating as recognized by the Intergovernmental Panel on Climate Change (IPCC), which includes DAC as a necessary technology to meet net-zero targets outlined in the Paris Agreement.[1] Additionally, the International Energy Agency (IEA) emphasizes the need for negative emissions technologies such as DAC to balance residual emissions from hard-to-abate sectors, with several national governments and private initiatives ramping up investments in this area.[2] As highlighted by Keith et al.(2018),[3] DAC systems that are modular, energy-efficient, and compatible with low-carbon heat sources offer a promising pathway toward cost-effective carbon removal. The potential for policy incentives, such as carbon credits and tax benefits (e.g., Section 45Q in the U.S.)],[4] further increases the viability of DAC as a component of global de-carbonization strategies.

During CENG 124A, our team completed a preliminary design and simulation of the plant. The core regeneration step, calcination, was modeled using an RSTOIC reactor and supported by a simplified heat exchanger network to preheat the sorbent feed to approximately 900°C using external heating. A gas-solid separator was implemented to split CO_2 from the solid products, and an initial compressor block was added to prepare CO_2 for compression and storage. This simplified process flowsheet provided estimates of key energy requirements, established methane as the primary heat source, and laid the groundwork for the more detailed, plant-wide simulation and equipment analysis being developed in this phase of the project.

2 Design Results

2.1 Basis of Design

The process design presented in this report is based on the ambient air CO_2 capture system described in the paper "A Process for Capturing CO_2 from the Atmosphere" by Keith et al. (2018).[3] All inlet streams were scaled from mentioned report to our target of a CO_2 capture rate of approximately 3032 kmol/h, equivalent to capturing 1.29 million metric tons of CO_2 per year delivered at 151 bar at 40 °C . The primary objective of the plant is to produce high-purity compressed CO_2 suitable for permanent practical storage or further uses. To meet this goal, the system integrates a series of primary unit operations including an air contactor, pellet reactor, calciner, slaker, and multiple auxiliary units such as heaters, separators and a final compressor to facilitate material and energy recovery across the process.

Key design requirements include maximizing the thermal integration between heating and cooling units to reduce external energy demands, operating all reactors near their optimal conversion efficiencies, while minimizing unreacted material recirculation. For example, the calciner is designed to operate at 900°C and achieve a 98% conversion of $CaCO_3$ to CaO and CO_2 in a single pass, as reported by Keith.[3] Subsequently, accumulation of un-reacted $CaCO_3$ is avoided by with the addition of a recovery loop in this design to approach near complete conversion, as will be discussed further.

Design constraints assume steady-state operation, negligible pressure drops across unit operations unless explicitly modeled, and ideal phase separation in separator units given a differential in the physical phase of separated components. Ambient air enters at ambient conditions and is here modeled at 21 °C, and 1 bar. The current design iteration operates under the assumption that key utility demands, such as water, electricity, and heat, are met by external sources. The ENTRTL-RK property method in Aspen Plus is selected as the main model to account for the thermodynamic and electrolyte behavior of all compounds (especially aqueous components) to ensure accuracy in representing multiphase systems. This basis serves as the foundation for evaluating unit performance, sizing of equipment, and further optimization in later iterations.

2.2 PFD

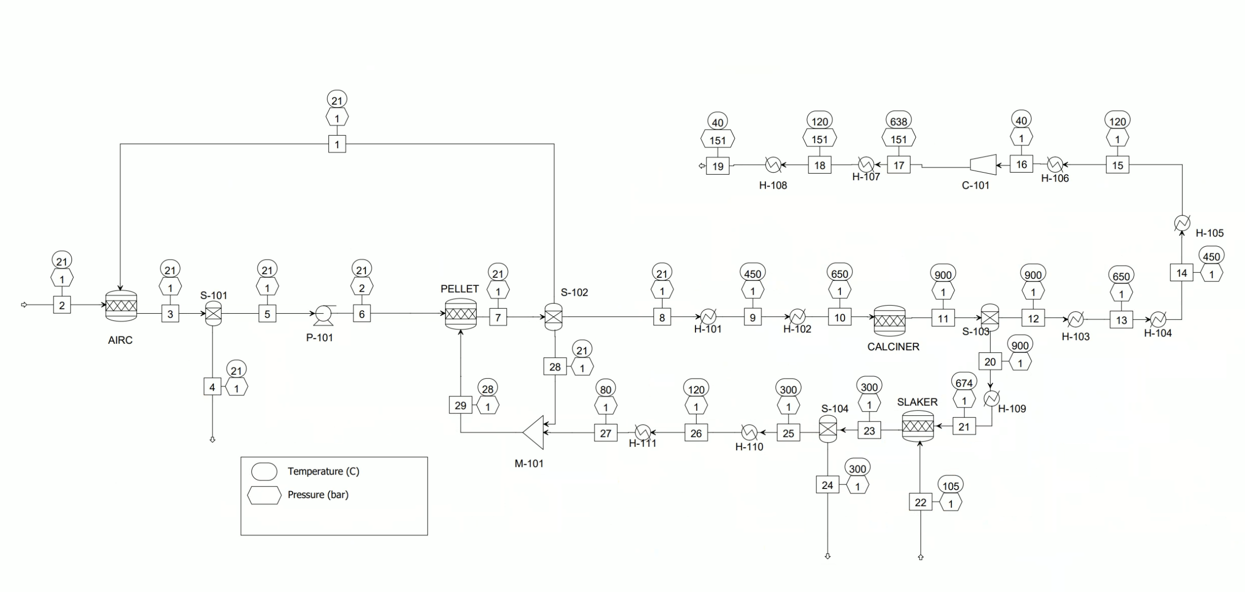


Figure 1: Overall PFD for CO_2 Capture Plant

2.3 Stream & Summary Tables

Table 1: Stream Tables for PFD in Fig. 1

Property/Component	**1**	**2**	**3**	**4**	**5**	**6**
Temperature (°C)	21	21	21.3	21.3	21.3	21.31
Pressure (bar)	1	1.013	1.013	1.013	1.013	1.52
Molar Vapor Fraction	0	1	0.239	1	0	0
Molar Liquid Fraction	1	0	0.761	0	1	1
Molar Solid Fraction 0	0	0	0	0	0	0
Molar Flows (kmol/hr)						
KOH	4129457	0	4124825	0	4124825	4124825
$K_2CO_{3(aq)}$	1141133	0	1143449	0	1143449	1143449
CO_2	0	3104	788.5	788.5	0	0
O_2	0	1636679	1636679	1636679	0	0
N_2	0	6174295	6174295	6174295	0	0
$Ca(OH)_2$	0	0	0	0	0	0
$CaCO_3$	0	0	0	0	0	0
CaO	0	0	0	0	0	0
H_2O	19812051	123867	19938233	0	19938233	19938233
Total Flows	25082641	7397945	33018270	7811762	25206508	25206508

Property/Component	**7**	**8**	**9**	**10**	**11**	**12**
Temperature (°C)	21	20.998	450	650	900	900
Pressure (bar)	1	1	1	1	1	1
Molar Vapor Fraction	0	0	0	0	0.433	1
Molar Liquid Fraction	0.999	0	0	0	0	0
Molar Solid Fraction	0.0002	1	1	1	0.567	0
Molar Flows (kmol/hr)						
KOH	25120534.39	3966.374	3966.374	3966.374	6998.794	3032.420
$K_2CO_{3(aq)}$	4129457.169	0	0	0	0	0
CO_2	1141133.443	0	0	0	0	0
O_2	0	0	0	0	3032.420	3032.420
N_2	0	0	0	0	0	0
$Ca(OH)_2$	336.935	336.935	336.935	336.935	336.935	0
$CaCO_3$	3094.306	3094.306	3094.306	3094.306	61.886	0
CaO	535.133	535.133	535.133	535.133	3567.552	0
H_2O	19845977.4	0	0	0	0	0
Total Flows	25120534.39	3966.374	3966.374	3966.374	6998.794	3032.420

Property/Component	**13**	**14**	**15**	**16**	**17**	**18**
Temperature (°C)	650	450	120	40	638.319	120
Pressure (bar)	1	1	1	1	151	151
Molar Vapor Fraction	1	1	1	1	1	0
Molar Liquid Fraction	0	0	0	0	0	1
Molar Solid Fraction	0	0	0	0	0	0
Molar Flows (kmol/hr)						
KOH	0	0	0	0	0	0
$K_2CO_{3(aq)}$	0	0	0	0	0	0
CO_2	3032.420	3032.420	3032.420	3032.420	3032.420	3032.420
O_2	0	0	0	0	0	0
N_2	0	0	0	0	0	0
$Ca(OH)_2$	0	0	0	0	0	0
$CaCO_3$	0	0	0	0	0	0
CaO	0	0	0	0	0	0
H_2O	0	0	0	0	0	0
Total Flows	3032.420	3032.420	3032.420	3032.420	3032.420	3032.420

Property/Component	**19**	**20**	**21**	**22**	**23**	**24**
Temperature (°C)	40	900	674	105	300	300
Pressure (bar)	151	1	1	1	1	1
Molar Vapor Fraction	1	0	0	1	0.069	1
Molar Liquid Fraction	0	0	0	0	0	0
Molar Solid Fraction	0	1	1	0	0.931	0
Molar Flows (kmol/hr)						
KOH	0	0	0	0	0	0
$K_2CO_{3(aq)}$	0	0	0	0	0	0
CO_2	3032.420	0	0	0	0	0
O_2	0	0	0	0	0	0
N_2	0	0	0	0	0	0
$Ca(OH)_2$	0	336.935	336.935	0	3369.355	0
$CaCO_3$	0	61.886	61.886	0	61.886	0
CaO	0	3567.552	3567.552	0	535.133	0
H_2O	0	0	0	3330.506	298.087	298.087
Total Flows	3032.420	3966.374	3966.374	3330.506	4264.461	298.087

Property/Component	**25**	**26**	**27**	**28**	**29**
Temperature (°C)	300	120	80	20.998	27.977
Pressure (bar)	1	1	1	1	1
Molar Vapor Fraction	0	0	0	0	0
Molar Liquid Fraction	0	0	0	1	0.895
Molar Solid Fraction	1	1	1	0	0.105
Molar Flows (kmol/hr)					
KOH	0	0	0	0	0
$K_2CO_{3(aq)}$	0	0	0	0	0
CO_2	0	0	0	0	0
O_2	0	0	0	0	0
N_2	0	0	0	0	0
$Ca(OH)_2$	3369.355	3369.355	3369.355	0	3369.355
$CaCO_3$	61.886	61.886	61.886	0	61.886
CaO	535.133	535.133	535.133	0	535.133
H_2O	0	0	0	33926.683	33926.683
Total Flows	3966.374	3966.374	3966.374	33926.683	37893.057

Table 2: Main Unit Operations in Fig. 1

Core Unit Operations	**AIRC**	**PELLET**	**CALCINER**	**SLAKER**
Temperature (°C)	21	21	900	300
Pressure (bar)	1.013	1	1	1
Heat Duty (MW)	292.5	-122.7	175.51	-106.2
Vapor Fraction	0.24	0	1	1
Single Pass Conversion	0.745	0.9	0.98	0.85

Table 3: Heat Exchangers in Fig. 1

Heat Exchangers	**H-101**	**H-102**	**H-103**	**H-104**	**H-105**	**H-106**
Outlet Temperature (°C)	450	650	650	450	120	40
Pressure (bar)	1	1	1	1	1	1
Heat Duty (MW)	43.83	23.45	-11.53	-8.68	-12.8	-2.69
Utility	Molten Salt	Molten Salt	BFW	BFW	BFW	CW
Process Side	Shell	Shell	Shell	Shell	Tube	Side

Heat Exchangers	**H-107**	**H-108**	**H-109**	**H-110**	**H-111**
Outlet Temperature (°C)	120	40	674	120	80
Pressure (bar)	151	151	1	1	1
Heat Duty (MW)	-35.19	-2.83	-15.38	-18.99	-3.99
Utility	BFW	CW	BFW	BFW	CW
Process Side	Tube	Tube	Shell	Shell	Shell

Table 4: Minor unit operations in Fig. 1

Other Unit Operations	**P-101**	**M-101**	**C-101**
Outlet Temperature (°C)	21	-28.33	638.32
Outlet Pressure (bar)	1.52	1	151
Net Work (MW)			24
Electrical Power (MW)	14		29
Efficiency	0.86		0.8

2.4 Air Contactor

The primary function of the Air Contactor (AIRC) system is the initial capture of dilute carbon dioxide from ambient atmospheric air (Stream 2, fed at 20 °C, 1 bar) via chemical absorption into a circulating aqueous potassium hydroxide (KOH) sorbent (Stream 1, 21 °C, 1 bar). Given the reaction takes place across different phases, the sorbent solution is pumped from top of a reactor through sprayer to increase surface area. The key reaction,

$$CO_{2(g)} + 2\,KOH_{(aq)} \longrightarrow K_2CO_{3(aq)} + H_2O_{(l)} \quad \Delta H_{rxn} = -95.8\ \text{kJ/mol} \tag{1}$$

which takes place in two different phases, requires high surface to volume ratio. A target capture efficiency of 74.5% is based on pilot performance reported by Keith *et al.*[3].

