Final Technical Report Cover Page

Recipient Organization:	West Virginia University Research Corporation
Project Title:	Unique nanotechnology converts carbon dioxide to valuable products
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Total Project Costs:	$1,018,205
DOE Share:	$800,000
Recipient Cost Share:	$218,205
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ACKNOWLEDGMENT

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*The **Table of Contents** should include a list of the elements of the Final Technical Report organized in the order in which the parts appear, and page numbers.*

NOTE: *When you have completed the Final Technical Report, please assure you also update the Table of Contents. Click anywhere on the Table of Contents and select "Update Table." When the box comes up, choose the "Update entire table" option to ensure that any sections you added/removed are reflected in the table. Please review the updated Table of Contents to ensure it is correct.*

Table of Contents

1.0 Executive Summary

Carbon capture and management are increasing challenges associated with global warming. Current commercial-scale carbon dioxide (CO_2) capture technologies are associated with a heavy economic penalty – they require at least one-third of the plant's steam and power to operate. The objective of this project was to develop and test an innovative nanotechnology that can utilize CO_2, from coal-based power systems or other industrial sources, as the primary feedstock to produce commercially valuable products to potentially offset the cost of CO_2 capture. The scope of this project includes conversion of CO_2 to nanomaterials using two unique amino acids in synthetic flue gases and the completion of a process design and techno-economic and lifecycle analyses to demonstrate the economic feasibility and environmental impact of the developed technology. The International Energy Agency predicts that fossil fuels will continue to play a significant role in meeting global energy demand. The goal of the research is to lead to an affordable and transformational CO_2 capture and reuse technology that will reduce the release of CO_2 thereby reducing global climate variability and its enormous impact on our daily lives.

2.0 Background

Provide a description of the Recipient, including the Recipient's long-term energy vision and goals, organizational structure, location, and demographics.

The recipient West Virginia University (WVU) is a public land-grant R1 research university with its main campus in Morgantown, West Virginia. WVU (Morgantown campus) offers more than 350 bachelor's, master's, doctoral, and professional degree programs throughout 13 colleges and schools. WVU has a long history of studying fossil energy, as does our partner institution for this project, the University of Pittsburgh. Among all U.S. universities, WVU ranks 2nd in competitive awards for fossil energy research and 34th in research expenditures from the U.S. Department of Energy. WVU maintains more than ten sustainable energy research centers and consortia and more than a dozen fossil energy research and consortia with 44 research specialties in everything from extraction and carbon capture to financial and economic modeling within energy sectors. The long-term vision and goal related to this project is to reduce the CO_2 emission from power plants. WVU in Morgantown, WV is the leading organization while the University of Pittsburgh in Pittsburgh, PA is a sub recipient. Both WVU and University of Pittsburgh are public universities.

Carbon dioxide, a main composition of greenhouse gases, is believed to be responsible for global warming; amine solvents and sorbents and others have been studied for CO_2 removal. However, the current technologies are costly and new approaches are needed to reduce the CO_2 management cost.

3.0 Project Objectives

Discuss project goals and objectives and the major tasks from the Statement of Project Objectives (SOPO) found as part of the award documents.

The project objective is to develop and test an innovative bicarbonate nanotechnology that can utilize CO_2 from coal-based power systems or other industrial sources as the primary feedstock to produce commercially valuable products to potentially offset the cost of CO_2 capture. The Recipient's bicarbonate nanotechnology process will be optimized to produce high-purity commercial quality sodium bicarbonate in synthetic flue gas while assessing the effects of contaminants on nanomaterial formation. Information and data gained throughout the project will be utilized in the development of a Life Cycle Analysis (LCA), initial technical and economic feasibility study, and Technology Maturation Plan (TMP).

Early in this project, a TMP will be developed, and a lab-scale unit will be modified for use. Initial testing will be completed to select the best candidate Amino Acid (AA) solution to allow the optimization of CO_2 conversion followed by the assessment of the effects of contaminants on bicarbonate nanomaterial formation. Finally, the LCA, techno-economic analysis (TEA), and TMP will be completed. The major tasks to be performed include:

Task 1.0 – Project Management and Planning

The Recipient shall manage and direct the project in accordance with a Project Management Plan to meet all technical, schedule, and budget objectives and requirements. The Recipient will coordinate activities in order to effectively accomplish the work. The Recipient will ensure that project plans, results, and decisions are appropriately documented, and project reporting and briefing requirements are satisfied.

The Recipient shall update the Project Management Plan 30 days after award and as necessary throughout the project to accurately reflect the current status of the project. Examples of when it may be appropriate to update the Project Management Plan include: (a) project management policy and procedural changes; (b) changes to the technical, cost, and/or schedule baseline for the project; (c) significant changes in scope, methods, or approaches; or (d) as otherwise required to ensure that the plan is the appropriate governing document for the work required to accomplish the project objectives.

Management of project risks will occur in accordance with the risk management methodology delineated in the Project Management Plan in order to identify, assess, monitor, and mitigate technical uncertainties as well as schedule, budgetary, and environmental risks associated with all aspects of the project. The results and status of the risk management process will be presented during project reviews and in Progress Reports with emphasis placed on the medium- and high-risk items.

Task 2.0 – Technology Maturation Plan

In this task, the Technology Maturation Plan will be developed according to the requirements listed in the SOPO Appendix A "Technology Maturation Plan Template."

Task 3.0 – Lab-scale unit modification

This task contains all work necessary to design, purchase, install, and commission equipment modifications to existing lab-scale unit that are necessary to achieve project objectives.

Task 4.0 – Selection of best candidate Amino Acid solution

This task contains all work necessary to optimize the conversion of CO_2 to bicarbonate nanomaterials in simulated flue gas while using several Amino Acid solutions. The effects of contaminants on bicarbonate nanomaterial formation, amounts of carbamates and bicarbonates formed, CO_2 absorption capacity and kinetics, and composition, structure, size, and density of the solid precipitates will be obtained and analyzed. Based upon test results, the best candidate AA solvent will be selected for further project testing.

Task 5.0 – Process optimization to produce high-purity nanomaterials

In this task, the best candidate AA solvent from Task 4 will be utilized to determine the optimum process conditions and procedures to obtain high-purity (>99.8%) bicarbonate nanomaterials upon AA interaction with CO_2.

Task 6.0 – Life Cycle Analysis

In this task, the Life Cycle Analysis will be developed.

Task 7.0 – Technical and Economic Feasibility Study

In this task, a high-level, return-on-investment (ROI) analysis based on experimental and modeling results shall be completed. Assumptions shall be used for the required rate of return-on-investment, capital and operating costs, other co-feeds (if applicable), etc., consistent with the products and markets targeted. The assumed purchase price of CO_2 and possibly other waste streams processed should be clearly stated, along with any potential tipping fees assumed. As appropriate, proposed changes to the power plant or industrial facility should be reflected in the study. Key components of this study shall include:

- Detailed accounting of capital costs
- Detail accounting of operation and maintenance (O&M) costs
- Required selling price (RSP) of the primary product relative to existing markets (co-products should be valued at no more than their current market value)
- Detailed market assessment for all value-added product(s), including assessment of all revenue streams, assumed unit costs, current and projected market volume and value, as well as the estimated quantity of CO_2 utilized.

4.0 Description of Activities Performed

Summarize project activities for the entire period of funding, including approaches used, and results.

Lab-scale unit modification

The lab-scale unit modification (Figure 1) was completed which allowed us to control the gas flow of each component that was used for the proposed studies.

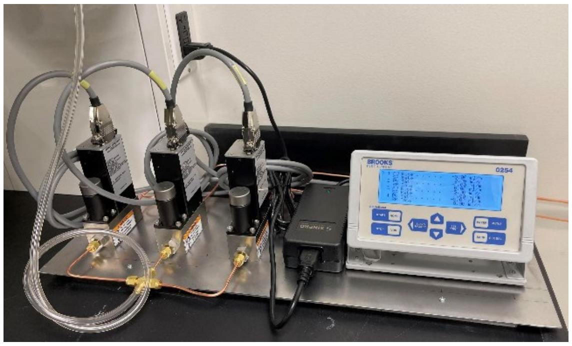


Figure 1. Three mass flow meters were purchased and assembled.

Selection of best candidate amino acid (AA) solvent

The selection of best candidate amino acid (AA) solvent was carried out by further screening and optimizing the AA solvents. The 20 conventional AAs were studied and optimized and techniques including scanning electronic microscopy (SEM) and nuclear magnetic resonance (NMR). Glycine (Gly) was selected and the CO_2 loading of Gly (25 wt%) salt solvents at various CO_2 levels (i.e., 0.04%, 2%, 4%, 10%, and 100% CO_2) were further studied. It was found that the CO_2 loading increased with increasing CO_2 levels (unpublished data not shown).

A phase-change AA nanotechnology concept (Figure 2) was proposed as shown below. A US patent was granted in 2020: Li B, et al. Amino acids react with carbon dioxide (CO_2) and form nanofibers and nanoflowers. US patent US10,583,388. Date of patent granted: March 2020.

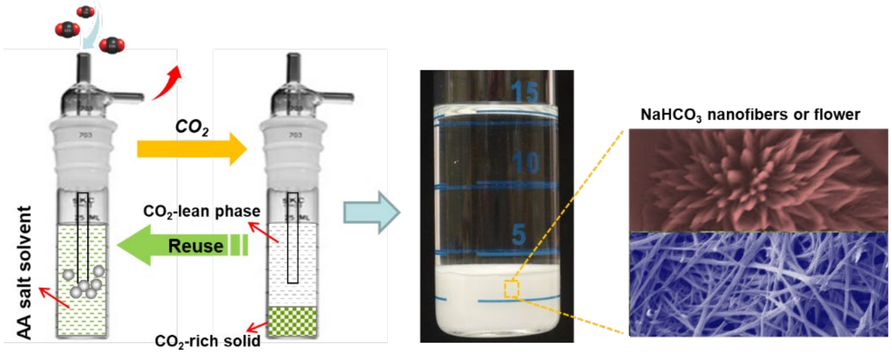


Figure 2. Proposed phase-change AA nanotechnology.

The formation of bicarbonate nanofibers was produced by multiple individuals at different times (Figure 3), confirming the reproducibility of the nanofiber products.

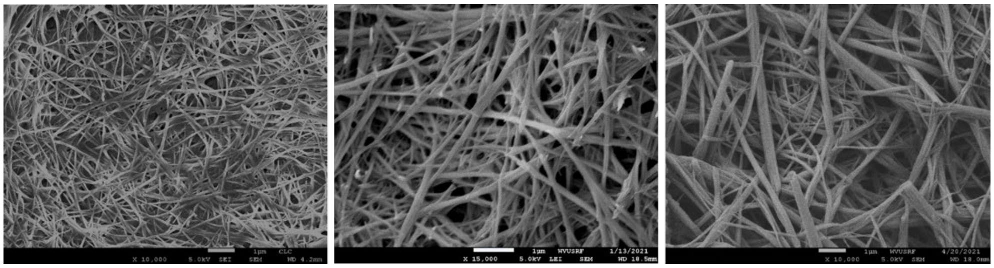


Figure 3. Nanofibers developed by multiple individuals and at different times.

Effects of contaminants

The effects of contaminants like SO_2 on CO_2 conversion using AA solvents were investigated. SO_2 levels between 0.03-3% were studied. Our data (unpublished) showed that SO_2 significantly influenced the CO_2 loading, and the pH and temperature of the AA solvents changed during CO_2 absorption in the presence of SO_2.

Process optimization to produce high-purity nanomaterials

To obtain high-purity products, we have used and optimized sodium bicarbonate saturated deionized water as rinsing medium, and we have also used deionized water as the rinsing medium. For example, 22 g G1N1 (Glycine:NaOH=1:1) solution was bubbled with CO_2 at 160 mL/min for 20 min, and the resulting solution was freeze dried at a temperature of -104 ^{o}C and at a vacuum pressure of 12 Pa. A small amount (0.8946 g) of freeze-dried powder was sampled for washing with saturated $NaHCO_3$ solution (10 g) to remove the impurities that are soluble in the saturated $NaHCO_3$ solution while the bicarbonate materials are not. The suspension was subsequently centrifuged to separate into upper solution and bottom residue, which was subjected to another rinsing using another 10 g saturated $NaHCO_3$ solution (2nd wash) followed by centrifugal separation at 4500 rpm for 5 min, and drying at 65 ^{o}C overnight. The dried powder was weighed as 0.8114 g, resulting in a recovery rate of 91%. Replacing saturated $NaHCO_3$ solution with pure deionized water (10 g) completely dissolved the ~0.9 g freeze-dried powder.