In the Aspen Plus simulation, the AIRC unit is modeled using a stoichiometric reactor block (RSTOIC) to impose the specified 74.5% CO_2 conversion, and thermodynamic properties were handled by the ENTRTL-RK (aqueous electrolytes) and RK-SOAVE (gaseous). After reaction, an ideal gas–liquid separator (S-101) vents the spent air (Stream 4). The split fraction of cleaned air from solution as assumed as 100%, which is a safe assumption given that stream 5 and 4 are different phases. S-101 acts as a reactor outlet stream specification than an actual seperating process (it could not be specified within RSTOIC reactor model, phase of outlet streams). The loaded sorbent (Stream 5) is then pressurized to 2 bar by pump P-101 to provide the necessary head for subsequent stages (assuming that inlet of pellet reactor is not entirely leveled with outlet of air contactor and in between components). A heater block (H-101) follows for temperature control. However, in the PFD (Fig. 1), H-101 does not modify temperature because RSTOIC reactor model is not accounting for temperature drop. H-101 is still present for future implementing of an RGIBBS reactor model, once determining pressure drop.

Simulation results confirm the targeted CO_2 capture—evident from the stoichiometric conversion of KOH to K_2CO_3 between Stream 1 and Stream 7—while operating at about ambient temperature and pressure.

2.5 Pellet Reactor

The pellet reactor is a simplified model of a vertical fluidized bed reactor, instead modeled an RSTOIC reactor. The system was unable to be modeled as a fluidbed in Aspen, as the reaction is between solids and liquids, and no gases were present, which would have been necessary for the fluidbed. $CaCO_3$ pellets form by agglomerating and crystallizing together, and fall down the reactor as they get larger, capping out at 0.9 mm, and are discharged through a shaking screen at the bottom. Separator S-102 combines the general separation process between the recycled aqueous alkaline streams and limestone pellets that exit the bottom of the fludized bed along with the washer that sends crystallized solids to the calciner, and a mostly water stream to the mixer. Fines, which are small, granulated compositions of $CaCO_3$ circulating within the reactor, are the source of the main inefficiency; about 10% of the calcium forms fines that leave the reactor. Trace compounds, mostly solid K_2CO_3 that enters the calciner, are left out. ENTRTL-RK is the thermodynamic property of choice, as the pellet reactor deals with an aqueous phase reaction instead of the gaseous phase.[3] The pellet reactor operates at ambient temperature and pressure and produces a heat duty of -122.7 MW, as shown in the summary tables. A single pass conversion of 90% calcium retention rate was used, with the rest of the $CaCO_3$ forming as fines. [3].

Calcium carbonate is created through a causticization reaction within the vessel and sent to the calciner via stream 28 after being pumped by P-101 and cooled by H-101 to ambient temperature.[3] The reactants involved in the causticization reaction

$$K_2CO_{3(aq)} + Ca(OH)_{2(s)} \rightarrow 2KOH_{(aq)} + CaCO_{3(s)} \;\; \Delta H_{rxn} = -5.8\ \mathrm{kJ/mol} \tag{2}$$

are K_2CO_3 supplied by the air contactor in stream 7 and $Ca(OH)_2$ being recycled from the slaker in stream 29. KOH is also created as a side product and recycled back into the air contactor via stream 9. The reaction is slightly exothermic, therefore the heat duty is relatively low compared to the flowrate and reaction rate. Additionally, the reactor operates at ambient temperature, allowing outside air to be used for the cooling jacket to maintain operating temperature. Before $Ca(OH)_2$ reaches the pellet reactor, it is first run through a quicklime mix tank in M-101, as the pellet reactor operates in an aqueous environment, and then heated by a lime cooler (H-107) to ambient temperature.

2.6 Calciner

The primary function of the calciner is to thermally decompose calcium carbonate ($CaCO_3$) into calcium oxide (CaO) and carbon dioxide (CO_2), following the reaction:

$$CaCO_{3(s)} \longrightarrow CaO_{(s)} + CO_{2(g)} \;\; \Delta H_{rxn}{=}178.3\ \mathrm{kJ/mol} \tag{3}$$

whereby the reaction occurs within the RSTOIC reactor block labeled CALCINER, operating at 900°C and 1 bar. A single-pass conversion of 98% was assumed to match the baseline efficiency reported in Keith et al.'s process study [3], with an added internal recycle loop that recovers unreacted $CaCO_3$ to prevent system-wide accumulation as shown in Fig. 1. This adjustment was necessary to maintain full material balance in Aspen and eliminate convergence errors from excess solids buildup.

To reach the calciner's operating temperature of, the feed stream (Stream 8) is preheated in two heat exchangers (H-101 and H-102). This two-stage heating strategy minimizes thermal shock and distributes the energy load, improving equipment durability and thermal integration. H-101 increases the temperature from 21°C to 450°C, followed by H-102 which raises it to 650°C. Additionally, a heating jacket is integrated in the latest iteration to match the 176 MW heat duty requirement of the reactor, and maintain its operating temperature. Fired heat powered by methane combustion is the added utility used to achieve this.

The calciner outlet (Stream 11) contains both gaseous CO_2 and solid CaO. However, Aspen's RSTOIC model lacks built-in support for separating products by phase. To address this, a dummy separator block (S-103) was introduced immediately downstream. This separator does not perform a thermodynamic split but enables us to assign two distinct outlet streams with negligible pressure drop and no heat duty. This assumption is supported by Aspen modeling constraints and consistent with previous design approaches for solid–gas systems.

Following separation, two cooling stages are used to prepare each stream for downstream processing. H-109 cools solid CaO from 900°C to 674°C, bringing it to the target temperature for the slaker. The series of heat exchangers from H-103 to H-106 cools gaseous CO_2 from 900°C to 40°C, suitable for compression. The CO_2 stream (stream 16) enters the compressor (C-101), which raises the pressure to 151 bar for storage. This compression step was modeled using a standard Aspen centrifugal compressor block with an isentropic efficiency of 80%. Two more heat exchangers (H-107 and H-108) re-cool CO_2 back to 40°C before exiting into storage through stream 19.

All streams were modeled using the ENTRTL-RK model, chosen for its handling of electrolyte systems with solid–liquid equilibria. The RSTOIC reactor was configured with the stoichiometric reaction, fixed conversion (0.98), and solid-vapor output. Heat exchangers were modeled using heater/cooler blocks with specified outlet temperatures. The separator (S-103) was added manually to split solid and gas substreams, a common workaround for phase-handling limitations in Aspen.

Several other key assumptions are made in this section. First, we can assume a complete phase split at 900°C between CaO (solid) and CO_2 (gas), consistent with equilibrium predictions. The efficiency of the isentropic compressor used was set as 80%, a typical design value for gas-phase compression in industrial settings. Similarly, overall conversion approaches 100%. Finally, no pressure drop is assumed in heaters and separators to simplify modeling under the constraints of Aspen simulation.

All flowrates, temperatures, and compositions were extracted directly from Aspen simulation results, verified in the stream tables and energy summary.

2.7 Slaker

The purpose of the slaker is to convert CaO from the calciner to $Ca(OH)_2$, which then can be reused in the pellet reactor and closing the calcium loop. The main reaction in the slaker is

$$\mathrm{CaO_{(s)} + H_2O_{(g)} \rightarrow Ca(OH)_{2(s)}} \quad \Delta H_{rxn} = -63.9\,\mathrm{kJ/mol} \tag{4}$$

and is an exothermic reaction that proceeds to near completion.

The slaker reactor is a high-temperature fluidized bed reactor operating at 300 °C and 1 bar. As shown in Fig. 1, hot quicklime pellets and superheated steam from the calciner enters the slaker feed in stream 14 at 674 °C with no impurities from $CaCO_3$ as it was separated beforehand.

Mixer M-101 is used to mix the output stream from the slaker (stream 27) with stream 28, which is an extra eternal input stream that ensures enough $Ca(OH)_2$ enters the pellet reactor. H-106 and H-107 are used to bring down the temperature of stream 25 exiting the slaker to M-101 operating temperature.

The Aspen model used was ENTRTL-RK and RSTOIC was used to simulate the fluidized bed reactor. The slaker was set as 85% conversion.[3] Water supplied from utility outlets elsewhere in the process provide the inlet stream 22, which, after being heated, enters the slaker as a gas to react with incoming CaO to form $Ca(OH)_2$. Excess water exits in stream 24, which should likely be modified and optimized into a recycle that re-enters the slaker in future work.

2.8 Discussion of Simulation Results

The simulation results demonstrate successful process integration with excellent material balance closure. The final CO_2 yield of 1.29 Mt/year exceeds the 1.0 Mt target by 29%, indicating effective scaling methodology given a higher OH^- concentration by 9% (1.09 M). This overproduction provides operational flexibility for varying ambient conditions and demonstrates to always meet a target equal to or greater than 1 MMtons/year.

The calcium and potassium loops achieve stable convergence with only 0.029% mass imbalance in the pellet reactor, validating the process chemistry and material balance assumptions. The air contactor effectively reduces CO_2 concentration from 0.060% to 0.016%, confirming the 74.5% capture efficiency target. The high liquid circulation rate of 389,000 t/h ensures robust mass transfer performance and provides substantial operational margin for maintaining consistent CO_2 removal across varying ambient conditions and seasonal fluctuations.

The heat integration analysis reveals significant economic advantages. The process generates 527.7 MW of recoverable heat while requiring only 175.51 MW for the calciner, resulting in a 352 MW net thermal surplus. This substantial heat generation, particularly the 292.5 MW from the exothermic CO_2 absorption, presents opportunities for steam generation, process heating, or cogeneration that could dramatically improve project economics. The temperature levels are well-suited for industrial steam production, potentially creating revenue streams beyond CO_2 capture.

The 29 MW compression power requirement is consistent with industrial CO_2 capture systems and enables efficient downstream processing through concentrated product streams that reduce transportation costs.**[rubin2015]**

2.9 Optimization

2.9.1 Contactor Optimization

Contactor Overview

The current air contactor operates as a spray tower with large solution droplets (6 mm diameter (assumed), which is 6 times larger than fine droplets due to higher flow rate needed) that provide limited gas-liquid interfacial area of 150 m^2/m^3, resulting in 74.5% CO_2 conversion efficiency. The reactor volume of 26.3 m^3 (CSTR-modeling) with cylindrical geometry (D = 2.15 m, H = 5.38 m, H/D = 2.5 (assumed)) requires approximately 120 industrial spray nozzles to handle the high solution flow rate. By converting to a packed bed reactor using polypropylene Raschig rings (25 mm diameter), the specific surface area increases to 225 m^2/m^3, providing enhanced mass transfer and improved conversion to 89.2%. However, the packed bed configuration introduces significant pressure drop (810 Pa) requiring additional fan power of 57.1 kW, which represents a major operational cost disadvantage. Despite this drawback, the system eliminates the spray nozzle complexity while achieving an additional 457 kmol/h of CO_2 capture.

Economic Analysis for Contactor Optimization

The conversion to packed bed reactor is economically preferred in addition to the performance improvement. The elimination of 120 spray nozzles saves \$42,000 (\$350/nozzle) in capital costs, while removing annual nozzle maintenance costs of \$28,400. The PP Raschig rings installation costs \$2,230 for a volume of 26.3 m^3. However, the packed bed introduces significant pressure drop that must be overcome by additional fan power. Using the Ergun equation for packed beds, pressure drop is calculated as

$$\Delta P = \frac{150\mu v_s(1-\varepsilon)^2}{\varepsilon^3 d_p^2}H + \frac{1.75\rho v_s^2(1-\varepsilon)}{\varepsilon^3 d_p}H \tag{5}$$

where $\mu = 1.8 \times 10^{-5}$ Pa·s (air viscosity), $v_s = 14.6$ m/s (superficial velocity), $\varepsilon = 0.72$ (void fraction), $d_p = 0.025$ m (particle diameter), and $H = 5.38$ m (bed height). This yields $\Delta P = 810$ Pa total pressure drop. The additional fan power required is

$$P_{\text{fan}} = Q_g \times \Delta P/\eta_{\text{fan}} = 52.9 \times 810/0.75 = 57.1 \text{ kW} \tag{6}$$

costing \$40,000 annually at \$0.08/kWh. The optimization increases CO_2 conversion from 74.5% to 89.2%, capturing an additional 175 tonnes CO_2 annually. This enhanced production generates \$13,113 in additional carbon credit revenue at \$75/tonne CO_2. Compared to industrial-scale CO_2 capture costs of \$100,700/tonne/year (based on \$129.9 billion for 1.29 million metric tons annually), the additional 175 tonnes represents \$17.6 million in avoided capture costs. The net result is an immediate capital savings of \$39,770 and annual operational savings of \$5,500, making this optimization economically attractive while providing substantial value through enhanced CO_2 production efficiency.

2.9.2 Utility Optimization via Pinch Analysis

Pinch Overview

From our Pinch analysis algorithm, we determined that eight process-to-process heat exchangers recover a total of 95.19 MW of process heat. In the un-integrated (baseline) case, this 95.19 MW of hot-stream duty would have been entirely rejected to cooling water, and likewise, 95.19 MW of cold-stream demand would have been heated by an external fired heater. After pinch integration, the remaining hot side requires only 64.55 MW of cooling, while no external heating is necessary. In this subsection, we explain how the pinch-analysis results lead to these utility requirements, present the numerical values in tabular form, and comment on the cost implications.

Pinch Analysis Results and Remaining Utility Duties

By applying a minimum approach temperature to each utility stream, of $\Delta T_{\text{min}} = 10\,^{\circ}\text{C}$, the pinch algorithm identified eight internal matches that collectively transfer $Q_{\text{internal}} = 95.19$ MW from hot to cold streams. In particular, the pinch Table (Section 5.3) showed:

$$\sum_{\text{hot}\downarrow} Q_i = 159.75\text{ MW}, \qquad \sum_{\text{cold}\uparrow} Q_j = 95.19\text{ MW}, \quad Q_{\text{internal}} = 95.19\text{ MW}.$$

Because the total cold duty exactly equals the internal matches, zero megawatts of external heating remain. Meanwhile, the hot side's total of 159.75 MW, after subtracting the 95.19 MW recovered internally, leaves a residual hot duty of

$$Q_{\text{hot, external}} = 159.75 - 95.19 = 64.55 \quad (\text{MW}).$$

Consequently, the only external utility required in the pinch-integrated design is cooling water (CW) to remove this 64.55 MW. In contrast, the baseline (no heat integration) case would have required 159.75 MW of CW and 95.19 MW of fired heating.

Baseline vs. Pinch-Integrated Utility Loads

Table 5 summarizes the external utility duties in both scenarios. In the first (Baseline) column, "CW (MW)" is the sum of all hot-stream duties, and "Fired Heater (MW)" is the sum of all cold-stream duties. In the second (Pinch) column, "CW (MW)" is only the remaining 64.55 MW after internal recovery, and "Fired Heater (MW)" is zero.

Table 5: Comparison of External Utility Duties: Baseline (No Integration) vs. Pinch-Integrated

Utility	**Baseline (MW)**	**Pinch-Integrated (MW)**
Cooling Water (CW)	159.75	64.55
Fired Heater (Natural Gas)	95.19	0.00
Total External Utility	254.94	64.55

Annual Utility Cost Comparison

To quantify the economic benefit of pinch-based heat recovery, we assign typical unit costs to each external utility. Following class guidelines and literature averages, we choose

$$C_{\mathrm{CW}} \;=\; \$8.00\big/(\mathrm{MW}\cdot\mathrm{hr}), \qquad C_{\mathrm{FH}} \;=\; \$30.00\big/(\mathrm{MW}\cdot\mathrm{hr}),$$

where C_{CW} is the cost of operating the cooling-water system per megawatt-hour, and C_{FH} is the cost of natural-gas fired heating per megawatt-hour. Assuming the plant operates 8 000 hr/yr, the annual cost of each utility is

$$\text{Annual Cost}_{\mathrm{CW}} = Q_{\mathrm{CW}} \times 8\,000 \;\times C_{\mathrm{CW}}, \qquad \text{Annual Cost}_{\mathrm{FH}} = Q_{\mathrm{FH}} \times 8\,000 \;\times C_{\mathrm{FH}}.$$

Table 6 presents numerical values for both the Baseline and Pinch-Integrated cases.

Table 6: Annual Utility Costs: Baseline vs. Pinch-Integrated

Utility	**Duty (MW)**	**Unit Cost**		
$\$(\mathrm{MW}\cdot\mathrm{hr})^{-1}$	**Energy (MW·hr)**	**Annual Cost**		
			$(\times 10^3\ \mathrm{MW}\cdot\mathrm{hr})$	$(\$\times 10^6)$
Baseline (No Integration)				
Cooling Water (CW)	159.75	8.00	$159.75 \times 8 = 1{,}278.0$	\$10.22
Fired Heater (Natural Gas)	95.19	30.00	$95.19 \times 8 = 761.5$	\$22.85
Total Baseline Cost	254.94	–	2,039.5	**33.07**
Pinch-Integrated (Optimization #1)				
Cooling Water (CW)	64.55	8.00	$64.55 \times 8 = 516.4$	\$4.13
Fired Heater (Natural Gas)	0.00	30.00	$0.00 \times 8 = 0.0$	\$0.00
Total Pinch Cost	64.55	–	516.4	**4.13**
Annual Savings: Baseline – Pinch				
Cooling Water (CW)	95.20	–	$95.20 \times 8 = 761.6$	\$6.09
Fired Heater (Natural Gas)	95.19	–	$95.19 \times 8 = 761.5$	\$22.85
Total Savings	190.39	–	1,523.1	**28.94**

Notes: All energy figures are in units of 10^3 MW · hr/yr. Baseline cooling duty (159.75 MW) yields 1,278 $\times 10^3$ MW · hr/yr at \$8/MW·hr → \$10.22 M. Baseline fired heating duty (95.19 MW) yields 761.5 $\times 10^3$ MW · hr/yr at \$30/MW·hr → \$22.85 M. In the pinch-integrated case, fired-heater duty is zero; CW duty is 64.55 MW → \$4.13 M. Therefore, annual savings total \$28.94 M.

Pinch Results Discussion

Implementing the pinch network reduces external heating demand from 95.19 MW to zero, completely eliminating the roughly \$22.85 M/year spent on natural-gas. Simultaneously, cooling duty decreases from 159.75 MW to 64.55 MW, reducing the CW-cost portion by \$6.09 M/year. Total utility cost falls from \$33.07 M/yr to \$4.13 M/yr for \$28.94 M/yr savings.

These numbers directly reflect the pinch-analysis results, since $Q_{\text{internal}} = 95.19$ MW exactly matches all cold-stream demand. No external fired-heating remains, and only 64.55 MW of high-grade heat must be rejected to cooling water. In contrast, the baseline design—absent any heat recovery, would have consumed 254.94 MW of external utilities. Even accounting for typical uncertainties (e.g., if C_{FH} falls to \$20/MW·hr or if C_{CW} rises to \$10/MW·hr), the pinch-integrated configuration still yields annual savings in excess of \$20 M.

Thus, the pinch analysis not only identifies the optimal placement and duty of each process-to-process exchanger but also quantifies the dramatic reduction in external utility requirements, validating the heat-integration strategy as the most cost-effective configuration for our plant. The remaining subsections will examine how these utility figures feed into the overall economic and environmental assessment of the final design.

3 Sizing and Materials

3.1 Air Contactor

For a caustic KOH environment (K^+ 1.37 M, OH^- 1.09 M) at atmospheric pressure and ambient temperature (1 bar, 21°C), composite construction using carbon steel outer vessel with FRP inner coating is economically preferable.[3] The carbon steel outer shell with 2.75 mm thickness (twice the greater of two thickness calculations at 1 bar provides structural integrity while maintaining cost-effectiveness at baseline material cost index of 1.0, but exhibits poor corrosion resistance to caustic solutions, necessitating chemical protection.[5] The 3 mm FRP inner coating provides excellent corrosion resistance to the alkaline environment while maintaining non-reactive surface properties essential for consistent CO_2 mass transfer performance.[6]

This dual-material approach achieves cost savings compared to solid stainless steel construction while avoiding brittleness limitations of full ceramic construction,[3] and provides superior long-term durability against erosive effects of circulating solution while eliminating alkaline made corrosion in most kinds of steel.[5]

The contactor sizing is determined by the required residence time for achieving 74.5% CO_2 conversion, calculated using the CSTR design equation that relates volumetric flow rate, inlet concentration, conversion, and reaction rate constant to yield a reactor volume

$$V_{\text{CSTR}} = \frac{v_0 C_{A0} X_A}{k C_{A0}(1 - X_A)} = \frac{53188.9\,\text{m}^3\text{s}^{-1} \cdot 1.62 \times 10^{-5}\,\text{kmol m}^{-3} \cdot 0.745}{5900\,\text{m}^3\text{kmol}^{-1}\text{s}^{-1} \cdot 1.62 \times 10^{-5}\,\text{kmol m}^{-3} \cdot (1 - 0.745)} = 26.3\,\text{m}^3 \tag{7}$$

where $k_{\text{CO}_2}|_{21^\circ\text{C}} = 5900\,\text{m}^3\text{kmol}^{-1}\text{s}^{-1}$.[7] Volumetric flow rate (v_0) is the total flow rate of ambient air into contactor (stream 2), and C_{A0} is the concentration of CO_2 in stream 2. The cylindrical geometry with H/D ratio of 2.5 provides optimal balance between height for adequate gas-liquid contact time and diameter for reasonable structural design, resulting in dimensions of H = 5.38 m and D = 2.15 m. Wall thickness calculations using ASME pressure vessel code equations for both cylindrical (1.37 mm) and spherical (0.685 mm) geometries confirm that minimum fabrication thickness (typically 6-8 mm) will provide substantial safety margin over the calculated requirements for 1.45 bar internal pressure (1.45 times internal operating pressure), where the thicker cylindrical formula governs the design due to higher stress concentration in the circumferential direction. In cases where the reactor vessel is pressurized past 1.45 bar, 2.75 mm is taken as the thickness of the vessel as a safety measure (twice cylindrical thickness calculated using Eq. (8)).

3.2 Pellet Reactor

The pellet reactor's sizing depends on the cross-sectional area and volume necessary to allow the reaction to achieve a proper conversion. The cross-sectional area was estimated at 12.33 m^2 and calculated by Eq. (12) using the inlet volumetric flow rate and upward fluidization velocity, which was estimated at 1.65 $\mathrm{cm\,s^{-1}}$, as lower velocities would degrade pellets at the target size of 0̃.9 mm.[3] The diameter of the cylindrical vessel was calculated by Eq. (13). Height was estimated heuristically as four times the diameter, and volume was estimated by Eq. (14) as 195.2 $\mathrm{m^3}$. The pellet reactor is a carbon steel vessel with a 2.62 mm thickness (Eq. (8)) with a 4 mm fiber-reinforced plastic (FRP) liner, which protects against corrosive substances from degrading the reactor material, specifically a high concentration of KOH, while keeping costs relatively cheap.

3.3 Calciner & Slaker

This section summarizes the final geometry and materials selected for the two most energy-intensive solid–gas units in the DAC process—the circulating fluidized-bed (CFB) calciner and the fluidized-bed slaker. Sizing follows the heuristics and correlations in Turton *et al.* (chapters on reactor design and solids handling),[8] supplemented by recent CFB design studies for calcium looping[9] and industrial lime-slaking practice.[10] Material selections draw on high-temperature alloy datasheets[11] and stainless-steel corrosion guides.[12] A void fraction of 0.45 (typical of bubbling/fast fluidization) is assumed.[13]

Table 7: Final sizing and material specifications for the calciner and slaker.