We conducted NMR characterization to monitor the species along with the washing process, and the corresponding spectra were shown in Figure 4. The amounts of Gly and carbamate left on the bicarbonate solid decreased with the washing course. To quantitatively determine the composition of the species in the product solid, we performed NMR quantitative analysis and the results were summarized in Table 1. We can see from Table 1 that the bicarbonate level was about 57% of the wet solid products before washing which increased to

76% after the first washing, and reached 100% purity after the second wash using saturated $NaHCO_3$ solution. The above results demonstrated that we can simply wash the obtained solid mixture using saturated bicarbonate solution to obtain high-purity bicarbonates.

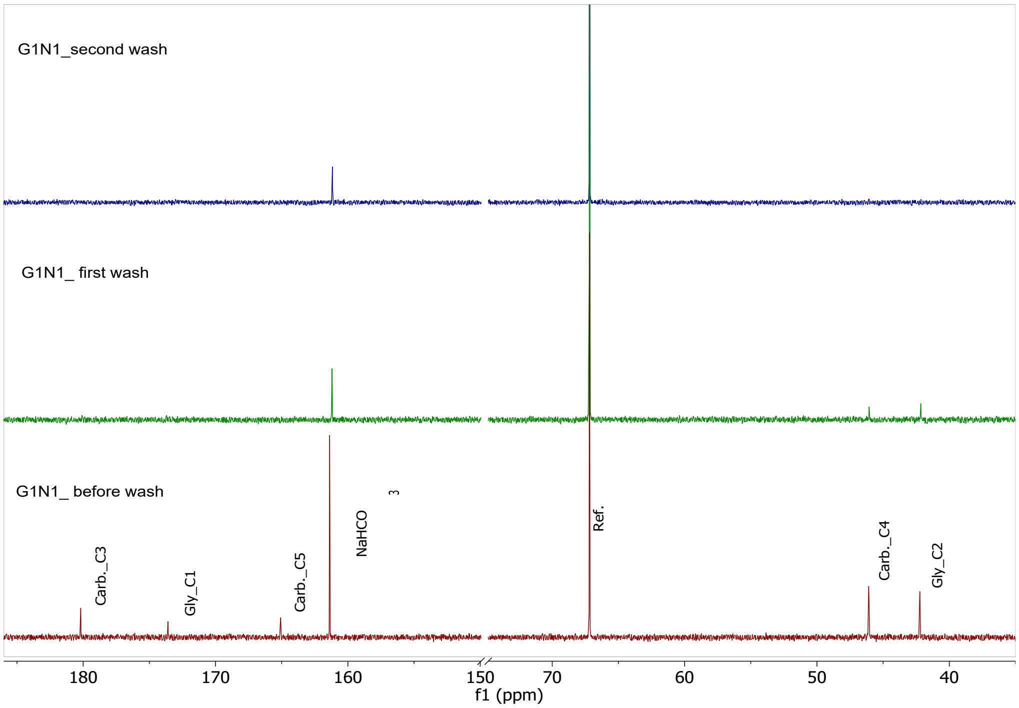


Figure 4. The ^{13}C NMR spectra of bicarbonate materials before washing and after 1st and 2nd washings.

Table 1. The composition of bicarbonate materials before washing and after 1st and 2nd washings.

	mol percentage (mol%)		
Bicarbonate nanomaterials	Gly	Carbamate	**Bicarbonate**
Before wash	20.6	22	**57.4**
1st $NaHCO_3$ washed	16.0	8.2	**75.8**
2nd $NaHCO_3$ washed	0	0	**100**

Process and techno-economic analysis (TEA) of phase-change AA nanotechnology

The objective of the TEA was to use Aspen Plus v.10 to perform TEA of the post-combustion CO_2 capture process using actual plant flue gas and Gly. A process for our phase-change nanotechnology was developed and two case studies were carried out. Using our validated Aspen Plus model, a continuous process flow diagram (PFD) was developed to capture more than 90% of CO_2 from a typical post-combustion flue gas stream using aqueous Gly salt solvents with the aim of producing pure sodium bicarbonates nanoparticles. A Block Flow Diagram (BFD) of the process is shown in Figure 5. The process consists of three main steps: (1) raw flue gas washing step, (2) CO_2 absorption from the washed flue gas step, and (3) separation of the sodium bicarbonate nanoparticles step. The main units of the process include washing unit (WU), CO_2 capture unit (CAU), reverse osmosis unit (ROU), NaOH makeup chamber, and ultrafiltration and $NaHCO_3$ production unit (UFU).

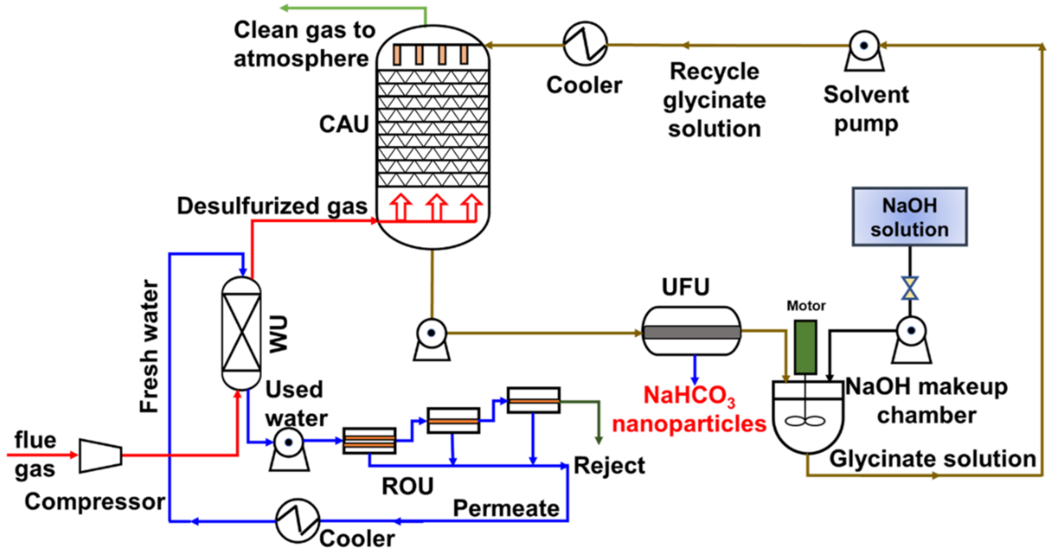


Figure 5. Process for CO_2 capture to produce $NaHCO_3$ nanomaterials.

Next, two case studies were conducted using actual flue gases from two power plants in the U.S. Case study 1: The flue gas from Wolverine Coal Power Plant (600 MWe) representing 10 MWe was studied. The gas pressure, temperature, and composition of the flue gas are shown in Table 2.

Pressure	1	atm
Temperature	353.15	K
Flow rate	12.43 12.38	kg/s m^3/s

Components	**mol %**	**wt %**
CO_2	13.33	20.18
H_2O	12.31	7.63
N_2	70.36	67.79
O_2	4.00	4.400
SO_2	2.35×10^{-3}	5.20×10^{-3}

Table 2. Flue gas pressure, temperature, and composition of Wolverine Coal Power Plant.

Constraints include 99.9% SO_2 removal, ≥ 90 mol% CO_2 absorption in CAU, no flooding in WU and CAU, packing height to diameter ratio ≥ 6, and the water content in CO_2 stream for sequestration ≤ 600 ppm. Calculations for capital cost, operating and maintenance cost, etc. were conducted as follows:

$$\mathbf{CAPEX} = \boldsymbol{Cost\ of\ all\ process\ units\ and\ rotating\ equipment}$$
$$\mathbf{OPEX_{2020}} = (\mathbf{37}\sum \mathbf{W}) + \mathbf{C_{NaOH}}\ \dot{m}_{NaOH} - \mathbf{C_{NaHCO3}}\ \dot{m}_{NaHCO3} + \mathbf{0.04}(\mathbf{CAPEX_{2020}})$$
$$\mathbf{LCOC} = (\boldsymbol{f_{CR}}/\boldsymbol{f_c})\sum(\boldsymbol{CAPEX}_{2020})/\dot{m}_{CO2} + \boldsymbol{OPEX}_{2020}/\dot{m}_{CO2}$$
$$\boldsymbol{f_{CR}} = (\boldsymbol{i}(\mathbf{1}+\boldsymbol{i})^{\wedge}\boldsymbol{N})/((\mathbf{1}+\boldsymbol{i})^{\wedge}\boldsymbol{N}-\mathbf{1})$$

f_{CR} = 0.106079 = Capital recovery factor, 1/yr

f_c = Capacity factor = 0.8

Electricity cost = 37 \$/MWh[1]
W = total power requirements, MWe
C_{NaOH} = NaOH makeup cost
$\dot{m}_{NaOH}$ = NaOH makeup, ton/h
C_{NaHCO3} = $NaHCO_3$ produced prices, \$/ton[2]
$\dot{m}_{NaHCO3}$ = $NaHCO_3$ produced, ton/h
O & M cost = 4% of the total CAPEX in \$/yr
$\dot{m}_{CO2}$ = CO_2 captured, ton/h
N = project lifetime, 30 yrs
i = discount rate = 10%/yr

Links:
[1] NREL, Commercial electricity rate in Industry, https://www.electricitylocal.com/states/pennsylvania/industry/#ref.
[2] $NaHCO_3$: https://www.alibaba.com/product-detail/Nahco3-Nahco3-Bicarbonate-Sodium-99-Stain_1600164672445.html?spm=a2700.galleryofferlist.normal_offer.d_title.1df1215fLzYXlB&s=p

The calculations showed that the levelized cost of CO_2 captured (LCOC) for our phase-change AA nanotechnology was \$35.49/ton CO_2 (Table 3) which was about 50% less compared to the cost of CO_2 capture using the conventional monoethanolamine (MEA) method (Table 4).

Cost category	**Cost**
Total CAPEX, 2020 \$	4,450,552
NaOH makeup, \$/h	3,460
$NaHCO_3$ production, \$/h	-3,278
Total OPEX, \$/h	233
$\dot{m}_{CO2}$, ton/h	8.47
$NaHCO_3$ produced, ton/h	16.15
Total LCOC, \$/ton CO_2	**35.49**

Table 3. TEA of the phase-change AA nanotechnology using the flue gas at Wolverine Coal Power Plant. Gly sodium salt is used for the TEA. CAPEX: Capital cost; OPEX: Operating cost; LCOC: Levelized cost of CO_2 captured.

Cost category	**Gly Pathway**	**MEA Pathway**
Total CAPEX, 2020 \$	4,450,552	\$14,596,990
NaOH makeup, \$/h	3,460	--
$NaHCO_3$ production, \$/h	-3,278	--
Total OPEX, 2020 \$/h	233	420
$\dot{m}_{CO2}$, ton/h	8.47	8.27
$NaHCO_3$ produced, ton/h	16.15	-
Total LCOC, \$/ton CO_2	**35.49**	**77.52**

Table 4. TEA comparison between CO_2 conversion from phase-change AA nanotechnology and the conventional MEA method using the flue gas from Wolverine Coal Power Plant.

Similar calculations were conducted using the flue gas from Longview Power Plant (780 MWe) representing 10 MWe. The gas conditions are given in Table 5, and the outcomes are shown in Table 6. In this case, the LCOC of phase-change AA nanotechnology is less than 50% of the MEA method (Table 6).