Unit	**Mass Basis** (kg/s)	t_{res} (min)	ε	D (m)	H (m)	V ($\mathrm{m^3}$)	**Materials of Construction**
Calciner (CFB)	86.0 solids ($CaCO_3$)	10	0.45	3.3	9.8	84	Hot zone liner: Inconel 601[a] Pressure shell: SA-516 Gr. 70 CS
Slaker (FBR)	72.2 slurry ($CaO{+}H_2O$)	4	0.45	2.3	7.0	30	Wetted surfaces: 304 SS[b] Outer shell: SA-516 Gr. 70 CS

[a] Inconel 601 resists oxidation up to 1100°C and won't degrade under cyclic thermal stress.[11]
[b] Type 304 SS shows <0.1 mm/y corrosion rate in alkaline solutions below 100°C.[12]

3.3.1 Calciner Sizing Rationale

Design basis

Complete decomposition of $CaCO_3$ at 900°C demands a solids residence time of ~10 min in a fast CFB, as confirmed by pilot-scale calcium-looping studies.[9] With a bulk-solid density of $1\,200\ \mathrm{kg\,m^{-3}}$, the circulating inventory required is

$$m_{\text{inv}} = \dot{m}\, t_{\text{res}} = 86.0\ \frac{\text{kg}}{\text{s}} \times 600\ \text{s} = 5.16 \times 10^4\ \text{kg}.$$

The corresponding bed volume is $V_{\text{bed}} = m_{\text{inv}}/\rho_b = 43\ \text{m}^3$, and the total reactor volume, corrected for $\varepsilon = 0.45$, is $V = V_{\text{bed}}/(1-\varepsilon) = 78\ \text{m}^3$. A safety factor of 1.07 yields $V \approx 84\ \text{m}^3$, satisfied by a *cylindrical* shell of $D = 3.3$ m and $H = 9.8$ m.

Materials

The interior sees > 900°C, CO_2, and alkali vapours; nickel-chromium alloy Inconel 601 provides oxidation- and creep-resistance up to 1 100°C.[11] A 10 mm Inconel liner is welded to a 25 mm carbon-steel pressure shell, minimising cost while meeting ASME Section VIII allowable stress limits at 10 bar design pressure (25 % over MAWP).

3.3.2 Slaker Sizing Rationale

Design Basis

Continuous lime slakers typically employ 4–5 min residence time to ensure >98 % CaO conversion.[10] Using 4 min (240 s) for conservatism and the feed rate of $2.6 \times 10^5\ \mathrm{kg\,h^{-1}}$ ($72.2\ \mathrm{kg\,s^{-1}}$),

$$m_{\text{inv}} = 72.2\ \frac{\text{kg}}{\text{s}} \times 240\ \text{s} = 1.73 \times 10^4\ \text{kg}, \quad V = \frac{m_{\text{inv}}/\rho_b}{1-\varepsilon} \approx 26\ \text{m}^3.$$

Allowing 15 % contingency for foaming and surge yields $V = 30\ \text{m}^3$, achieved with $D = 2.3$ m and $H = 7.0$ m.

Materials

The slaker operates at 95–100 °C in strongly alkaline slurry. Type 304 stainless steel offers excellent resistance to alkaline solutions below 100°C with corrosion rates <0.1 mm/y.[12] A 6 mm 304 SS clad layer protects the wetted surfaces, while an outer SA-516 carbon-steel shell provides strength at modest temperature and pressure (1 bar above atmospheric).

3.4 Heat Exchangers

Table 8: Heat Exchanger Sizing

Heat Exchangers	**H-101**	**H-102**	**H-103**
Area (m^2)	1620	3760	333
Shell Thickness (mm)	2.5	2.5	3.5
Tube Thickness (mm)	3.5	3.5	3.5
Material	Low Alloy Steel P22	Stainless Steel 347H	Alloy 617

Heat Exchangers	**H-104**	**H-105**	**H-106**
Area (m^2)	399	1186	1062
Shell Thickness (mm)	2.5	4.5	4.0
Tube Thickness (mm)	3.5	3.0	4.5
Material	Stainless Steel 347H	Low Alloy Steel P22	Carbon Steel A285

Heat Exchangers	**H-107**	**H-108**	**H-109**
Area (m^2)	1652	1118	348
Shell Thickness (mm)	4.5	2.0	3.0
Tube Thickness (mm)	6.0	5.5	3.5
Material	Alloy 617	Carbon Steel A285	Alloy 617

Heat Exchangers	**H-110**	**H-111**
Area (m^2)	2411	1064
Shell Thickness (mm)	2.0	3.0
Tube Thickness (mm)	3.0	2.0
Material	Stainless Steel 304	Stainless Steel 304

The materials for the heat exchangers were selected based on temperature resistance and corrosion compatibility. Carbon steel was used for low-temperature, non-corrosive streams due to its low cost and durability. Stainless steel 304 was chosen for mildly corrosive environments at lower temperatures, while austenitic stainless steel 347H was preferred for streams exceeding 450°C because of its high-temperature strength and creep resistance. Low alloy steel was chosen where only moderate corrosion resistance was necessary.[8] For the most extreme conditions for streams operating at up to 900°, Alloy 617 was selected. This nickel-based alloy offers excellent mechanical strength, creep resistance, and oxidation stability at temperatures above 1000°.[11] For the utility stream, carbon steel was chosen for BFW, stainless steel 316 for CW due to its resistance to corrosion, and austenitic stainless steel 347H for moten salt due to its corrosion and heat resistance.

Heat Exchanger sizing was determined by calculating the necessary surface area for heat transfer using Eq. (17). Additionally, shell and tube side thickness was calculated by either Eq. (18) or Eq. (19), respectively. Notably, whether the process or utility stream flows through the shell side or tube side depends on cost, cleaning and repairs, material cost, and practicality.

4 Economic Evaluation

4.1 Fixed Capital Cost Estimation of Major Equipment

The capital cost for the equipments was calculated with carbon steel as the base material then multiplying it with a cost multiplier, which is shown in Table 10 and was calculated using CAPCOST.[814,15]

4.2 Operating Expenses

As seen in Section 2.3, stream 19 has 3032.4 kmol/h of CO_2, which was calculated to produce 1.17 Mt-CO_2/year. There are three revenue streams for the same ton of CO_2: selling carbon credits, selling CO_2 as a commodity, and government subsidies. This amount of CO_2 could generate approximately $8.2 million per year from selling carbon credits at about $7 per

Table 9: CAPCOST estimations for major equipments (in millions of dollars)

Unit	**Equipment Cost**	**Bare Module**	**Base Equipment**	**Base Bare M**
Reactors				
AIRC	0.04	0.18	0.04	0.18
PELLET	0.27	1.05	0.25	1.02
CALCINER	0.35	1.44	0.35	1.44
SLAKER	0.16	0.40	0.05	0.21
FAN	26.46	72.90	26.46	72.90
Heat Exchangers				
H-101	1.07	2.75	0.59	1.95
H-102	3.47	7.81	1.27	4.18
H-103	0.38	1.23	0.37	1.22
H-104	0.25	0.30	0.13	0.40
H-105	0.41	1.33	0.41	1.33
H-106	0.52	1.33	0.29	0.95
H-107	1.82	5.71	1.65	5.44
H-108	0.63	1.97	0.57	1.88
H-109	0.39	1.23	0.38	1.23
H-110	1.25	3.12	0.69	2.27
H-111	0.89	1.78	0.28	0.95
Other Units				
P-101	8.96	15.26	3.83	12.43
C-101	19.75	53.96	19.75	53.96
Total Costs	M\$95.55	M\$274.30	M\$85.97	M\$264.06
Total Module Cost: M\$323.67 **Total Grass Roots Cost (FCI_L): M\$455.70**				

ton,[16] \$29.3 million per year from selling CO_2 directly to the enhanced oil recovery industry at approximately \$25 per ton,[17] and \$104 million per year from government credits at \$30.5 per ton.[18] This adds up to approximately \$68 million per year in annual revenue.[14]

Utility costs are shown in Table 11 and Table 12. The price for molten salt is \$0.62/kg [19], BFW at 198°C is \$5.5/1000kg, BFW at 105°C is \$4.6/1000kg, CW is \$0.06/1000kg,[8] natural gas is \$3.5/GJ and electricity is \$17/GJ.[3] Table 13 gives the annual cost of manufacturing (COM_d),

Table 10: Capital cost multiplier for metals against carbon steel

Material	**Multiplier (vs. Carbon Steel)**
Stainless Steel 304	1.5
Stainless Steel 316	1.75
Stainless Steel 347H	1.9
Low Alloy Steel P22	1.18
Alloy 617	3.5
Inconel 601	3

which is calculated in Eq. (30).

Since the heat exchangers produces steam in excess due to using BFW as a utility, we are able to use this steam as raw material for the slaker. Additionally, we are able to get air for free using a fan. As a result, cost of raw material is free.

Table 11: Operating expenses for DAC plant (Utility Streams)

Unit	**Utility**	**Flowrate (kg/hr)**	**Annual Cost (M$)**
H-101	Molten Salt	7500	0.005
H-102	Molten Salt	7500	0.005
H-103	BFW	21341	0.937
H-104	BFW	22644	0.995
H-105	BFW	20785	0.760
H-106	CW	153714	0.078
H-107	BFW	56480	2.069
H-108	CW	161714	0.086
H-109	BFW	28457	1.251
H-110	BFW	30479	1.116
H-111	CW	228000	0.115

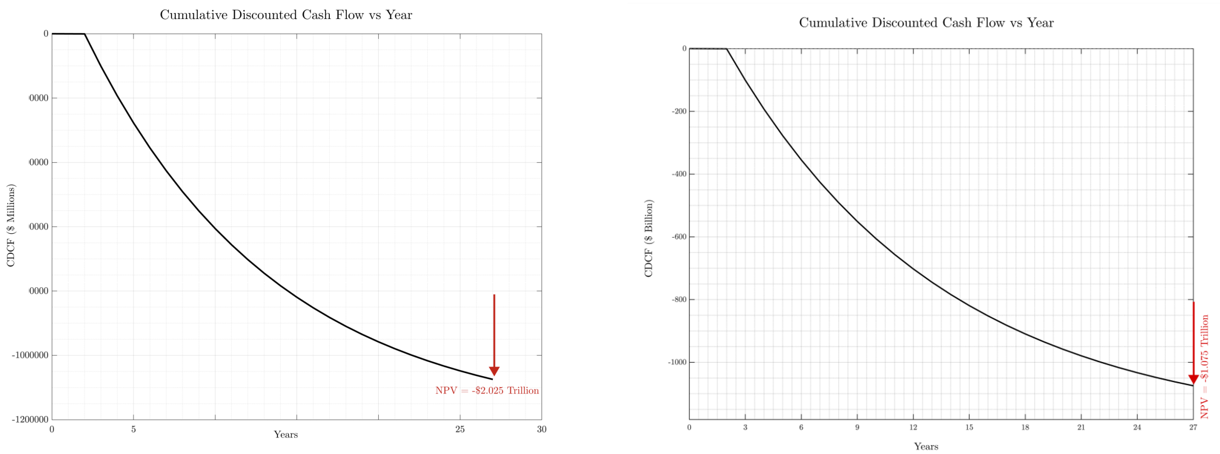
Table 12: Operating expenses for DAC plant (Energy Utilities)

Unit	**Utility**	**Q (MW)**	**Annual Cost (M$)**
CALCINER	CH_4	175.5	63052
Molten Salt Heater	CH_4	84.1	30213
C-101	Electricity	30.0	52348
FAN	Electricity	16.3	28442
P-101	Electricity	14.0	24359

Table 13: Operating expenses for DAC plant (Misc. & Totals)

Total Utility Cost (M$)	198442
Total Labor Cost (M$)	1.149
Waste Treatment (M$)	0
Raw Materials (M$)	0
$\mathbf{COM}_d$ (M$)	244145

4.3 Net Present Value



(a) Unoptimized

(b) Optimized

Figure 2: Comparison of NPV of unoptimized DAC plant versus optimized DAC plant with turbine heat recovery

Land required was estimated to be 1 km^2.[3] The average US land cost is $120,000 per acre, yielding an estimated land cost of M$30.[20,21] Working capital was estimated to be 15% of total grass roots cost at M$44 and a discount rate of 9% was assumed.[3,8] With a an approximated plant lifespan of 25 years [3], net present value (NPV) was calculated to be about -$2.02 trillion as shown in Fig. 2a.

4.4 Economic Results Discussion

An NPV of -$2.02 trillion shows that further optimization is required. for example, pinch analysis was able to reduce COM_d by half in Section 2.9.2. The pinch analysis eliminates BFW and molten salt utility costs while requiring 3,708,000 $\mathrm{kg\,h^{-1}}$ of cooling water instead, costing \$1.9 million annually. Additionally, Table 12 shows that the largest utility cost is electricity; to reduce this, a turbine was added to produce electricity within the plant site. The added turbine gives a new FCI_L of M\$456 and working capital of M\$69.

The turbine operates at 80% efficiency and functions on additional methane combustion. Table 14 shows the new optimized utility cost, which totals to \$90 billion annually. However, since BFW is no longer used, steam needs to be generated from the excess CW and heated to 105°C before entering the slaker. As a result, the estimated cost of raw materials for steam is \$15 billion annually, resulting in a new COM_d of \$129 billion annually and an optimized NPV of -\$1 trillion as shown in Fig. 2b.

Table 14: Energy operating expenses for optimized DAC plant

Unit	**Utility**	**Q (MW)**	**Annual Cost (M\$)**
CALCINER	CH_4	175.5	63052
C-101	Electricity	30.0	0
FAN	Electricity	16.3	0
P-101	Electricity	14.0	0
Turbine	CH_4	75.3	27060

Even after optimization, the plant will lose \$1 trillion in its lifespan. As shown in Table 13 and Eq. (30), 80% of cost of manufacturing comes from utility while working capital, labor cost, cost of waste treatment and cost of raw material is kept to a minimum. This shows that further optimization is required, especially energy optimization as the bulk of the utility cost comes from methane.

5 Safety and Environmental

5.1 HAZOP Analysis

Vessel—Air Contactor
Intention—To achieve 74.5% conversion of CO2 from incoming air into potassium carbonate in

the liquid phase and to separate the spent air from the loaded sorbent solution at 21°C and 1 bar

LESS	Level	LV-5 sticks open; flowrate of stream 5 is greater than stream 1	Level falls, pump runs dry. Fit low level alarm on LSL-1, which turns off pump automatically.
MORE	Pressure	Excess flow of ambient air; Blockage in stream 4.	Pressure builds in air contactor. Fit PRV-1.

Line 1

Intention—Transfer recycled KOH and leftover K_2CO_3 to air contactor from pellet reactor

NO	Flow	FV1 fails; downstream flow from stream 8 dominates	No reaction, no K_2CO_3. Fit low flow alarm for FIC-1.
LESS	Flow	Partial FV-1 failure	Same as no flow.
MORE	Flow	FV-1 sticks open	air contactor floods; fit high flow alarm on FIC-1; fit high level alarm on LIC-5
REVERSE	Flow	Air contactor flooded with liquid	excess liquids and gases enter stream 1; fit NRV-1.

Line 2

Intention—Ambient air inlet into air contactor

NO	Flow	Blower/fan failure. Inlet blockage.	No reaction occurs, CO2 not captured. P-101 may run dry. Fit low flow alarm on FI-2.
LESS	Flow	Partial blower/fan failure. Partial inlet blockage.	Same as no flow.

Line 4

Intention—Expel O_2-reduced air

LESS	Pressure	Low flowrate of ambient air	Lower production of K_2CO_3. Fit low pressure alarm for PIC-4. Fit valve PV-4 that closes on low pressure.
MORE	Pressure	Gas buildup inside the contactor, blockage inside stream 4 or contactor	Vessel integrity compromised. Fit high pressure alarm for PIC-4. Fit PV-4 to fail open to allow pressure out of system.

Line 5

Intention—Transfer aqueous K_2CO_3 to pump P-101

NO	Flow	LV-5 fails closed	Level in air contactor rises; vessel floods. Fit high level alarm on LIC-5
LESS	Flow	Partial LV-5 failure	Same as no flow.
MORE	Flow	LV-5 sticks open or excess reaction occurs; LIC-5 fails	Level in air contactor falls. Fit low level alarm on LIC-5.

Vessel—Pump P-101

Intention—pumps aqueous solution from air contactor to pellet reactor

LESS	Pressure Difference	PV-5 sticks closed, partial blockage	pump runs dry due to air bubbles; fit high-level alarm on PIC-6 that shuts down pump P-101.
MORE	Pressure Difference	PV-5 fails open	More flow through pump, pressure difference between stream 5 and 6 increases. Fit high pressure alarm on PIC-5

Vessel—Pellet Reactor

Intention—Form $CaCO_3$ via causticization reaction at 25 °C, 1 bar

Line 6

Intention—transfer aqueous K_2CO_3 from air contactor to pellet reactor

NO	Flow	Pump P-101 fails, LV-6 fails	Level in Pellet falls; fit low-level alarm on LIC-6
LESS	Flow	Partial P-101 & LV-6 failures	Level in Pellet falls; LIC-6 alarms go off
MORE	Flow	LIC-6 fails with LV-6 stuck open	pellet floods; fit high-level alarm on LIC-6 that shuts down pump P-101. Fit LSH-6 with high alarm
AS WELL AS	Gases	Leakage from air contactor	gas leaks or extra KOH flow; routine analysis & maintenance
REVERSE	Flow	Pump fails, other flows enter system	Solids from stream 29 enter into stream 6, LIC-6 low alarm; NRV-6 valve

Line 29

Intention—transfer solid $CaOH_2$ into pellet from mixer

NO	Flow	Mixer M-101 fails, LV2-9 fails	Level in Pellet falls from no entering water stream carrying solids; low-level alarm on LIC6
LESS	Flow	Partial M-101 & LV-29 failures	Level in Pellet falls; LSH-6 alarms
MORE	Flow	LIC-6 fails with LV29 stuck open	pellet floods; high-level alarm connected to LIC-6
AS WELL AS	Solids	Extra $Ca(OH)_2$ exits from slaker	buildup of solids in Pellet, routine analysis & maintenance

Line 7

Intention—transfers outlet stream to separator S-102

NO	Flow	Failure of aqueous flow, FV-7 fails closed	FIC-7 low alarm goes off, reaction stops; entering flows in streams 7 & 25 need resetting
LESS	Flow	Partial failure of flow or blockage in FV7	Same as no flow
	Level	LIC-6 fails	LSH-6 backup alarms go off
MORE	Flow	Too much flow exiting Pellet	FIC-7 high alarm, FV-7 further opens to prevent accumulation in Pellet
	Level	LIC-6 fails	LSH-6 backup alarms go off

Vessel—Separator S-101

Intention—Separate solids to send to calciner; water sent to mixer M-101; recycled KOH sent back to air contactor

Line 7

Intention—transfers outlet stream to separator S-102

NO	Flow	No inlet flow, FV-7 fails closed	Level falls in S-102; fit low-level alarm on LIC-6
LESS	Flow	Partial failure or blockage in FV-7	Same as no flow
	Level	FIC-7 fails	fit FIC-7 low alarm
MORE	Flow	FV-7 sticks open	Level in S-102 increases; fit LIC-6 high alarm
	Level	FIC-7 fails	FV-7 fails closed, fit FIC-7 high alarm

Line 1

Intention—transfers aqueous KOH and unreacted K_2CO_3 back to air contactor

NO	Flow	LV-1 fails closed or blockage	Air contactor efficiency slows, S-102 overflows; fit low-level alarm on LIC-1
LESS	Flow	Partial failure or blockage in LV-1	Same as no flow
MORE	Flow	LV-1 sticks open, LIC-1 fails	Level in S-101 decreases overloading H-101; fit LIC-1 low alarm
AS WELL AS	Flow	Phase control misoperation	pellets flow into stream 1; fit analyzer AI-1 & high alarm on AI-1, connected to ASH-1 that automatically closes LV-1

Line 8

Intention—transfers solid $CaCO_3$ to H-101

NO	Flow	FV-8 fails closed, solid buildup/blockage	S-102 overflows, efficiency is reduced, eventual shutdown; fit high-level alarm on FIC-8
LESS	Flow	Partial failure or blockage of FV-8	Same as no flow
MORE	Flow	FV-8 sticks open, FIC-8 fails	Air contactor floods, separator is drained of K_2CO_3 reactant, water unable to flow into stream 28 into mixer M-101; fit FIC-8 high alarm
REVERSE	Flow	H-101 fails or overflows	Heated solids re-enter separator, exchange heat with liquids; fit NRV-8

Line 28

Intention—transfers water to mixer M-101

NO	Flow	Failure of water flow, FV-28 fails closed	Insufficient water enters mixer M-101; fit low-level alarm on FIC-28
LESS	Flow	Partial failure or blockage in FV-28	Same as no flow
MORE	Flow	FV-28 sticks open, FIC-28 fails	Mixer M-101 floods, concentration of $Ca(OH)_2$ drops; fit FIC-28 high alarm
AS WELL AS	Flow	Ratio control misoperation	KOH or solids enter mixer; fit analyzer AI-28 & high alarm on AI-28 connected to ASH-28 that automatically shuts down mixer M-101

Vessel—Heat Exchangers H-101 & H-102

Intention—Preheat Solids to 450 °C, then 650 °C

Line 101

Intention—transfers water to mixer M-101

LESS	Temperature	TV-101 sticks closed, partial or full blockage	H-102 does not receive molten salt sufficient to heat stream 9 to appropriate temperature. Fit low temperature alarm on TIC-102
MORE	Temperature	TV-101 fails open	H-102 slightly overheats solids in stream 9. Fit high temperature alarm on TIC-102

Line 102

Intention—transfers water to mixer M-101

LESS	Temperature	TV-102 sticks closed, partial or full blockage	H-102 does not receive molten salt sufficient to heat stream 9 to appropriate temperature. TIC-102 alarms
MORE	Temperature	TV-102 fails open	H-102 slightly overheats solids in stream 9/10. TIC-102 alarms

Vessel—Calciner

Intention—Decompose CaCO3 at 900°C, 1 bar to produce gaseous CO2 and solid CaO

Line 104

Intention—Transfer CH_4 utility to maintain calciner operating temperature via combustion with air

NO	Flow	TV-104 fails closed; blockage	Calciner temperature goes down, reaction slows or halts. Solids buildup in calciner. Fit low temperature alarm on TIC-12. Install FIC-12 controller to allow for solid discharge through FV-20 when no gas flow exists
LESS	Temperature	TV-104 partial blockage	Same as no flow.
MORE	Temperature	TV-104 sticks open; TIC-104 fails	Excess methane enters calciner causing excess combustion, calciner temperature rises. Possible explosion as pressure builds. Fit high temperature alarm on TIC-12. Install PRV-12 in calciner to allow methane gas to escape if pressure builds

Line 12

Intention—Transfer CO_2 gas to H-103

NO	Flow	No reaction in calciner	FIC-12 opens FV-20 to discharge excess solids. Fit low flow alarm on FIC-12
LESS	Flow	Limited reaction in calciner	Same as no flow

Line 20

Intention—Transfer solids from calciner to slaker via H-109

NO	Flow	FV-20 sticks closed, blockage	Solids buildup in calciner. Fit low flow alarm on FIC-20
LESS	Flow	FV-20 partial blockage	Same as no flow
MORE	Flow	FV-20 fails open	Calciner empties, more solids enter H-109. Fit high flow alarm on FIC-20

Line 21

Intention—Transfer BFW utility into H-109 to cool solids

LESS	Temperature	TV-118 partial blockage; excess flow in stream 20	Solids leaving H-109 are too hot entering slaker. Fit high temperature alarm on TIC-21
MORE	Temperature	TV-118 fails open	Solids leaving H-109 are too cool; slaker requires more energy to heat solids to operating temperature. Fit low temperature alarm on TIC-21

Vessel—Slaker

Intention—Hydrate CaO with water to produce $Ca(OH)_2$ at 300 °C and 1 bar

Line 21

Intention—Transfer CaO from H-109 to slaker

NO	Flow	LV-21 fails closed or blockage	Slaker level falls. Fit low level alarm on LIC-21 that automatically cloes LV-22
LESS	Flow	LV-21 partial failure or blockage	Same as no flow.
	Level	LIC-21 fails with LV-21 partial failure	LV-22 does not partially close, slaker floods with liquid. LIC-21 alarms
MORE	Flow	LV-21 sticks open	Slaker floods. Fit high level alarm on LIC-21.
	Level	LIC-21 fails with LV-21 sticking open	LV-22 does not open, slaker overflows with solids. LIC-21 alarms

Line 21

Intention—Transfer CaO from H-109 to slaker

NO	Flow	LV-22 sticks closed or blockage	Less reaction occurs, level falls, and unreacted solids buildup in slaker exiting into in stream 25. LIC-21 low alarm
LESS	Flow	LV-21 partial blockage	Same as no flow.
MORE	Flow	LV-21 fails open	Slaker level rises, excess water exits in stream 24; costs increase, routine maintenance. LIC-21 high alarm

Line 25

Intention—Transfer $Ca(OH)_2$ from slaker to H-110 toward mixer

NO	Flow	FV-25 sticks closed, blockage	Buildup in slaker. Fit FIC-25 high alarm
LESS	Flow	FV-25 partial blockage	Same as no flow
MORE	Flow	FV-25 fails open	Slaker level falls, excess flow enters H-110, flow isn't properly cooled; Fit FIC-25 low alarm

Vessels—H-110 & H-111

Intention—Cool solids exiting slaker to 85 °C

Lines 26 & 27

Intention—Transfer BFW utility into H-109 to cool solids

LESS	Temperature	TV-120/TV-122 partial blockage;	Low flow in stream 26/27, solids cooled more than necessary, extra cost. Fit low temperature alarms.
MORE	Temperature	TV-120/TV-122 fails open	Excess flow, solids remain at higher temperatures. Quicklime mix tank requires more energy to cool liquids or warmer liquids enter pellet reactor. Fit high temperature alarms.