Pressure, atm	1	
Temperature, K	324.82	
Flow rate	11.82 10.52	kg/s m^3/s
Components	**mol %**	**wt %**
CO_2	12.022	17.668
CO	3.144e-3	2.94e-3
O_2	4.79	5.12
N_2	79.198	74.086
H_2O	0.03	1.805
Ar	0.98	1.307
SO_2	3.319e-3	7.10e-3
NO_2	3.547e-3	5.45e-3

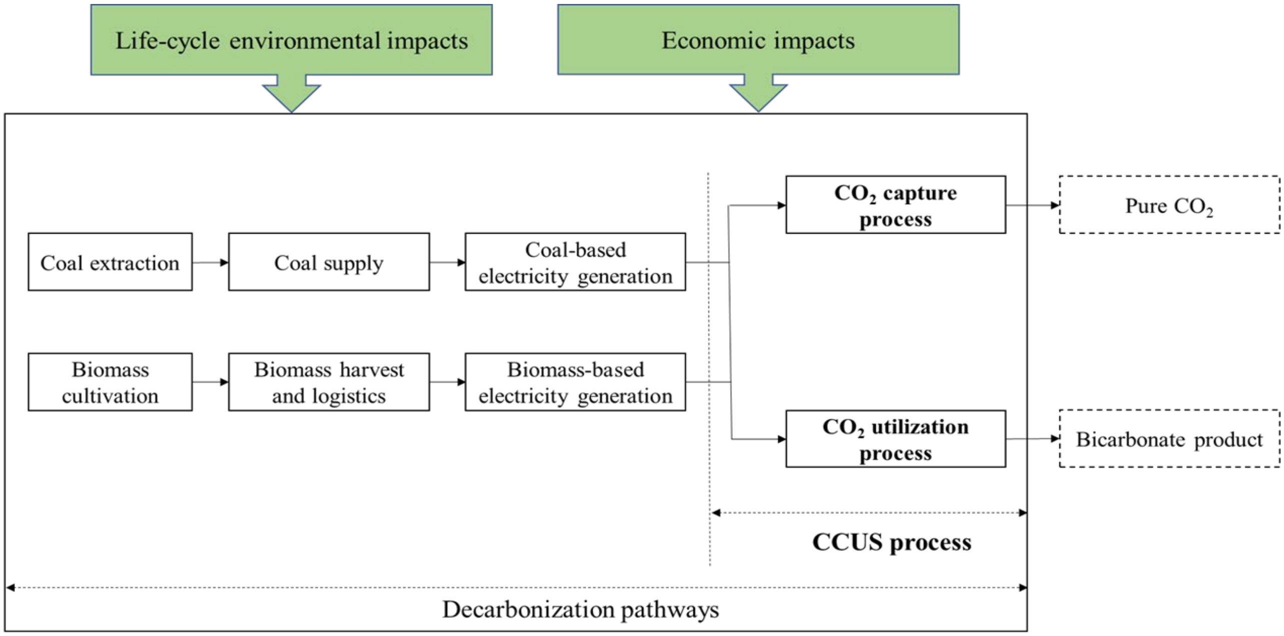
Table 5. Flue gas pressure, temperature, and composition of the flue gas from Longview Power Plant.

Cost category	Gly Pathway	MEA Pathway
Total CAPEX, 2020 $	4,171,205	$13,177,583
NaOH makeup, $/h	2,823	--
$NaHCO_3$ production, $/h	-2,674	--
Total OPEX, 2020 $/h	175	322
$\dot{m}_{CO2}$, ton/h	6.90	6.95
$NaHCO_3$ produced, ton/h	13.17	-
Total LCOC, $/ton CO_2	**34.51**	**75.03**

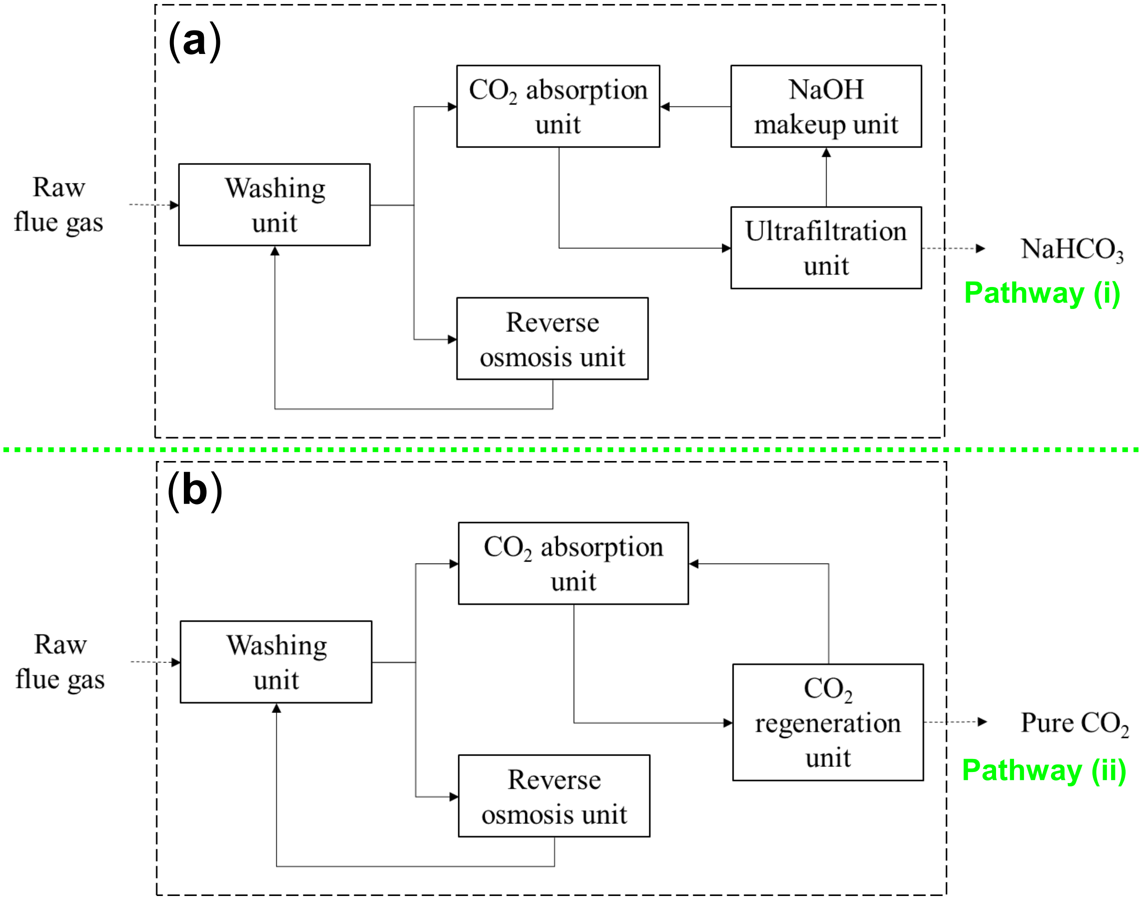
Table 6. TEA comparison between phase-change AA nanotechnology and the conventional MEA method using flue gas from the Longview Power Plant.

Life cycle assessment (LCA) of phase-change AA nanotechnology

The objective of the LCA was to develop a cradle-to-gate LCA model to quantitatively evaluate the environmental impacts, especially the global warming potential (GWP) impact, of the AA-based phase-change processes for CO_2 utilization; therefore, the process for CO_2 sequestration was studied and compared. Integrated consequential and attributional cradle-to-gate LCA with TRACI 2.1 was used to quantify the life-cycle environmental impacts. The same CO_2 utilization process established above was studied and a CO_2 capture process from biomass processes was compared. The modeling framework and simplified process were shown in Scheme 1 and Scheme 2 below.

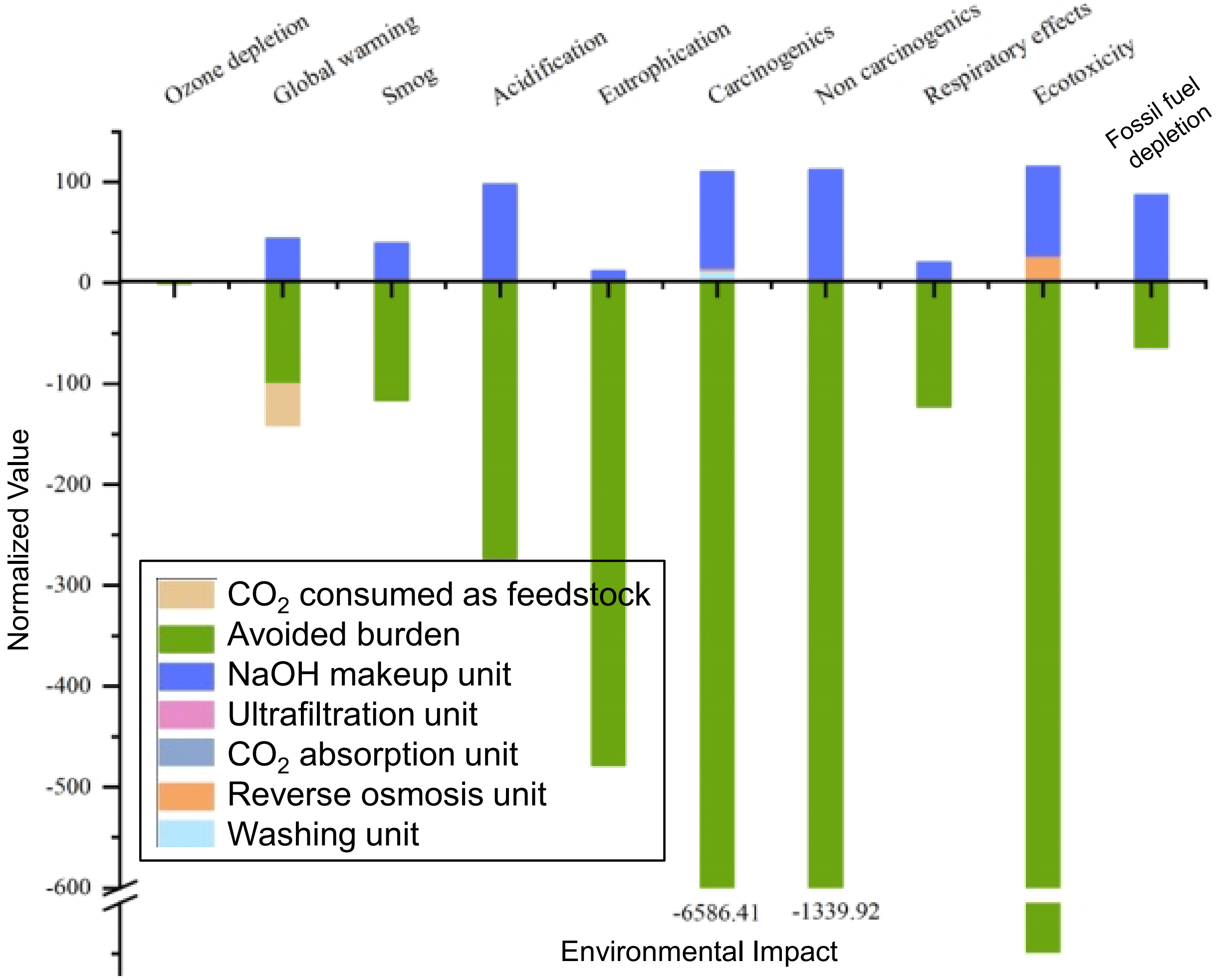


Scheme 1. Analysis modeling framework of LCA.



Scheme 2. (a) CO_2 utilization process to produce nanomaterials as Pathway i and (b) CO_2 capture process to obtain CO_2 for sequestration as Pathway ii.

The environmental impact of the two pathways (i.e., Pathway i and Pathway ii) was calculated and normalized (Figure 6). It shows that the CO_2 utilization may have less impact on the environment (Figure 6).



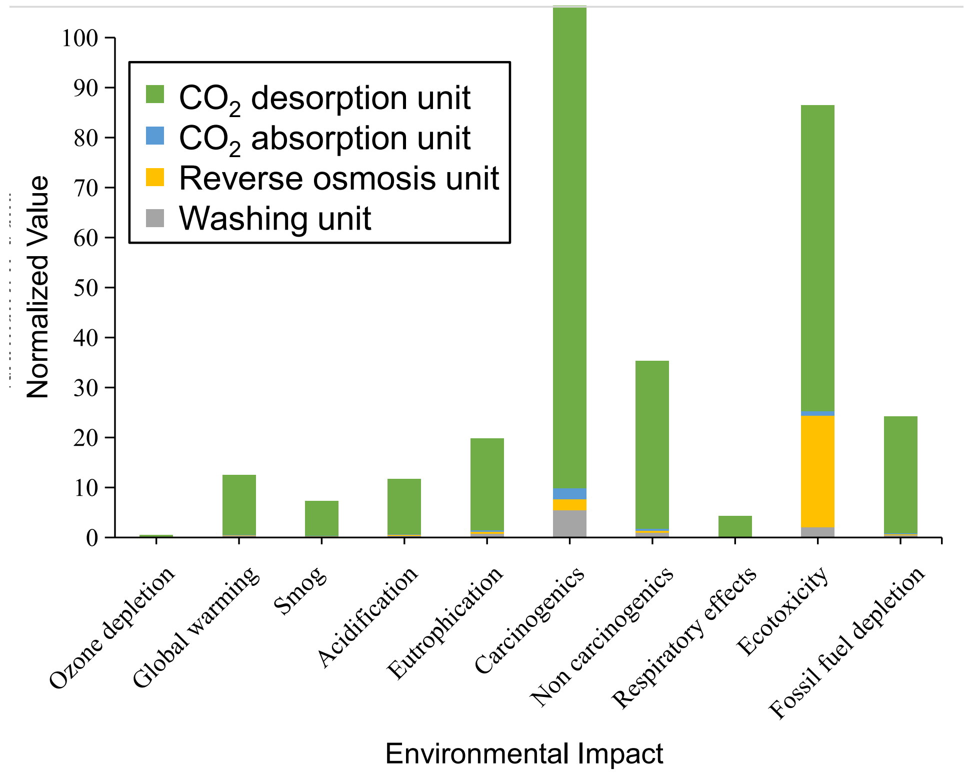


Figure 6. Normalized life-cycle environmental impact of CO_2 utilization process (top, Pathway i) and CO_2 capture process (bottom, Pathway ii) for coal-fired flue gas by impact and unit process.

As to the environmental impact, it was found that:

- CO_2 utilization process (Pathway i): the overall GWP impact is (-2367.61) metric ton CO_2 eq./1,000 metric ton CO_2 utilization.
- CO_2 capture process (Pathway ii): the overall GWP impact is 303.47 metric ton CO_2 equivalent (eq.)/1,000 metric ton CO_2 captured.

As to the economic impact, it was found that:

- CO_2 utilization process (Pathway i): The operation of 1,000 ton CO_2 utilization can provide 2.44-3.25 employment, $196,591-261,591 labor income, $150,663-476,659 value-added, and $1,045,944-1,528,849 industry output.
- CO_2 capture process (Pathway ii): The operation of 1,000 ton CO_2 capture can provide 0.29-0.35 employment, $21,231-25,199 labor income, $50,246-52,300 value-added, and $102,777-107,570 industry output to the national economy.

5.0 Conclusions and Recommendations

Discuss project results and accomplishments and their specific contributions to the Tribe/Tribal community's energy vision. Provide a list of any other publications of project results, networks or collaborations fostered, and technologies or techniques used. Where required, include twelve months of data monitoring and verification to demonstrate energy savings or generation.

In summary,

- We have established a productive collaboration with researchers in the field of nanotechnology, carbon management, TEA, and LCA. We have established a strong collaboration among researchers and engineers from WVU, University of Pittsburgh, and Longview Power Plant, and such a collaboration builds a strong foundation for future pilot or large scale studies.
- We have successfully developed an innovative phase-change AA nanotechnology for carbon reduction or utilization, and have optimized the process and obtained high-purity products.
- Our LCA has indicated that the CO_2 utilization process could be carbon negative. The operation of 1,000 ton CO_2 utilization can annually provide 2.44-3.25 employment, \$196,595-261,591 labor income, \$150,663-476,659 value-added, and \$1,045,944-1,528,849 industry output to the US economy.
- Using the actual flue gases from two power plants in the U.S., our TEA has shown that the unique phase-change AA nanotechnology is cost-effective and achieves much lower LCOCs compared to MEA, as shown below (Table 7):

Cost category	**Wolverine Coal Power Plant**			**Longview Power Plant**		
	Gly Pathway (i)	**Gly Pathway (ii)**	**MEA Pathway (ii)**	**Gly Pathway (i)**	**Gly Pathway (ii)**	**MEA Pathway (ii)**
Total CAPEX, 2020 \$	4,450,552	12,085,346	\$14,596,990	4,171,205	10,749,326	\$13,177,583
Total OPEX, 2020 \$/h	233	250	420	175	191	322
Total LCOC, \$/ton CO_2	**35.49**	**52.68**	**77.52**	**34.51**	**51.34**	**75.03**

Table 7. TEA comparison between phase-change AA nanotechnology and the conventional MEA method.

- We have educated 11 students and two postdoctoral research associates from WVU and University of Pittsburgh in this project.
- We have been awarded one US patent, authored 7 manuscripts, and had 12 abstracts from this project, as listed below:

US patent:

- Li B*, et al. Amino acids react with carbon dioxide (CO_2) and form nanofibers and nanoflowers. US patent US10,583,388. Date of patent granted: March 10, 2020.

Manuscripts:

- Bao Z, Li Q, Akhmedov NG, Li BA, Xing M, Wang J, Morsie BI, Li B*. (2022). Innovative cycling reaction mechanisms of CO_2 absorption in amino acid salt solvents. Chem Eng J Adv 10:100250.
- Li Q, Bao Z, Akhmedov N, Li BA, Duan Y, Xing M, Wang J, Morsi BI, Li B*. (2022). Unravelling the role of glycine in K_2CO_3 solvent for CO_2 removal. Ind Eng Chem Res 61(34):12545-54.
- Wickramasinghe S, Wang J, Morsi B, Li B*. (2021). Carbon dioxide conversion to nanomaterials: Methods, applications, and challenges. Energy & Fuels 35(15):11820-34.
- Wang X, Bao Z, Akhmedov NG, Hopkinson D, Hoffman J, Duan Y, Egbebi A, Resnik K, Li B*. (2022). Unique biological amino acids turn CO_2 emission into novel nanomaterials with three switchable product pathways. (submitted).
- Wang R, Ashkanani HE, Li B, and Morsi B. (2022) Development of an innovative process for post-combustion CO_2 capture to produce high-value $NaHCO_3$ nanoparticles. Int J Greenhouse Gas Control 120:103761.
- Wang R, Ashkanani H, Li B, Morsi B. (2022). TEA of a unique three-pathways process for post-combustion CO_2 capture. J Energy Power Technol 4(4):033.

- Zhang X, Wang J, Li B, Morsi B, Wang R. (2022). Environmental and economic impacts of an innovative amino-acid-based CO_2 capture and utilization technology and its decarbonization pathways. (Submitted).

Abstracts:

- Bao Z, Li Q, Akhmedov NG, Li BA, Wang J, Morsi BI, Li B. Oral presentation. Investigation of potential cycling reaction mechanisms in CO_2 solvents. 39th Annual International Pittsburgh Coal Conference, Pittsburgh, Sept. 19-22, 2022 (virtual).
- Wang R, Ashkanani HE, Li B, Morsi BI. Oral presentation. TEA of a unique two-pathways process for CO_2 capture from post-combustion applications using two amino acid salts. 39th Annual International Pittsburgh Coal Conference, Pittsburgh, Sept. 19-22, 2022 (virtual).
- Li B, Morsi B, Wang J. Oral presentation. Unique nanotechnology converts carbon dioxide to valuable products. U.S. DOE 2022 Carbon Management Project Review Meeting, Pittsburgh, PA, August 15-19, 2022.
- Li B. Oral presentation. Conversion of carbon dioxide into nanomaterials using amino acids. 2022 North American Biochar & Bioenergy Conference, Morgantown, WV, August 8-11, 2022.
- Bao Z, Li B. Oral presentation. Innovative cycling reaction mechanisms of CO_2 absorption in amino acid salt solvents. 2022 North American Biochar & Bioenergy Conference, Morgantown, WV, August 8-11, 2022.
- Zhang X, Wang J, Li B. Oral presentation. Life-cycle assessment of an innovative nanotechnology converting CO_2 from power plant flue gas to valuable products. 2021 Conference of American Center of Life Cycle Assessment. Sep. 21-24, 2021, ACLCA: Virtual, US.
- Li B, Morsi B, Wang J. Oral presentation. Carbon Management and Oil and Gas Research Project Review Meeting, Carbon Utilization. National Energy Technology Laboratory, DoE. Aug 30-31, 2021 (virtual).
- Wang R, Ashkanani HE, Li B, Morsi BI. Oral presentation. TEA of a unique process for producing high-value nanomaterials or CO_2 capture and sequestration. 38th Annual International Pittsburgh Coal Conference, Pittsburgh, Sept. 20-23, 2021 (virtual).
- Wang R, Li B, Morsi B. Poster presentation. Nanotechnology converts CO_2 from power plants flue gas to valuable products. U.S. DOE 2020 Virtual Integrated Project Review Meeting, Carbon Utilization sessions, October 21-22, 2020.
- Wang R, Ashkanani HE, Li B, Morsi BI. Poster presentation. Development of a continuous nanotechnology process for converting carbon dioxide to valuable products. 37th Annual International Pittsburgh Coal Conference (Virtual Conference), Pittsburgh, Sept. 8-11, 2020.
- Wang R, Ashkanani H, Li B, Morsi B. Poster presentation. Modeling of CO_2 absorption from gas mixtures using chemical absorbents in adiabatic packed-beds. 36th Annual International Pittsburgh Coal Conference, September 3-6, 2019, Pittsburgh, PA.
- Li B, Wafle T. Oral and poster presentations. Unique nanotechnology converts carbon dioxide to valuable products. Addressing the Nation’s Energy Needs Through Technology Innovation – 2019 Carbon Capture, Utilization, Storage, and Oil & Gas Technologies Integrated Review Meeting, Pittsburgh, PA, August 26-30, 2019.

6.0 Lessons Learned

Discuss obstacles and challenges encountered during the course of the project, how these challenges were addressed, and the lessons learned.

Technically, we had met with difficulties in enhancing the purity of $NaHCO_3$ through one of the approaches we previously proposed (i.e., using deionized water as the rinsing medium). This probably was due to the quick dissolution of the product in the rinsing water. Instead, we achieved high purity products via the use of $NaHCO_3$ saturated water as the rinsing medium.

Overall, this project was a successful one with a productive collaboration that led to multiple joint proposals and publications. Looking back, the beginning part was slow and we could have done a better job. There was a lack of communication between the collaborators and our university grants personnel, which led to a delay of funding availability and a subsequent delay (about 5 months behind schedule) in getting started on the project. The delay was discussed with the project manager at DoE and a no-cost extension was requested and approved to have time to finish the proposed activities. We did not have such challenges in the subsequent months and years after we started to have better communication and better interactions; ultimately, we have become familiar with each other among the principal investigator and the co-investigators. We have communicated with each other easily via phone calls, emails, and Zoom meetings, and our communication was excellent after the first year. The lesson learnt is that, after approval of a grant, we should immediately be prepared and should communicate with all people involved in a timely manner.

Another small challenge was related to changes in research team members. As we know, students and postdoctoral research associates may join and leave. We had a few changes in research personnel; the changes were normal and we were able to fit in other graduate students or postdoctoral research associates.

Finally, we thank everyone (students, postdoctoral research associates, collaborators, DoE project manager, and staff) involved for their dedication to this project. It was their dedication that led to the success of this project.