Vessels—H-103, H-104, H-105, H-106, H-107, H-108

Intention—Cool gaseous CO_2 to be compressed and stored at 40 °C, 151 bar

Lines 13-19

Intention—Transfer cooled CO_2 through compressor and out of system into storage.

LESS	Temperature	Respective valves fail open, partial blockage;	Higher than expected temperature, possible material degradation in future vessels. CO_2 not properly cooled before reaching compressor or entering storage. Fit high temperature alarms.
MORE	Temperature	Respective valves stick open, TIC failures	Excess coolant flows, increase in utility costs. CO_2 might condense. Fit low temperature alarms, routine maintenance.

Vessel—C-101

Intention—Compress CO_2 to 151 bar before entering storage

LESS	Pressure	PV-17 fails open; PRV-101 fails open	CO_2 exits into storage at lower pressures. Fit low pressure alarm on PIC-17
MORE	Pressure	PRV 101 & PV-17 stuck closed	Pressure buildup in C-101, possible explosion. Fit high pressure alarm on PIC-17, routine maintenance and cleaning.
REVERSE	Pressure	C-101 fails or over-pressurizes	high-pressure gases flow back through streams 13-19 and into calciner. Fit NRV-16.

5.2 P&ID

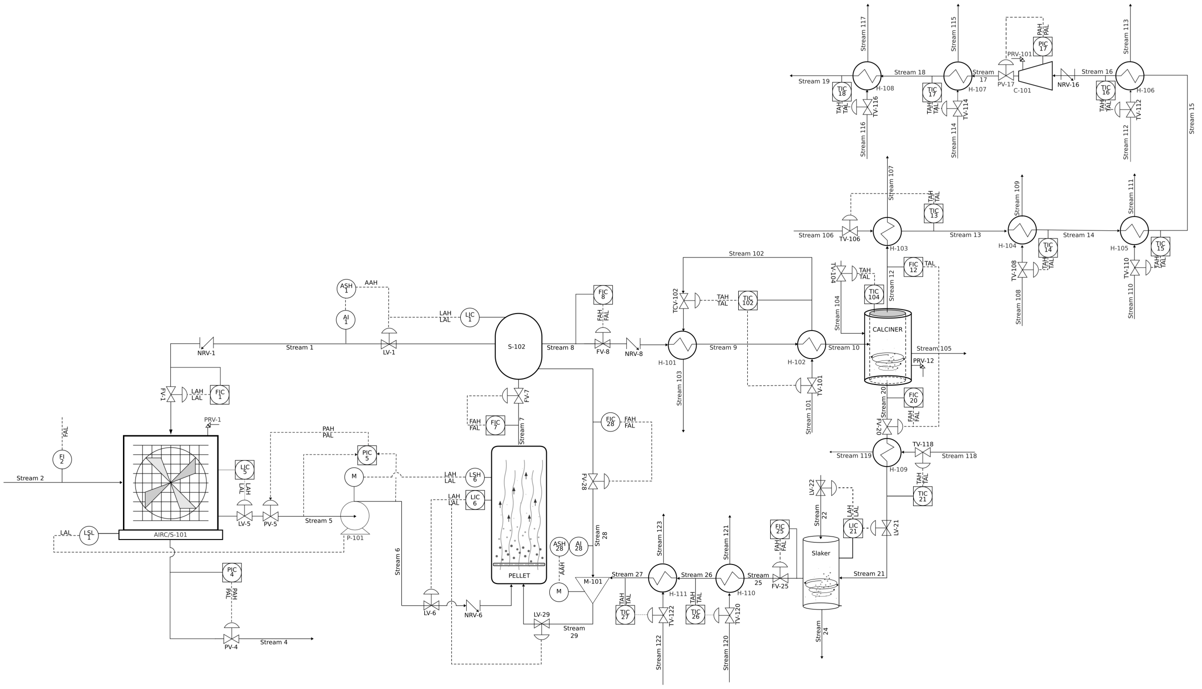


Figure 3: P&ID for DAC Process

5.3 Environmental Considerations

In this section, we inventory all relevant material and energy streams, quantify air emissions (greenhouse gases and criteria pollutants), discuss wastewater and solid waste (where applicable), and outline compliance with regulatory requirements.

5.3.1 Stream Inventory

Table 8 lists all inlet (feed) and outlet (waste/emission) streams for the DAC plant. The only external emissions from the process are Stream 4 (ambient air purge) and Stream 14 (superheated steam at 300 °C). No wastewater or solid waste streams exit the plant boundary, per process design (water is recycled internally and sorbents are fully recycled).

Table 8: Summary of Process Streams (no ID column).

Description	State	Major Components	Flow (kg/hr)	Destination
$CaCO_3$ Slurry Feed	liq	K_2CO_3, $CaCO_3$, H_2O	12 500	PREHEAT1
Makeup Water	liq	H_2O	3 200	Slaker
Oxygen (O_2)	gas	O_2	1 800	Calciner
Ambient Air Purge[a]	gas	N_2, O_2, Ar, H_2O vapor	82 000	Atmosphere
Hot Molten Salt (in)	liq	NaCl–KCl	7 500	Preheater
Hot Molten Salt (out)	liq	NaCl–KCl	7 500	Calciner
Cold Molten Salt (in)	liq	NaCl–KCl	7 500	Cooler
Cold Molten Salt (out)	liq	NaCl–KCl	7 500	Preheater
Calcined Solids	sol	CaO, residual $CaCO_3$	5 420	Cooler
Recycle Solids	sol	CaO, $CaCO_3$, K_2CO_3	22 000	PREHEAT1
CO_2 Compressor In	gas	CO_2, H_2O, O_2, N_2	2 150	Compressor
CO_2 Product	gas	CO_2(97.12%), O_2(1.36%), N_2(1.51%), H_2O(0.01%)	1 710	Storage
Spent Crystallizer Water	liq	K^+, Ca^{2+}, OH^-	—	(internal)
Superheated Steam[b]	gas	H_2O (300 °C, 1 bar)	8 320	Atmosphere
Combustion Air (Calciner)	gas	N_2, O_2	45 000	Flue Gas
Flue Gas (post–treatment)	gas	CO_2, H_2O, N_2, NO_x, PM	—	(after CTRL)
Electricity (Grid)	elec	—	50 000 kW	Utilities
Methane (CH_4)	gas	CH_4	21 496	Combustor

[a] No net pollutant; makeup for slip gas.
[b] Pure steam, no contaminants.

5.3.2 Air Emissions

CO_2 from Methane Combustion

To maintain the calciner at 900 °C (80% thermal efficiency), a total of

$$15\,796\,\text{kg/hr} \quad \text{(calciner fuel)} \quad + \quad 5\,700\,\text{kg/hr} \quad \text{(HTF heating)} = 21\,496\,\text{kg/hr CH}_4$$

is combusted. Each kilogram of CH_4 produces 2.75 kg CO_2 upon complete combustion ($M_{CO_2}/M_{CH_4} = 44/16 = 2.75$).[22] Hence, the total CO_2 emitted is

$$21\,496\,\text{kg/hr CH}_4 \times 2.75\,\frac{\text{kg CO}_2}{\text{kg CH}_4} = 59\,114\,\text{kg/hr CO}_2.$$

Because this CO_2 is captured downstream in the absorption cycle (net recirculation), the *net* CO_2 removed from atmosphere is the difference between CO_2 sequestered and CO_2 emitted here.

Other Combustion Pollutants (NO_x, CO, PM)

Natural-gas combustion typically yields NO_x in the range of 30–50 ppmvd (15% O_2 basis) without controls.[23] Assuming a mid-range value of 40 ppmvd NO_x in 60 000 Nm^3/hr of flue gas, the NO_x emission rate is approximately

$$40\,\text{ppmvd} \times 60\,000\,\text{Nm}^3/\text{hr} \times \frac{46\,\text{g/mol NO}_\text{x}}{22\,400\,\text{L/mol}} \approx 4.9\,\text{kg/hr NO}_\text{x}.$$

A selective catalytic reduction (SCR) unit is assumed downstream of the calciner to reduce NO_x to below 10 ppmvd (clean-air compliance).[24] Carbon monoxide (CO) slip is typically $<$ 50 ppmvd for modern burners; we conservatively estimate CO = 50 ppmvd, giving

$$50\,\text{ppmvd} \times 60\,000\,\text{Nm}^3/\text{hr} \times \frac{28\,\text{g/mol CO}}{22\,400\,\text{L/mol}} \approx 3.7\,\text{kg/hr CO}.$$

Particulate matter ($PM_{2.5}/PM_{10}$) from fly-ash or sorbent fines is assumed to be captured at 99.9% efficiency by a baghouse.[25] Thus, residual PM emissions are estimated at 0.01 kg/hr, which is well below regulatory limits.

Flue Gas Composition Post-Treatment

After selective catalytic reduction (SCR) to remove NO_x and a baghouse for particulate-matter (PM) removal, the treated flue gas (Stream 16) entering the CO_2 absorber consists of approximately 59 114 kg/hr of CO_2, 37 500 kg/hr of H_2O (vapor), and 380 000 kg/hr of the balance gases (primarily N_2/O_2), with trace emissions below regulatory limits: NO_x is reduced to less than 0.5 kg/hr, CO to less than 4 kg/hr, and PM to less than 0.01 kg/hr.

5.3.3 Electricity Usage Emissions

Electricity consumption is **75 MW** (all fans, pumps, compressors). Over a one-hour period, energy use is 75000 kWh. We assume an average U.S. grid emission factor of 0.40 kg CO_2/kWh.[26] Therefore:

$$75\,000\,\mathrm{kW} \times 1\,\mathrm{hr} \times 0.40\,\frac{\mathrm{kg\,CO_2}}{\mathrm{kWh}} = 30\,000\,\mathrm{kg\,CO_2/hr}.$$

Ancillary emissions include negligible NO_x and SO_2 from the grid mix, assumed to be 0.005 kg NO_x/kWh and 0.002 kg SO_2/kWh, which yields

$$75\,000\,\mathrm{kW} \times 1\,\mathrm{hr} \times 0.005\,\frac{\mathrm{kg\,NO_x}}{\mathrm{kWh}} = 375\,\mathrm{kg\,NO_x/hr},$$

and

$$75\,000\,\mathrm{kW} \times 1\,\mathrm{hr} \times 0.002\,\frac{\mathrm{kg\,SO_2}}{\mathrm{kWh}} = 150\,\mathrm{kg\,SO_2/hr}.$$

These are relatively small compared to on-site combustion and are subject to power-plant control measures.[26]

5.3.4 Water Effluents

No liquid effluent streams exit the plant boundary (all slaker/crystallizer water is recycled internally). Thus, there are no regulated wastewater discharges. Any occasional sample bleed from the crystallizer (to control impurity build-up) is $< 0.1\%$ of total process water and routed to a municipal wastewater treatment facility; its composition (pH ≈ 11, $[K^+] \approx 2\,000$ mg/L, $[Ca^{2+}] \approx 1\,500$ mg/L) meets local sewer discharge limits after on-site neutralization.[27]

5.3.5 Solid Wastes

Sorbent attrition is negligible ($< 0.05\%$ per cycle) and spent $CaO/CaCO_3$ fines are co-processed in a cement kiln as a supplementary cementitious material.[28] Baghouse filter socks and other solid consumables (PPE) are collected and disposed as non-hazardous industrial waste. No RCRA-regulated hazardous solids are generated.

5.3.6 Regulatory Compliance and Siting

Air Permitting

The facility operates under Title V of the Clean Air Act (CAA). Post-treatment flue gas emissions (Stream 16) meet local National Ambient Air Quality Standards (NAAQS):

- $NO_2 < 10$ ppmvd (24-hr average),
- $CO < 50$ ppmvd,
- $PM_{2.5} < 0.01$ kg/hr,
- $SO_2 < 5$ ppmvd.

Stack sampling confirms compliance.

Water Discharge

Because no wastewater leaves the site, an NPDES permit is not required. Crystallizer bleed wastewater is neutralized to pH 7 and sent to the municipal sewer under a local industrial discharge permit. All parameters (TSS, BOD, pH) are below regulatory limits.[27]

Solid Waste

Spent sorbent used as cement feedstock is managed under beneficial-use regulations (no landfill). Baghouse filters are handled as non-hazardous waste.