TEA of the CO_2 Capture Process in the Longview Power Plant

DEFE0031707

“Unique Nanotechnology Converts Carbon Dioxide to Valuable Products”

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1. Introduction

The Longview Power Plant (LPP) located near Maidsville, West Virginia, USA is a clean coal-fired facility, which produces 700 net MW of electric power and its heat rate of 8,750 kWh is greater than those of other coal-fired power plants in North America. The plant is provided with a supercritical boiler for high energy conversion and advanced air pollution control systems, leading to significantly less CO_2 emission than most other coal-fired power plants.

The flue gas mass flow rate emitted from the plant is 3,039 metric ton/h at 51.67 ^{o}C and 1 atmosphere (101.325 kPa). The composition of this flue gas is given in Table 1, and as can be observed, it contains 12.02 mol% CO_2, 33.19 ppmv SO_2 and 35.47 ppmv NO_2. A schematic of a post-combustion power plant, such as LPP, is presented in Figure 1.

Table 1: Flue gas composition of the LPP

Component	Gas composition, mol%
CO_2	12.02
O_2	4.79
N_2	79.20
Ar	0.98
H_2O	3.00
CO	3.144e-3 (31.44 ppmv)
SO_2	3.319e-3 (33.19 ppmv)
NO_2	3.547e-3 (35.47 ppmv)

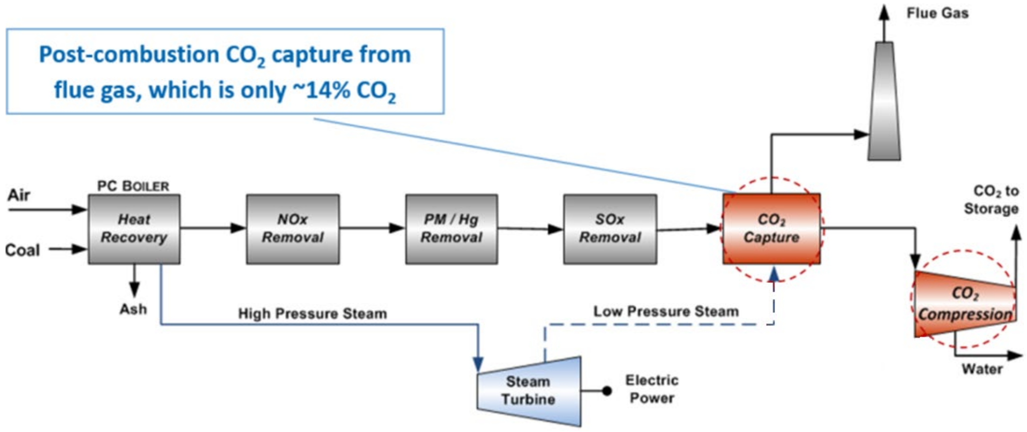

Figure 1: Schematic of a post-combustion power plant [1]

In this figure, coal and air are fed to a boiler and upon combustion, the flue gas, containing contaminants, such as SOx, NOx, CO_2, particulate matter, and mercury (Hg), has to be cleaned before emission into atmosphere. The heat recovered in the boiler converts water to high-pressure steam, which drives stream turbine to generate electric power. The objective of this part in our project was to perform Techno-Economic Analysis (TEA) of the CO_2 capture process in the LPP.

2. Techno-Economic Analysis (TEA) performed in this project

Considering the huge flue gas mass flue rate (3,039 ton/h) emitted from the LPP, and the unavailability of the total plant costs, particulate matters removal costs, and Hg removal costs, the TEA presented here is for a split stream of (456 ton/h), representing 15 wt% of the total flue gas emitted from the plant. Thus, the TEA was performed for a conceptual process developed in Aspen Plus v.12 and designed to remove SO_2 and NO_2 and capture CO_2 from the split flue gas stream. The process includes two main units, one unit for SO_2 and NO_2 scrubbing from the raw flue gas stream, and another unit for CO_2 capture from the polished flue gas stream, which is SO_2 and NO_2 free. Aspen Plus v.12 was used to simulate the conceptual process and calculate the capital cost (CAPEX), operating cost (OPEX) of the SO_2 and NO_2 scrubbing process, and the CAPEX, OPEX, and levelized cost of the CO_2 capture (LCOC) process.

In our project, since aqueous sodium glycinates solutions (SGS) were used to capture CO_2 from the flue gas streams, the reaction products exhibited a unique phase separation into a CO_2-rich phase and CO_2-lean phase. This behavior allowed for two process pathways. In Pathway (I), the nanomaterials in the CO_2-rich phase were separated and sold to offset the overall cost of the CO_2 capture process; and in Pathway (II), the nanomaterials in the CO_2-rich phase were regenerated, and the released CO_2 was compressed in preparation for subsequent sequestration. The TEA for each pathway is presented in this report. It should be emphasized, however, that the TEA presented herein should be handled with caution, since we did not consider the total plant costs, and the particulate matters and Hg removal costs.

In the following, a process for SO_2 and NO_2 scrubbing form the raw split flue gas stream is discusses. Also, two processes for CO_2 capture from the polished flue gas stream following Pathways (I) and (II) are described.

3. Process for SO_2 and NO_2 scrubbing from raw flue gas using DIW

Conventionally, sulfur-containing and nitrogen-containing compounds in the flue gas are removed using catalytic beds [2]. In this project, we used deionized water (DIW) to completely remove SO_2 and NO_2 in a countercurrent adiabatic packed-bed scrubber. The packing used in the scrubber was non-catalytic Mellapak 250Y, which has a specific surface area of 256 m^{-1} and voidage of 98.7%.

3.1 Chemical reactions in the scrubber

The chemical reactions between DIW and SO_2 and NO_2 take place in the scrubber. SO_2 is oxidized by O_2 and NO_2 as in Reactions (1) and (2) to become SO_3, while NO_2 in Reaction (2), is reduced by SO_2 to become NO. SO_3 then reacts with H_2O to become H_2SO_4 as in Reaction (3); whereas NO and NO_2 react with H_2O to become HNO_2 and HNO_3, as in Reactions (4) and (5), respectively.

Reaction (1):	$2SO_2 + O_2 \rightleftharpoons 2SO_3$	$\Delta G^o = -140.5\ kJ/mol$ $\Delta H^o = -196.9\ kJ/mol$
Reaction (2):	$SO_2 + NO_2 \rightleftharpoons SO_3 + NO$	$\Delta G^o = -35.5\ kJ/mol$ $\Delta H^o = -41.9\ kJ/mol$
Reaction (3):	$SO_3 + H_2O \rightleftharpoons H_2SO_4$	$\Delta G^o = -136.8\ kJ/mol$ $\Delta H^o = -227.9\ kJ/mol$
Reaction (4):	$4NO + O_2 + 2H_2O \rightleftharpoons HNO_2$	$\Delta G^o = 76.7\ kJ/mol$ $\Delta H^o = 90.4\ kJ/mol$
Reaction (5):	$2NO_2 + H_2O \rightleftharpoons HNO_2 + HNO_3$	$\Delta G^o = -28.7\ kJ/mol$ $\Delta H^o = -108.5\ kJ/mol$

According to the ELECNRTL model in Aspen Plus v.12, the reversible Reactions (1) through (5) are equilibrium reactions throughout the process [3].

3.2 Mass transfer in the scrubber

For mass transfer considerations, the Henry's Law constant (He) for all flue gas species listed in Table 1, including reactive (SO_2 and NO_2) and non-reactive (CO_2, O_2, CO and N_2) in DIW are available in Aspen Plus v.12 [3].

3.3 Flow diagram of the SO_2 and NO_2 scrubbing process

Aspen Plus v.12 was used to simulate the SO_2 and NO_2 scrubbing process from the split flue gas stream emitted from LPP. Table 1 shows the raw flue gas stream contains 33.2 ppmv SO_2 and 35.5 ppmv NO_2. The constraints imposed on the scrubbing process were: (1) 100 mol% SO_2 and NO_2 removal in scrubber, (2) no flooding in the scrubber to ensure smooth operation, and (3) the height to diameter ratio for the scrubber should be equal or greater than 6 to avoid gas-liquid channeling and wall effects. The SO_2 and NO_2 scrubbing process flow diagram is depicted in Figure 2; and all equipment used are listed in Table 2.

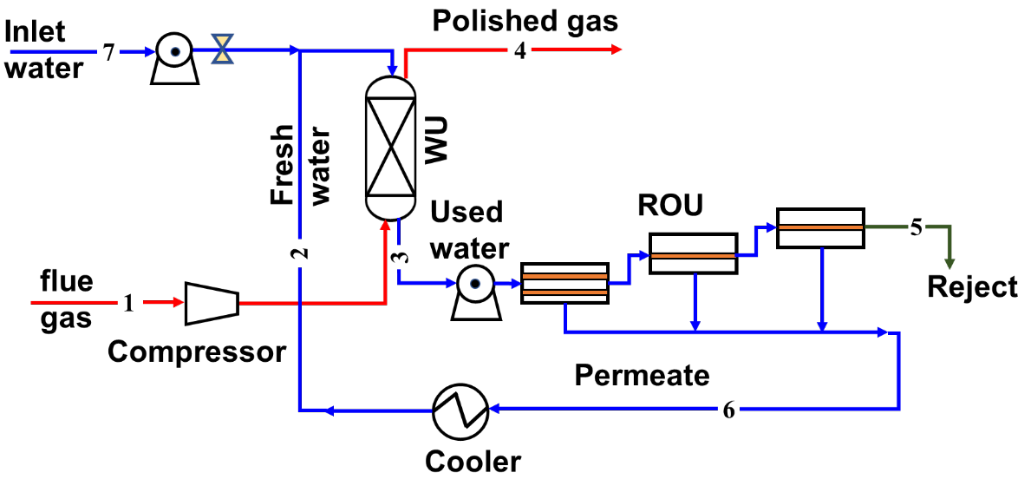

Figure 2: Schematic of the SO_2 and NO_2 scrubbing process

Table 2: Equipment used in the SO_2 and NO_2 scrubbing process

Unit	Number
Compressor	1
Pump	2
Packed-bed (Scrubber)	1
Cooler	1
ROU	1

In the scrubbing process, DIW enters the scrubber at the top (stream 7) whereas the raw flue gas enters from the bottom (stream 1). The chemical reactions occurring in the scrubber are given in Section 3.1. The polished flue gas existing from the top of scrubber (stream 4) is sent to the CO_2 absorber, whereas the used-DIW exiting from the bottom (stream 3) is sent to a reverse osmosis unit (ROU) for removing the dissolved sulfate and nitrate ions. After 99.5% H_2SO_4 and HNO_3 rejection, the clean-DIW (stream 6) or permeate is sent back to the scrubber for removing anew more SO_2 and NO_2, whereas the concentrated water-dissolved impurities (stream 5) or reject could be disposed of or used to react with KOH to produce K_2SO_4 and KNO_3 which are high-value salable product. Details for ROU are given in the following.

3.3.1 ROU

The ROU is a pressure-driven crossflow filtration unit that employs a semipermeable membrane acting as a barrier to salts [4]. The BW30-400 membrane manufactured by Dow with the properties given in Table 3, was selected to reject 99.5% of H_2SO_4 and HNO_3 from the used DIW. Following the design guideline by Dow [5], the ROU used in this process includes three stages with 17, 9 and 4 elements, respectively. Each element consists of 6 (BW30-400) membranes arranged in series.

Table 3: Specifications of the BW30-400 reverse osmosis membrane [166]

Active area of membrane	400, ft^2 (37.16, m^2)
Length of membrane	40, in (1.02, m)
Diameter of the membrane	7.9, in (0.20, m)
Feed space	0.034, in (0.00086, m)
Feed flow rate range	3.52 ~ 83.65, gpm (0.8 ~ 19.0, m^3/s)
Permeate flow	7.292, gpm (1.66 m^3/s)
Stabilized contaminant rejection	99.5, mol%
Operating pressure	15.5, bar (1.55 MPa)
Permeability constant of pure water	7.50E-09, $kg/m^3/s/Pa$
Permeability constant of salt	6.20E-05 $kg/m^2/s$
Cost of membrane	900, USD

At steady state, all conditions and compositions of the scrubbing process streams simulated with the rate-based model in Aspen Plus v.12 are given in Table 4.

Table 4: Inlet and outlet streams of SO_2 and NO_2 scrubber

Stream	**1**	**2**	**3**	**4**	**5**	**6**	**7**
T, (K)	324.82	298.15	304.35	300.26	304.35	304.35	298.15
P, (bar)	1.013	1.013	1.013	1.168	1.013	1.013	1.013
ρ, (kg/m^3)	1.124	997.168	995.49	1.213	10.836	995.393	997.168
Mwt, (kg/kmol)	29.946	18.015	18.021	29.863	25.856	18.016	18.015
$\dot{m}$, (kg/s)	126.630	74.788	74.300	127.118	0.079	74.221	0.568
Q, (m^3/s)	112.627	0.075	0.075	104.771	0.007	0.075	0.0006
	Composition						
Component	**Wt %**						
H_2O	1.805	100.000	99.952	2.206	56.833	99.998	100.000
O_2	5.118	-	1.75E-04	5.096	0.157	8.77E-06	-
CO_2	17.668	-	0.015	17.591	13.391	7.49E-04	-
CO	2.94E-03	-	-	2.93E-03	0.000	-	-
N_2	74.086	-	1.31E-03	73.801	1.175	6.57E-05	-
Ar	1.307	-	4.89E-05	1.302	0.044	-	-
H_3O^+	-	-	1.16E-04	-	0.104	5.80E-06	-
OH^-	-	-	-	-	3.35E-07	-	-
HCO_3^-	-	-	3.72E-04	-	0.333	1.86E-05	-
SO_2	7.10E-03	-	-	-	-	-	-
SO_3	-	-	-	-	7.71E-04	-	-
NO_2	5.45E-03	-	-	-	4.59E-05	-	-
HNO_2	-	-	-	-	7.75E-04	-	-
HNO_3	-	-	1.27E-02	-	11.384	6.37E-04	-
H_2SO_4	-	-	1.85E-02	-	16.579	9.27E-04	-

These results indicate that only 0.075 m^3/s of DIW is required to scrub 99.99 mol% of SO_2 and NO_2 from 112.63 m^3/s flue gas flow rate at 324.82 K and 101.325 kPa in a countercurrent packed-bed scrubber (5.8 m ID and 21.5 m packing height) containing a structured packing (Mellapak 250Y). Also, because of heat transfer between the flue gas and DIW, the flue gas is cooled down from 324.82 to 300.26 K, while the DIW is heated from 298.15 to 304.35 K.

The hydraulics (two-phase pressure drop, liquid holdup, and the normalized packing specific wetted area) and gas-liquid mass transfer coefficients were calculated under the scrubber operating conditions. The results indicated that the pressure drop was only 20 kPa through the packing height of 21.5 m. The average liquid holdup was 5.76%; and the normalized packing specific wetted area appears to follow the same trend of the liquid holdup and with an average value of 24.25%. Also, the liquid-side mass transfer coefficient was order of magnitudes lower than the gas-side mass transfer coefficient, indicating that resistance to mass transfer is located in the liquid-film next to the gas-liquid interface.

4. Process for CO_2 capture using aqueous sodium glycinates (SGS)

The polished flue gas which contains CO_2 coming from the top of the scrubber enters at the bottom of the CO_2 absorber, which is a packed-bed with Mellapak 250Y. When aqueous sodium glycinate solution (SGS) enter from the top of the CO_2 absorber, the following reactions will take place:

4.1 Reactions in the CO_2 absorber

According to Reaction (6), H_2O is ionized $\mathrm{OH^-}$ and $\mathrm{H_3O^+}$. Glycine undergoes zwitterion transformation according to Reaction (7) to protonate the amino group and becomes completely unreactive with CO_2 [6]. However, in a basic environment, such as NaOH, the amino group is deprotonated and becomes reactive with CO_2 to form SGS as expressed in Reaction (8). CO_2 then reacts with H_2O and $\mathrm{OH^-}$ to produce bicarbonate and carbonate ions according to Reactions (9), (10), and (11). CO_2 also reacts with SGS to form carbamate, which rapidly undergoes hydrolysis in water to produce glycine and bicarbonate ions following Reaction (12) [7]. It should be noted that Reactions (8) to (10) are equilibrium reactions and their corresponding equilibrium constants can be obtained using the change of the standard Gibbs free energy (ΔG^o), however, Reactions (11) and (12) are kinetic reactions and their forward and backward rate constants are required.

Reaction (6):	$\mathrm{2\,H_2O \rightleftharpoons OH^- + H_3O^+}$	$\Delta G^o = 79.91\ kJ/mol$ $\Delta H^o = 55.82\ kJ/mol$
Reaction (7):	$\mathrm{NH_2CH_2COOH \rightleftharpoons NH_3{}^+CH_2COO^-}$	
Reaction (8):	$\mathrm{NH_3{}^+CH_2COO^- + OH^- \rightleftharpoons NH_2CH_2COO^- + H_2O}$	$\Delta G^o = -24.17\ kJ/mol$ $\Delta H^o = -11.63\ kJ/mol$
Reaction (9):	$\mathrm{CO_2 + 2\,H_2O \rightleftharpoons H_3O^+ + HCO_3{}^-}$	$\Delta G^o = 36.36\ kJ/mol$ $\Delta H^o = 7.62\ kJ/mol$
Reaction (10):	$\mathrm{HCO_3{}^- + H_2O \rightleftharpoons CO_3{}^{2-} + H_3O^+}$	$\Delta G^o = 58.97\ kJ/mol$ $\Delta H^o = 14.84\ kJ/mol$
Reaction (11):	$\mathrm{CO_2 + OH^-} \xleftrightarrow[k_{-1}]{k_1} \mathrm{HCO_3{}^-}$	
Reaction (12):	$\mathrm{NH_2CH_2COO^- + CO_2 + H_2O} \xleftrightarrow[k_{-2}]{k_2} \mathrm{NH_3{}^+CH_2COO^- + HCO_3{}^-}$	

For Reaction (11), Pinsent et al. [8] suggested Equations (1) and (2) to calculate its forward (k_1) and the backward (k_{-1}) rate constants, respectively. The forward rate constant (k_2) of Reaction (12) is represented by Equation (3), proposed by Lee et al. [9]. For the backward rate constant (k_{-2}) in Reaction (12), we used the standard Gibbs free energy change (ΔG^o) and the equilibrium rate constant by Ziemer et al. [10] to obtain Equation (4). The units for k_2 and k_{-2} are in m^3/kmol·s.

$k_1 = 4.32 \times 10^{13} \exp(\frac{-6,667.5}{T})$	(1)
$k_{-1} = 2.38 \times 10^{17} \exp(\frac{-14,821.1}{T})$	(2)
$k_2 = 1.95 \times 10^{13} \exp(\frac{-7,670}{T})$	(3)
$k_{-2} = 3.82 \times 10^{12} \exp(\frac{-9,508}{T})$	(4)

4.2 Process pathways

The CO_2 reaction with SGS in the absorber leads to a unique phase separation into a CO_2-rich phase (represents 25 vol% of the total liquor volume and contains 62 mol% $NaHCO_3$ nanomaterials) and a CO_2-lean phase. Therefore, the stream coming from the bottom of the CO_2 capture unit allows for two process pathways. Pathway (I): the nanomaterials in the CO_2-rich phase can be separated and sold to offset the overall cost of the CO_2 capture process; and Pathway (II): the nanomaterials in the CO_2-rich phase can be regenerated, and the CO_2 released is compressed in preparation for sequestration in geological formation or for use in other applications, such as enhanced oil recovery (EOR), beverages, etc.

4.2.1 Process design for Pathway (I)

The process flow diagram for Pathway (I) is shown in Figure 3. The SO_2 and NO_2 scrubbing unit and the Reverse Osmosis Unit (ROU) was detailed in Section 3. The constraints imposed on the CO_2 capture process were: (1) at least 90 mol% CO_2 capture from the flue gas, (2) like the SO_2 and NO_2 scrubber, no flooding in the CO_2 absorber to ensure smooth operation, and (3) the packing height to diameter ratio for the CO_2 absorber should be equal or greater than 6 to avoid gas-liquid channeling and wall effects.

The process flow diagram for Pathway (I) consists of other 3 main units: (1) CO_2 absorption unit (CAU), (2) Ultrafiltration Unit (UFU) for $NaHCO_3$ solid nanoparticles separation, and (3) NaOH makeup chamber for hydroxide replenishment as needed. In this pathway, the polished flue gas from the scrubber is sent to CO_2 absorber to capture CO_2 and produce $NaHCO_3$ nanomaterials. Following CO_2 and SGS reactions, the CO_2 effluent stream coming from the bottom of absorber is pumped to an UFU to separate the nanomaterials from the solution. The filtrate from the UFU is then mixed with NaOH makeup solution in a makeup chamber, which is a continuously stirred tank reactor (CSTR) to convert the glycine to sodium glycinate. After pumping and cooling, the sodium glycinate solution is recycled back to the absorber. All equipment used in the CO_2 capture process for Pathway (I) are given in Table 5.

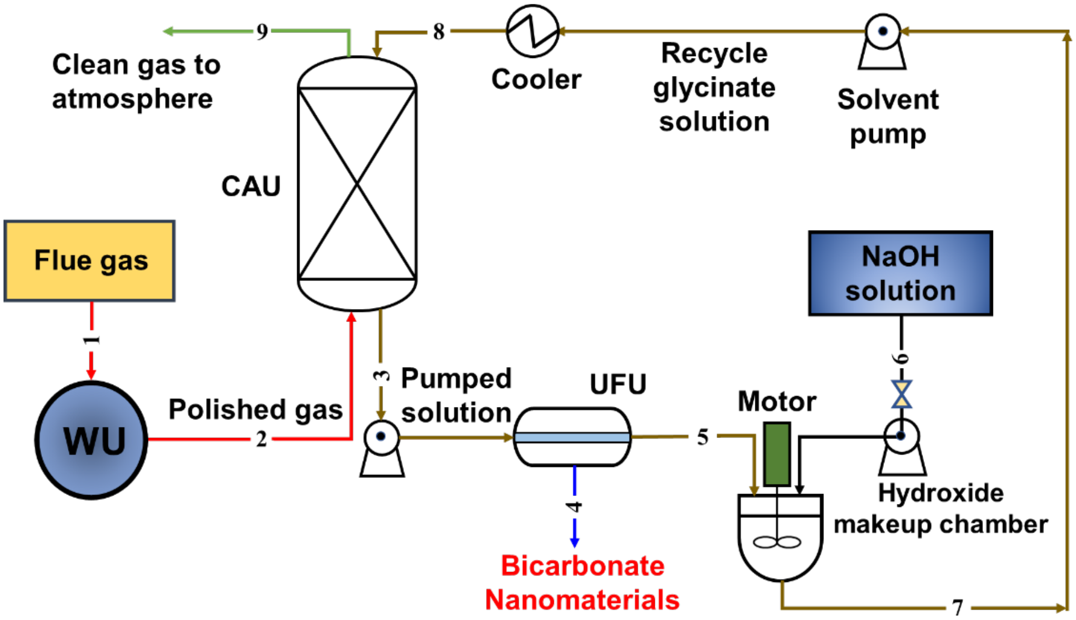

Figure 3: Process flow diagram of the CO_2 capture process for producing bicarbonate nanomaterials (Pathway (I))

Table 5: Equipment used in Pathway (I)

Unit	Number
CSTR	1
Pump	3
Packed-bed (Absorber)	1
Cooler	1
UFU	1

4.2.1.1 UFU

The liquid exiting from the bottom of the CO_2 absorber consists of water, glycine, unreacted SGS, and $NaHCO_3$ solid nanoparticle with an average size of 25 nm [11]. In order to separate the nanoparticles from the solution, an UFU using SFP-2860 membrane by DOW was employed. The UFU relies on the pressure difference through the semipermeable membrane to separate the solid particles from the solution as a retentate. The water, glycine and unreacted SGS passes through the membrane as a permeate. The specifications of SFP-2860 ultrafiltration membrane are given in Table 6. Based on the total flow rate of liquid and average feed flow rate for one membrane, 454 membranes operating with transmembrane pressure at 3.2 MPa are required to separate $NaHCO_3$ nanoparticles from the liquid-phase for SGS. Using this specific semipermeable membrane, 38.48 kg/s of $NaHCO_3$ solid nanoparticles were obtained.