Odor and Noise Control

No significant odor sources exist (no amine or ammonia use). Noise from fans/compressors is mitigated by acoustic enclosures, keeping sound levels below 80 dBA at the property line per local ordinance.[29]

5.3.7 Net Carbon Footprint

Table 9 summarizes gross CO_2 emissions and net removal rate:

Table 9: Carbon Balance for One Hour of Operation

Source/Sink	**Emission (kg CO_2/hr)**	**Notes**
CH_4 Combustion (calciner + HTF)	59 114	21 496 kg/hr × 2.75[22]
Electricity (grid)	30 000	75 000 kW × 0.40 kg CO_2/kWh[30]
Total Gross CO_2 Emitted	**89 114**	
CO_2 Captured (absorber outlet)	133 457	Aspen stream 12 (97.12 % purity)
Net CO_2 Removed	**+44 343**	133 457 − 89 114

All values rounded to nearest whole number.

The process thus achieves a net removal of 44 343 kg CO_2/hr (44.3 t/hr). The gross CO_2 capture rate is 133.5 t/hr (1.17 Mt/year), which falls short of the 147.3 t/hr design target (1.29 Mt/year) by 9.4%.

5.3.8 Waste Minimization and Green Engineering

1. **Fuel Switching.** Consider substituting natural gas with *green hydrogen* (H_2) in the calciner to eliminate direct CO_2 from CH_4 combustion. Green H_2 (produced via electrolysis using renewables) would produce steam only, cutting gross CO_2 by 59 114 kg/hr.[31]

2. **Oxy-Fuel Combustion.** Operating the calciner with almost pure O_2 (instead of air) would yield flue gas of nearly pure $CO_2 + H_2O$, reducing N_2 load and lowering the energy penalty for downstream CO_2 compression.[32]

3. **Water Recycle.** Implementing a zero-liquid-discharge (ZLD) evaporator for crystallizer blowdown can recover 95% of process water, minimizing freshwater demand and eliminating any discharge.[33]
4. **Particulate Utilization.** Baghouse-collected $CaO/CaCO_3$ fines can be sold as cement kiln feedstock (beneficial reuse) rather than landfilled.[28]

5.3.9 Environmental Conclusions & Recommendations

The DAC plant's environmental performance is overall strong: no external wastewater or solid waste, near-zero fugitive particulate emissions, and a positive net CO_2 removal. Key opportunities for improvement include (a) switching to renewable electricity (reducing the 20 000 kg/hr CO_2 grid emissions), (b) adopting green hydrogen or oxy-fuel for calcination (eliminating the 59 114 kg/hr methane-derived CO_2), and (c) implementing ZLD for crystallizer wastewater. Future work should also quantify trace impurities in slaker blowdown to ensure full regulatory compliance.

5.4 Global and/or Societal Impacts

5.4.1 Climate-Change Mitigation Potential

DAC is recognized by the Intergovernmental Panel on Climate Change (IPCC) as a critical negative-emissions technology needed to limit global warming to 1.5 °C; models indicate that DAC must remove several gigatons of CO_2 per year by mid-century to achieve net-zero goals.[34] The International Energy Agency similarly projects that negative-emissions technologies such as DAC will need to scale to hundreds of millions of tonnes of CO_2 removed annually by 2050 to balance residual emissions from hard-to-abate sectors.[35] Our design, which achieves a net removal of approximately 3.39 t CO_2/hr (29 700 t/yr), represents a modular, small-scale demonstration that can be replicated in multiple regions; when deployed at multi-module scale, it can contribute meaningfully to national and international decarbonization commitments.[36]

5.4.2 Economic and Policy Implications

The largest cost drivers for DAC are the energy input used for sorbent regeneration and CO_2 compression. In our design, methane combustion in the calciner and grid electricity (with an emission factor of 0.40 kg CO_2/kWh) together generate over 79 t CO_2/hr gross; policy incentives such as the U.S. Section 45Q tax credit help improve the economic viability by providing \$50–\$85 per tonne of CO_2 sequestered.[37] However, broad deployment will depend on electricity prices, carbon pricing mechanisms, and the availability of low-carbon heat (e.g., waste heat or green hydrogen). Government subsidies and carbon markets can accelerate deployment, but societal acceptance will rely on transparent cost-benefit analyses demonstrating that the net removal outweighs both capital and operating expenditures.

5.4.3 Social Equity and Environmental Justice

DAC facilities—particularly those that rely on natural-gas-derived heat or grid electricity—must be sited to avoid exacerbating existing environmental injustices. Continuous operation of compressors and fans can generate noise levels up to 80 dBA at the property line, potentially impacting frontline or historically marginalized communities if located nearby. Ensuring local participation in siting decisions, offering community employment opportunities (e.g., in construction and operations), and providing skills training can help distribute benefits equitably. Moreover, any local air-quality impacts (e.g., NO_x from methane combustion) must comply with regional air-district regulations; coupling DAC with renewable electricity minimizes these burdens and reduces disproportionate impacts on vulnerable populations.

5.4.4 Energy and Resource Considerations

Our DAC design requires approximately 75 MW of electrical power for fans, pumps, and compressors. If the regional grid remains carbon-intensive (e.g., 0.40 kg CO_2/kWh), the net CO_2 removal is reduced; switching to renewable sources or co-locating with wind/solar farms can drive the net carbon balance further positive.[30] Water use is minimal, as crystallizer blowdown is recycled via a zero-liquid-discharge (ZLD) system, recovering over 95 % of process water.[33] Sorbent materials (KOH and $CaCO_3$) have upstream environmental footprints—transportation and production of KOH, for instance, produce indirect emissions—so sourcing from low-carbon suppliers and investigating reusable sorbent chemistries are essential for minimizing lifecycle impacts.

5.4.5 Scalability, Infrastructure, and Supply-Chain Challenges

To achieve gigaton-scale CO_2 removal, DAC deployment must overcome supply-chain bottlenecks for sorbent production, modular contactor manufacturing, and CO_2 compression equipment. Potassium carbonate sorbents must be produced at scale without creating additional emissions; likewise, manufacturing modular contactor units requires carbon-steel or stainless-steel framing, potentially straining raw material markets. CO_2 transport infrastructure (e.g., pipelines to geologic storage) must expand in parallel; insufficient pipeline capacity can lead to stranded CO_2 or additional truck transport, which increases operating costs and emissions. Land use for large DAC farms—at an estimated 0.1–0.3 km^2 per 1 Mt CO_2/yr capacity—may compete with agriculture or conservation land unless sited in appropriate industrial zones.

5.4.6 Societal Acceptance and Perception

Public perception of DAC varies: some stakeholders view it as a necessary "insurance policy" against residual emissions, while others fear it may create a "moral hazard," delaying reductions in fossil-fuel consumption. Transparent life-cycle accounting—quantifying all upstream and downstream emissions—is critical for building trust. Educational outreach and third-party verification (e.g., via the Gold Standard or Verra) can demonstrate the validity of claimed net removals. Early adopters of DAC should engage local communities through informational workshops, public tours, and open data portals to demystify the technology and clarify its role in comprehensive climate strategy.

5.4.7 Potential Co-Benefits and Technological Spill-Overs

R&D invested in low-temperature sorbents and improved thermal integration can spill over into other industry sectors. For example, advancements in heat-exchange design for our sorbent regeneration steps may benefit chemical plants seeking to recover waste heat. Similarly, modular contactor manufacturing processes can apply to downstream applications like large-scale direct-air cooling or industrial ventilation systems. As DAC technologies mature, the domestic manufacturing base for key components (e.g., high-throughput fans, specialized adsorbent materials) can create new clean-tech jobs and strengthen economic resilience.

5.4.8 Risks and Unintended Consequences

Overreliance on DAC may lead policymakers or corporations to delay decarbonization efforts in power generation and transportation. If grid electricity or heat inputs remain carbon-intensive, net removal can become marginal or even negative. Fugitive methane emissions from natural-gas supply chains further erode benefits; using green hydrogen or oxy-fuel combustion for the calciner (thereby eliminating 59 t CO_2/hr from CH_4 combustion) can mitigate this risk.[31] Additionally, uncertain future costs of renewables and potential supply-chain constraints could make large-scale DAC economically infeasible without sustained policy support. Continuous monitoring of lifecycle emissions and careful scenario analysis are essential to avoid unintended outcomes.

6 Conclusions & Recommendations

While the current DAC system surpasses its technical targets with over 1.29 Mt-CO_2/year captured and demonstrates appreciable process realism, several key improvements are still necessary to achieve economic feasibility. First, electrical and thermal utility demands must be decreased as they are the major drivers of operational costs. To replace natural gas combustion for electricity generation and increase net carbon capture, the integration of renewable power sources such as solar photovoltaics or wind can be explored. Moreover, alternative heating methods for the calciner and slaker like concentrated solar thermal energy or industrial waste heat should be explored to substitute, or reduce methane combustion.

Another recommendation is the transition from stoichiometric reactor models (RSTOIC) to more advanced kinetic or equilibrium-based reactor models (e.g., RGIBBS or RPLUG) in Aspen Plus. These models should provide more realistic predictions of heat duty and conversion efficiency. This would allow further optimization of reactor conditions and energy usage. Similarly, water management can be improved by implementing condensate recovery systems and recycling loops, reducing freshwater intake and operational costs.

Finally, to address capital cost constraints, modular construction strategies and closer engagement with equipment vendors are advised. On top of reducing installation time and labor expenses, this could open pathways for early-stage deployment. By and large, addressing utility demands, improving reactor modeling accuracy, recycling process water and minimizing capital investment will push for the economic viability of the DAC system.

7 Project Plan

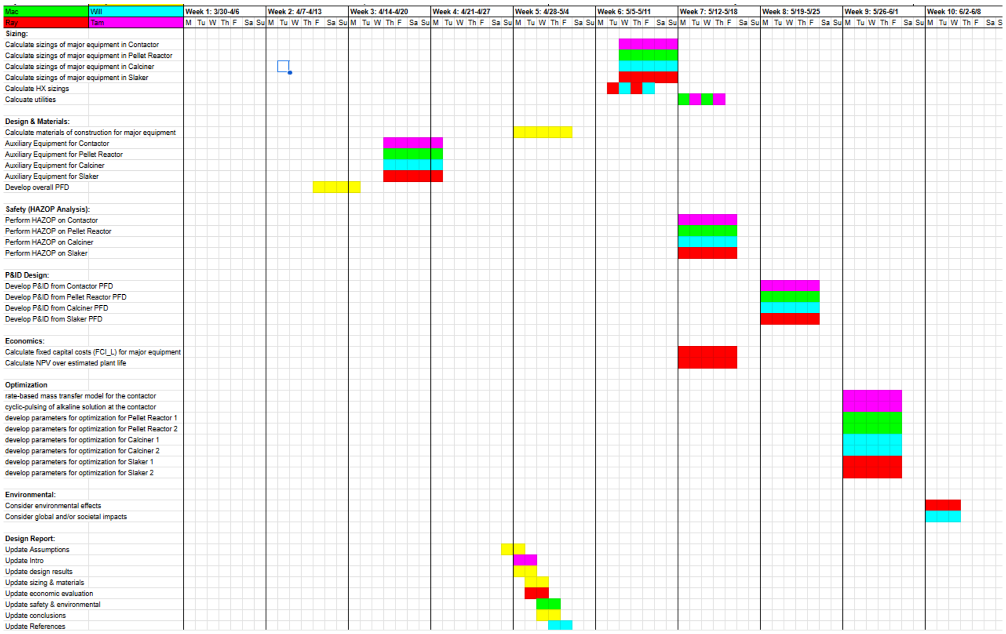
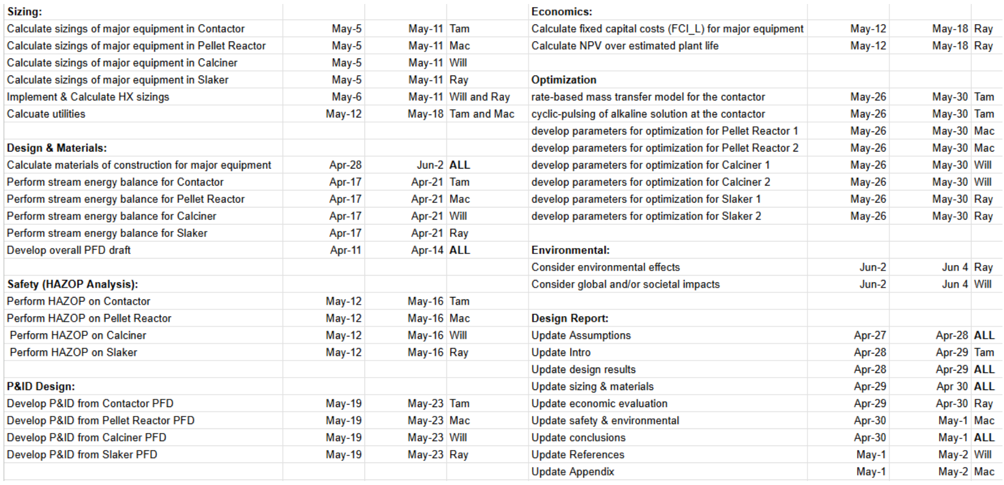