Table 6: Specifications of SFP-2860 ultrafiltration membrane [12]

Active area of membrane	355, ft^2 (32.98, m^2)
Flow range	5.9 – 17.3, gpm (1.34 – 3.93 m^3/s)
Length of the membrane	73.2, in (1.86, m)
Diameter of the membrane	6.5, in (0.17, m)
Nominal pore diameter	0.03 µm
Maximum transmembrane pressure	36, psi (0.25 MPa)
Operating pH	2 - 11

4.2.1.2 Sodium Hydroxide Makeup Chamber

The permeate from the UFU is a mixture of H_2O, glycine and unreacted SGS. The SGS permeate contains 75.43 wt% H_2O, 12.78 wt% NaGly, 11.76 wt% glycine. In order to convert the glycine in the permeate once again to SGS, a highly concentrated solution of NaOH is added to the mixture in the NaOH makeup chamber, which is a conventional continuous stirred tank reactor (CSTR) provided with an agitator and a propeller. The volume of the CSTR used is 2.3 m^3, with 1.38 m inside diameter for SGS. Also, the agitator in the CSTR is designed to provide agitation at 200 revolution per minute (rpm). The agitation was delivered by a pitched blade turbine and the power required for this unit is 10.77 kW. In the CSTR, the aqueous NaOH reacts exothermally with glycine according to Reaction (8) and the heat of reaction increases the temperature of the aqueous SGS produced up to 335.3 K. The hot aqueous SGS solution is cooled to 298.15 K with a cooler and then is pumped back to the CAU for more CO_2 capture.

At steady state, all conditions and compositions of the CO_2 capture process streams simulated with the rate-based model in Aspen Plus v.12 are given in Table 7.

Table 7: Stream results of CO_2 capture from the polished flue gas - Pathway (I)

Stream	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
T, (K)	324.817	300.262	310.395	310.545	310.545	298.150	335.311	298.150	308.626
P, (bar)	1.013	1.017	1.013	1.013	1.013	1.013	1.000	1.013	1.013
ρ, (kg/m^3)	1.124	1.214	1,169.419	2,158.99	1,084.537	1,771.394	1,083.662	1,108.606	1.107
Mwt, (kg/kmol)	29.946	29.863	23.624	42.003	22.340	19.885	22.916	22.871	28.010
$\dot{m}$ (kg/s)	126.630	127.118	331.794	38.477	293.317	19.321	312.638	312.638	107.947
Q, (m^3/s)	112.627	104.752	0.284	0.018	0.270	0.011	0.289	0.282	97.530
	Composition								
Component	**Wt %**								
CO_2	17.668	17.591	3.77E-03	-	5.16E-05	-	4.84E-05	7.52E-10	2.030
CO	2.94E-03	2.93E-03	2.80E-06	-	3.16E-06	-	2.97E-06	2.97E-06	3.44E-03
N_2	74.086	73.801	4.80E-04	-	5.43E-04	-	5.10E-04	5.10E-04	86.907
AR	1.307	1.302	1.75E-05	-	1.98E-05	-	1.86E-05	1.86E-05	1.533
O_2	5.118	5.096	6.31E-05	-	7.14E-05	-	6.70E-05	6.70E-05	6.001
SO_2	7.10E-03	-	-	-	-	-	-	-	-
NO_2	5.45E-03	-	-	-	-	-	-	-	-
H_2O	1.805	2.206	66.688	-	75.427	5.181	73.728	73.575	3.526
NaGly	-	-	11.347	-	12.784	-	26.227	25.403	-
HGLYOH	-	-	10.363	-	11.762	-	0.026	0.664	1.59E-09
Na^+	-	-	3.174	27.366	0.012	54.499	0.008	0.203	-
HCO_3^-			8.423	72.634	0.006		0.005	0.006	
OH^-	-	-	1.06E-04		0.008	40.320	0.004	0.149	-
H_3O^+	-	-	-	-	-	-	-	-	-

These data indicate that the size of the absorber required in Pathway (I) was 8 m ID and the packing (Mellapak 250Y) height was 48 m. The polished flue gas flow rate was 127.12 kg/s, and its composition is given as (stream 2) in Table 7. In order to meet the constraint of at least 90 mol% CO_2 capture, the required 3M (3 mol/Liter) SGS solvent flow rate was 282 L/s as given in stream 8 of Table 7. The liquid-phase enters at the top of the packing at 298.15 K and leaves at the bottom of the packing at higher temperatures of 300.26 K, whereas the polished gas enters from the bottom of the absorber at 300.26 K and leaves at the top of the packing at 307.19 K. Also, the polished flue gas enters the absorber with 11.94 CO_2 mol% and exits with 1.3 mol% CO_2, which confirms that the CO_2 capture efficiency is more than 90 mol%, set as one of the process constraints.

The hydraulics (two-phase pressure drop, liquid holdup, and the normalized packing specific wetted area) and gas-liquid mass transfer coefficients were also calculated using Aspen Plus v.12 for Pathway (I). Under the operating conditions used, the resulting pressure drop was 15.5 kPa for a packing height of 48 m. The average liquid holdup was 7.90%; and the normalized packing specific wetted area appears to follow the same trend of the liquid holdup and the average value was 38.2%. Also, the liquid-side mass transfer coefficient was order of magnitudes lower than the gas-side mass transfer coefficient, indicating that resistance to mass transfer is located in the liquid-film next to the gas-liquid interface.

4.2.2 Process design for Pathway (II)

The process flow diagram for Pathway (II) is shown in Figure 4. The SO_2 and NO_2 scrubbing unit and the Reverse Osmosis Unit (ROU) was detailed in Section 3 The constraints imposed on the CO_2 capture process were: (1) at least 90 mol% CO_2 capture from the flue gas, and like in Pathway I, (2) no flooding in the CO_2 absorber to ensure smooth operation, (3) the packing height to diameter ratio for the absorber should be equal or greater than 6 to avoid gas-liquid channeling and wall effects, and (4) the H_2O in the CO_2 stream ready for sequestration should be less than 600 ppm to avoid the potential formation of ice-like CO_2 hydrates in the CO_2 transportation pipelines to sequestration sites. The process flow diagram for Pathway (II) consists of other 4 main units: (1) an absorber for CO_2 capture from the polished flue gas, (2) a decanter for phase separation, (3) a stripper for regenerating the CO_2-rich solution coming from the bottom of the absorber, and (4) a multistage-compressor for CO_2 compression in preparation for sequestration. In this pathway, the polished flue gas from the scrubber is sent to CO_2 absorber to capture CO_2 and the liquor coming from the bottom of absorber is separated into two phases in a decanter. The CO_2-rich phase is heated in cross-flow heat exchanger and regenerated in a stripper. The released pure CO_2 stream is compressed in multistage-compressor to 152.7 bar in preparation for sequestration in geological formation or for use in other applications, such enhanced oil recovery (EOR), beverages, etc. The regenerated SGS is mixed with CO_2-lean phase, pumped and cooled for recycling to CO_2 absorber. All equipment used in Pathway (II) are given in Table 8.

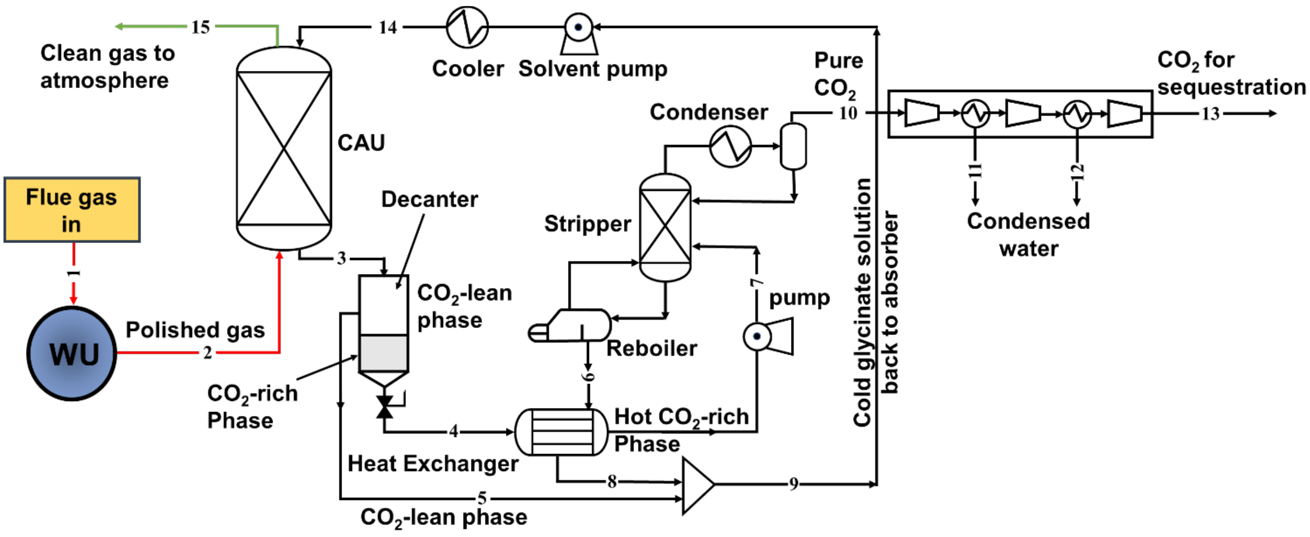

Figure 4: Process flow diagram of the CO_2 capture process for regeneration and CO_2 sequestration (Pathway (II))

Table 8: Equipment used in Pathway (II)

Unit	Number
Multi-stage compressor	1
Cross-flow heat exchanger	1
Reboiler	1
Condenser	1
Stripper	1
Decanter	1
Cooler	3
Pump	3

4.2.2.1 Stripper

The energy required for the CO_2-rich phase stream in this process includes the sensible heat to raise the temperature of liquid from that of the crossflow heat exchanger to the reboiler temperature, heat of evaporation in the reboiler to produce a gas-phase composed of CO_2 and H_2O which is condensed in the overhead condenser, and the heat required for the endothermic CO_2 desorption reaction. Therefore, regenerating only the CO_2-rich phase (stream 4) instead of the entire CO_2-rich solution (stream 3) is an energy-saving strategy.

Table 9 shows the size and packing of the stripper used for regenerating solvents, the CO_2-rich phase flow rate, the reboiler duty and the condenser duty.

Table 9: Operating conditions for the stripper

Pressure, atm	1
Column diameter, m	4
Packing height, m	24
Packing type	Mellapak 250Y
CO_2-rich phase flow rate, kg/s	127.69
Reboiler heat duty, MW	41.01
Condenser heat duty, MW	-8.74

In the stripper, the CO_2-rich solution is heated with the reboiler to generate CO_2 and water vapor moving upward through the stripper to reach the condenser where water vapor is partially condensed, and pure CO_2 stream is recovered in stream 10. This CO_2 stream should be further compressed to 152.7 bar in three-stages compressor for sequestration purposes. The three-stages compressor with intercooling knocks out H_2O in streams 11 and 12, so that the H_2O vapor content in final CO_2 (stream 13) is 504.7 ppm (< 600 ppm) to avoid the formation of CO_2 hydrates in CO_2 transportation pipelines to the sequestration sites.

At steady state, all conditions and compositions of the CO_2 capture process streams simulated with the rate-based model in Aspen Plus v.12 are given in Tables 10 and 11.