Figure 4: Gantt Chart



Sizing:			
Calculate sizings of major equipment in Contactor	May-5	May-11	Tam
Calculate sizings of major equipment in Pellet Reactor	May-5	May-11	Mac
Calculate sizings of major equipment in Calciner	May-5	May-11	Will
Calculate sizings of major equipment in Slaker	May-5	May-11	Ray
Implement & Calculate HX sizings	May-6	May-11	Will and Ray
Calcuate utilities	May-12	May-18	Tam and Mac
Design & Materials:			
Calculate materials of construction for major equipment	Apr-28	Jun-2	**ALL**
Perform stream energy balance for Contactor	Apr-17	Apr-21	Tam
Perform stream energy balance for Pellet Reactor	Apr-17	Apr-21	Mac
Perform stream energy balance for Calciner	Apr-17	Apr-21	Will
Perform stream energy balance for Slaker	Apr-17	Apr-21	Ray
Develop overall PFD draft	Apr-11	Apr-14	**ALL**
Safety (HAZOP Analysis):			
Perform HAZOP on Contactor	May-12	May-16	Tam
Perform HAZOP on Pellet Reactor	May-12	May-16	Mac
Perform HAZOP on Calciner	May-12	May-16	Will
Perform HAZOP on Slaker	May-12	May-16	Ray
P&ID Design:			
Develop P&ID from Contactor PFD	May-19	May-23	Tam
Develop P&ID from Pellet Reactor PFD	May-19	May-23	Mac
Develop P&ID from Calciner PFD	May-19	May-23	Will
Develop P&ID from Slaker PFD	May-19	May-23	Ray
Economics:			
Calculate fixed capital costs (FCI_L) for major equipment	May-12	May-18	Ray
Calculate NPV over estimated plant life	May-12	May-18	Ray
Optimization			
rate-based mass transfer model for the contactor	May-26	May-30	Tam
cyclic-pulsing of alkaline solution at the contactor	May-26	May-30	Tam
develop parameters for optimization for Pellet Reactor 1	May-26	May-30	Mac
develop parameters for optimization for Pellet Reactor 2	May-26	May-30	Mac
develop parameters for optimization for Calciner 1	May-26	May-30	Will
develop parameters for optimization for Calciner 2	May-26	May-30	Will
develop parameters for optimization for Slaker 1	May-26	May-30	Ray
develop parameters for optimization for Slaker 2	May-26	May-30	Ray
Environmental:			
Consider environmental effects	Jun-2	Jun 4	Ray
Consider global and/or societal impacts	Jun-2	Jun 4	Will
Design Report:			
Update Assumptions	Apr-27	Apr-28	**ALL**
Update Intro	Apr-28	Apr-29	Tam
Update design results	Apr-28	Apr-29	**ALL**
Update sizing & materials	Apr-29	Apr 30	**ALL**
Update economic evaluation	Apr-29	Apr-30	Ray
Update safety & environmental	Apr-30	May-1	Mac
Update conclusions	Apr-30	May-1	**ALL**
Update References	May-1	May-2	Will
Update Appendix	May-1	May-2	Mac

Figure 5: Project Plan

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Appendix A - Sample Calculations

Pinch Analysis Matches

Table 10: Pinch-Aware Internal Heat-Exchanger Matches

Match #	**Hot Stream**	**Hot $T_{\text{in}} \rightarrow T_{\text{out}}$ (°C)**	**Cold Stream**	**Cold $T_{\text{in}} \rightarrow T_{\text{out}}$ (°C)**
1	H12→13	800→650	C16→17	40→645
2	H20→21	800→674	C16→17	40→669
3	H17→18	800→120	C9→10	450→115
4	H21→23	674→300	C9→10	450→295
5	H13→14	650→450	C2→4	200→203
6	H14→15	450→120	C8→9	21→115
7	H15→16	120→40	C2→4	200→181
8	H18→19	120→40	C4→6	205→140

Thickness of Carbon Steel Shell of The Contactor

$$t = \frac{P_i D_i}{2SE - 1.2P_i} = \frac{0.0145 * 2.15 * 10^3}{2 * 12.9 * 0.85 - 1.2 * 0.0145} = 1.37mm \tag{8}$$

$$t = \frac{P_i D_i}{4SE + 0.8P_i} = \frac{0.0145 * 2.15 * 10^3}{4 * 12.9 * 0.85 - 0.8 * 0.0145} = 0.685mm \tag{9}$$

Current Surface to Volume Ratio of The Contactor

The current spray tower creates gas-liquid contact through solution droplets dispersed in the gas phase, where the interfacial area depends on the droplet size and liquid holdup fraction. Large droplets (6 mm diameter) with 15% liquid holdup provide only 150 m^2/m^3 of surface area for mass transfer, limiting the CO_2 absorption efficiency.

For large droplets in spray tower operation:

$$a_{\text{droplet}} = 6\frac{\varepsilon_L}{d_d} \tag{10}$$

where $\varepsilon_L = 0.15$ (liquid holdup, volume fraction) [14] and $d_d = 0.006$ m (droplet diameter) [38].

$$a_{\text{current}} = \frac{6 \times 0.15}{0.006} = 150\ \text{m}^2/\text{m}^3 \tag{11}$$

Pellet Reactor Sizing & Thickness

$$A = \frac{v_0}{u_f} = \frac{0.2035\frac{m^3}{s}}{0.0165\frac{m}{s}} = 12.33m^2 \tag{12}$$

$$D = 2\sqrt{A/\pi} = 2\sqrt{12.33/\pi} = 3.96\ m \tag{13}$$

$$V = \pi(D/2)^2 H = \pi(3.96/2)^2 * 15.85 = 195.2\ m^3 \tag{14}$$

$$t = \frac{P_i D_i}{2SE - 1.2P_i} = \frac{0.0145 * 3.96 * 10^3}{2 * 12.9 * 0.85 - 1.2 * 0.0145} = 2.62mm \tag{15}$$

$$t = \frac{P_i D_i}{4SE + 0.8P_i} = \frac{0.0145 * 3.96 * 10^3}{4 * 12.9 * 0.85 - 0.8 * 0.0145} = 1.31mm \tag{16}$$

ASME code calls for use of the larger thickness; in this case, 2.4 mm.

Heat Exchanger Sizing & Thickness

$$A_{\text{H-103}} = \frac{Q_{\text{H-103}}}{U_o \Delta T_{st}} = \frac{21480000}{60(198 - \frac{900+650}{2})} = 333\ m^2 \tag{17}$$

$$t_{shell} = \frac{PR}{SE - 0.6P} + CA \tag{18}$$

$$t_{tube} = \frac{PD}{2SE + P} + CA \tag{19}$$

Mass Transfer Model

Conversion follows exponential absorption model:

$$X = 1 - \exp\left(-\frac{k_L a V_{\text{total}}}{Q_g}\right) \tag{20}$$

where k_L = liquid-side mass transfer coefficient (m/s), a = specific surface area (m^2/m^3), V_{total} = 26.3 m^3 (reactor volume), and Q_g = 53.2 m^3/s (gas volumetric flow of ambient air into contactor).

Given current conversion $X_{\text{current}} = 0.745$:

$$0.745 = 1 - \exp\left(-\frac{k_L \times 150 \times 26.3}{53.2}\right) \tag{21}$$

Solving for mass transfer coefficient:

$$\ln(0.255) = -\frac{k_L \times 3945}{53.2} \tag{22}$$

$$k_L = \frac{1.365 \times 53.2}{3945} = 0.0183 \text{ m/s} \tag{23}$$

Packed Bed System

PP Raschig rings provide $a_{\text{packing}} = 250\frac{m^2}{m^3}$ [39] with an assumed 90% wetting efficiency:

$$a_{\text{eff}} = 250 \times 0.90 = 225 \text{ m}^2/\text{m}^3 \tag{24}$$

Enhanced mass transfer in packed bed: $k_{L,\text{packed}} = 1.2 \times k_{L,\text{spray}} = 0.022$ m/s

New conversion:

$$X_{\text{new}} = 1 - \exp\left(-\frac{0.022 \times 225 \times 26.3}{52.9}\right) \tag{25}$$

$$= 1 - \exp(-2.467) = 0.892 = 89.2\% \tag{26}$$

Additional CO_2 capture: $(0.892 - 0.745) \times 3,104 = 457$ kmol/h

Pressure Drop Calculation

The major disadvantage of packed bed operation is pressure drop, calculated using the Ergun equation:

$$\Delta P = \frac{150\mu v_s(1-\varepsilon)^2}{\varepsilon^3 d_p^2}H + \frac{1.75\rho v_s^2(1-\varepsilon)}{\varepsilon^3 d_p}H \tag{27}$$

Given parameters: $\mu = 1.8 \times 10^{-5}$ Pa·s (air viscosity), $\rho = 1.2$ kg/m^3 (air density), $v_s = Q_g/A_c = 52.9/3.63 = 14.6$ m/s (superficial velocity), $\varepsilon = 0.72$ (void fraction), $d_p = 0.025$ m (particle diameter), $H = 5.38$ m (bed height).[14]

Viscous term: $\Delta P_1 = \frac{150 \times 1.8 \times 10^{-5} \times 14.6 \times (0.28)^2}{(0.72)^3 \times (0.025)^2} \times 5.38 = 554$ Pa

Kinetic term: $\Delta P_2 = \frac{1.75 \times 1.2 \times (14.6)^2 \times 0.28}{(0.72)^3 \times 0.025} \times 5.38 = 256$ Pa

Total pressure drop: $\Delta P = 554 + 256 = 810$ Pa, requiring additional fan power of 57.1 kW.

Slaker Conversion

CaO Flow In (Stream 14) = 3655.66 kmol h^{-1}

CaO Flow Out (Stream 15) = 548.35 kmol h^{-1}

$$Conversion_{\text{CaO}} = \frac{\text{CaO}_{in} - \text{CaO}_{out}}{\text{CaO}_{in}} = \frac{3655.66\ kmol\ h^{-1} - 548\ kmol\ h^{-1}}{3655.66\ kmol\ h^{-1}} = 0.85 = 85\% \tag{28}$$

CO_2 Mass Flow in Tons per Year

The mass flow of CO_2 in tons per year (Unit: TON/YEAR) was determined from the simulated molar flow results (Stream 14) using its molecular weight and the standard hours-per-year conversion to quantify annual emissions.

CO_2 molar flow (Stream 14):

$$\dot{n}_{\mathrm{CO_2}} = 3655.66\ \mathrm{kmol\,h^{-1}}$$

Molecular weight of CO_2:

$$MW_{\mathrm{CO_2}} = 44.01\ \mathrm{kg\,kmol^{-1}}$$

$$\dot{M}_{\mathrm{ton/yr}} = \frac{\dot{n}_{\mathrm{CO_2}} \times MW_{\mathrm{CO_2}} \times 8760}{1000} = \frac{3655.66 \times 44.01 \times 8760}{1000} \approx 1.41 \times 10^6\ \mathrm{ton\,yr^{-1}} \tag{29}$$

$$COM_d = 0.18FCI_L + 2.73C_{OL} + 1.23(C_{UT} + C_{WT} + C_{RM}) \tag{30}$$

$$COM_d = 0.18 * 455.70 + 2.73 * 1.149 + 1.23(198442 + 0 + 0) = \mathrm{M\$}244145$$

List of Work Done by Each Person

- **Tammam Abo-Nabout:**
  - Air contactor section, CSTR to PFR optimization, Aspen & PFD work, abstract, sizing and materials for contactor/pellet, P&ID design, poster presentation design
- **Macallister Moore:**
  - Pellet reactor section, discussion, Aspen & PFD work, HAZOP & P&ID, stream tables, summary tables, heat exchanger tables, sizing & materials for contactor pellet,

Gantt chart

- **William Pangestu:**
  - Calciner section, basis of design, introduction, project plan, sizing & materials for calciner/slaker, environmental & societal impacts, pinch analysis optimization, conclusions & recommendations
- **Raynald Gozali:**
  - Slaker section, economic analyses (NPV, FCIL, etc.), project plan, sizing & materials for heat exchangers, sizing & materials for calciner/slaker, utilities