Table 10: Stream results of CO_2 capture from the polished flue gas - Pathway (II)

Streams	1	2	3	4	5	6	7	8
T, (K)	324.817	300.262	308.594	308.594	308.594	379.619	372.334	312.590
P, (bar)	1.013	1.144	1.013	1.013	1.013	1.013	1.013	1.013
ρ, (kg/m^3)	1.124	1.214	1,170.866	1,233.180	1,149.591	1,139.775	1,189.156	1,186.566
Mwt, (kg/kmol)	29.946	29.863	23.605	21.809	24.235	18.336	21.808	18.336
$\dot{m}$ (kg/s)	126.63	127.118	532.519	127.691	404.828	105.107	127.691	105.107
Q, (m^3/s)	112.627	104.752	0.455	0.104	0.352	0.092	0.107	0.089
Composition								
Component	**Wt %**							
CO_2	17.668	17.591	3.87E-03	-	5.09E-03	-	0.013	-
CO	0.003	2.93E-03	2.91E-06	-	3.83E-06	-	-	-
N_2	74.086	73.801	4.89E-04	-	6.43E-04	-	-	-
AR	1.307	1.302	1.79E-05	-	2.36E-05	-	-	-
O_2	5.118	5.096	6.45E-05	-	8.48E-05	-	-	-
SO_2	0.007	-	-	-	-	-	-	-
NO_2	0.005	-	-	-	-	-	-	-
H_2O	1.805	2.206	66.699	69.540	65.803	82.381	69.540	82.381
NaGly	-	-	10.999	-	14.469	-	-	-
HGLYOH	-	-	10.522	-	13.841	-	-	-
Na+	-	-	3.222	8.336	1.609	10.127	8.336	10.127
HCO_3^-	-	-	8.552	22.124	4.272	0.000	22.107	-
OH^-	-	-	9.35E-05	-	9.23E-05	7.492	0.005	7.492
H_3O^+	-	-	-	-	-	-	-	-

Table 11: Stream results of CO_2 capture from the polished flue gas - Pathway (II) Cont.

Streams	**9**	**10**	**11**	**12**	**13**	**14**	**15**
T, (K)	318.081	293.150	293.150	293.150	293.150	298.150	298.607
P, (bar)	1.013	1.013	5.392	28.694	152.700	1.013	1.013
ρ, (kg/m^3)	1,122.463	1.813	996.085	989.278	288.874	1,133.123	1.154
Mwt, (kg/kmol)	23.188	43.384	18.107	18.409	43.978	23.182	28.253
$\dot{m}$ (kg/s)	511.363	20.578	0.167	0.031	20.380	511.363	105.962
Q, (m^3/s)	0.456	11.348	1.68E-04	3.11E-05	0.071	0.451	91.836
Composition							
Component	**Wt%**						
CO_2	4.03E-03	99.001	0.858	3.614	99.950	3.34E-06	1.873
CO	3.03E-06	-	-	-	-	3.03E-06	0.004
N_2	5.09E-04	-	-	-	-	5.09E-04	88.536
AR	1.87E-05	-	-	-	-	1.87E-05	1.562
O_2	6.72E-05	-	-	-	-	6.72E-05	6.113
SO_2	-	-	-	-	-	-	-
NO_2	-	-	-	-	-	-	-
H_2O	70.937	0.999	99.141	96.383	0.050	70.914	1.911
NaGly	20.242	-	-	-	-	20.117	-
HGLYOH	4.160	-	-	-	-	4.257	-
Na+	1.274	-	-	-	-	1.304	-
HCO_3^-	3.382	-	1.46E-03	2.71E-03	-	3.387	-
OH^-	-	-	-	-	-	2.02E-02	-
H_3O^+	-	-	4.54E-06	8.46E-06	-	-	-

These data indicate that the size of the absorber required in Pathway (II) was 8 m ID and the packing (Mellapak 250Y) height was 48 m. The polished flue gas flow rate was 127.12 kg/s, and its composition is given stream 2 in Table 10. In order to meet the constraint of at least 90 mol% CO_2 capture, the required 3M (3 mol/Liter) SGS solvent flow rate was 451 L/s as given in stream 14 of Table 11. The liquid-phase enters at the top of the packing at 298.15 K and leaves at the bottom of the packing at higher temperatures of 300.26 K, whereas the polished gas enters from the bottom of the absorber at 300.26 K and leaves at the top of the packing at 298.61 K as stream 15 of Table 7. Also, the polished flue gas enters the absorber with 11.94 CO_2 mol% and exits with 1.20 mol% CO_2, which confirms that the CO_2 capture efficiency is more than 90 mol%, set as one of the process constraints. The hydraulics (two-phase pressure drop, liquid holdup, and the normalized packing specific wetted area) and gas-liquid mass transfer coefficients were also calculated using Aspen Plus v.12 for Pathway (II). Under the operating conditions used, the resulting pressure drop was 13.1 kPa for a packing height of 48 m. The average liquid holdup was 9.72%; and the normalized packing specific wetted areas appear to follow the same trend of the liquid holdup and the average value was 46.55%. Also, the liquid-side mass transfer coefficient was order of magnitudes lower than the gas-side mass transfer coefficient, indicating that resistance to mass transfer is located in the liquid-film next to the gas-liquid interface.

5. Techno-Economic costs

The CAPEX of a process includes the cost of all equipment, in addition to the installation and material cost factors. These costs are detailed in literature [13]. Table 12 lists the costs of the solvent (Sodium glycinate), the packing and the membrane used in the TEA calculations. The total OPEX of the process includes all rotating equipment electricity, heat exchanger (cooler) electricity, operating and maintenance (O&M) cost, initial solvent cost, and solvent makeup cost.

Table 12: Materials, packing and membrane costs used in the TEA

Material	Cost
Mellapak 250Y [14]	178 $/m^3$
SFP-2860 membrane [15]	1,650 $/module
$NaHCO_3$ [16]	203 $/ton
Cost of 3M SGS solution [17]	1.15 $/L
NaOH [18]	450 $/ton
BW30-400 membrane [19]	900 $/module

The LCOC includes the total capital and operating costs per ton of CO_2 captured, which is used to provide a fair quantification of the CO_2 capture process [20]. LCOC depends on other factors, such as plant lifetime (N), discount rate (i), capacity factor (f_c), and the capital recovery factor (f_{CR}). The parameters for LCOC calculation in Table 13 can be found elsewhere [13]. The CAPEX in USD/ton of CO_2 captured for Pathways (I) and (II) was calculated using Equation (5).

$$CAPEX\ (USD/ton.CO2) = \frac{f_{CR}\sum CAPEX_{2020}}{f_c \times \dot{m}_{CO2}} \tag{5}$$

The OPEX in USD/ton of CO_2 captured for Pathway (I) was calculated using Equation (6).

$$OPEX\ (USD/ton.CO2) = \frac{\left[(E\sum W) + (C_{NaOH}\dot{m}_{NaOH} - C_{NaHCO3}\dot{m}_{NaHCO3}) + \frac{0.04(CAPEX_{2020})}{7{,}200}\right]}{\dot{m}_{CO2}} \tag{6}$$

Where $\dot{m}_{NaOH}$ and $\dot{m}_{NaHCO3}$ are NaOH makeup rate and $NaHCO_3$ production rate in ton/h, respectively.

The OPEX in USD/ton of CO_2 captured for Pathway (II) was calculated using Equation (7).

$$OPEX\ (USD/ton.CO2) = \left[(E\sum W) + \frac{0.04(CAPEX_{2020})}{7{,}200}\right]/\dot{m}_{CO2} \tag{7}$$

The LCOC in USD/ton of CO_2 capture for Pathways (I) and (II) was calculated using Equation (8)

$$LCOC\ (USD/ton.CO2) = CAPEX\ (USD/ton.CO2) + OPEX\ (USD/ton.CO2) \tag{8}$$

The recovery factor in Equation (5) was calculated using Equation (9)

$$f_{CR} = \frac{i(1+i)^N}{(1+i)^N - 1} \tag{9}$$

Where $\dot{m}_{CO2}$ is the CO_2 captured in ton.CO_2/year.

As can be observed, all the calculated costs are in USD-2020.

Table 13: Parameters used for LCOC calculations [13]

Parameter	Value
Cost of electricity [21]	$37/MWh
i	10%/year
N	30 years
fc	0.8
$f_{O\&M}$	4% of the Total CAPEX, $/year
f_{CR}	0.10608

5.1 TEA of the SO_2 and NO_2 scrubbing process

Aspen Plus v.12 calculations of the CAPEX and OPEX of SO_2 and NO_2 scrubbing unit are given in Tables 14 and 15. As can be observed the CAPEX and OPEX of SO_2 and NO_2 scrubbing process are $3,045,668 and 29.22 $/h, respectively.

Table 14: CAPEX of the SO_2 and NO_2 scrubbing unit

Unit	
Cooler	$756,818
Packing cost	$100,924
Packed-bed scrubber	$1,601,598
Initial DIW cost	$137,068
ROU	$160,200
Rotating equipment	$289,060
Total CAPEX	**$3,045,668**

Table 15: OPEX of the SO_2 and NO_2 scrubbing unit

Unit	
Cooler	0.204 MW
Rotating equipment	0.129 MW
O&M	16.92 $/h
Total OPEX	**29.22 $/h**

5.2 TEA of the CO_2 capture process in Pathway I

Aspen Plus calculations of the CAPEX, OPEX, and LCOC of the Pathway (II) without the scrubbing unit are given in Tables 16, 17, and 18, respectively. As can be observed in these tables, the CAPEX, OPEX and LCOC of this process are 14,232,481 USD, 2,008 USD/h, and 30.62 USD/ton of CO_2 captured. Also, according to Table 18, the contributions of OPEX and CAPEX to the LCOC are 27.65 and 2.97 USD/per ton.CO_2 captured, respectively. In addition, the process was able to capture 72.61 ton/h of CO_2 and produce 138.52 ton/h of $NaHCO_3$ solid nanomaterials.

Table 16: Total CAPEX of the of the CO_2 capture process in Pathway (I)

Unit	
Cooler	$5,071,374
Packing cost	$429,468
CO_2 absorber	$4,197,566
UFU	$934,594
Reaction chamber	$716,785
Initial solvent cost	$450,119
Rotating equipment	$2,432,575
Total CAPEX	**$14,232,481**

Table 17: Total OPEX of the CO_2 capture process in Pathway (I)

Unit	
Cooler	4.713 MW
Rotating equipment	5.281 MW
Product of $NaHCO_3$	28,119 $/h
Cost of NaOH makeup	29,678 $/h
O&M	79.069 $/h
Total OPEX	**2,007.85 $/h**

Table 18: Total LCOC of the CO_2 capture process in Pathway (I)

Parameter	
CO_2 capture rate, ton/h	72.6
$NaHCO_3$ produced, ton/h	138.52
CAPEX, USD/ton.CO_2	2.97
OPEX, USD/ton.CO_2	27.65
Total LCOC, USD/ton.CO_2	**30.62**

It should be noted that if the SO_2 and NO_2 scrubbing process costs are included in the TEA calculations, the CAPEX, OPEX, and LCOC of Pathway (I) will be 17,278,149 USD, 2,036.8 USD/h, and 31.65 USD/ton of CO_2 captured, respectively.

5.3 TEA of the CO_2 capture process in Pathway II

Aspen Plus calculations of the CAPEX, OPEX, and LCOC of the Pathway (I) without the scrubbing unit are given in Tables 19, 20, and 21, respectively. These tables show the CAPEX, OPEX and LCOC of this process are 34,519,579 USD, 2,470 USD/h, and 42.34 USD/ton of CO_2 captured. Also, according to Table 21, the contributions of the OPEX and CAPEX to LCOC are 33.67 and 8.67 USD/per ton of CO_2 captured.

Table 19: CAPEX of the CO_2 capture process in Pathway (II)

Unit	
Stripper	$1,009,791
Coolers	$20,912,520
Packing Cost	$483,152
CO_2 Absorber	$4,197,566
Initial solvent	$450,119
Rotating equipment	$7,466,431
Total capital cost	**$34,519,579**

Table 20: OPEX of the CO_2 capture process in Pathway (II)

Unit	
Heat exchanger	47.698 MW
Rotating equipment	13.876 MW
O&M	191.78 $/h
Total OPEX	**2,470 $/h**

Table 21: Total LCOC of the CO_2 capture process in Pathway (II)

Parameter	
CO_2 capture rate, ton/h	73.355
CAPEX, USD/ton.CO_2	8.67
OPEX, USD/ton.CO_2	33.67
Total LCOC, USD/ton.CO_2	**42.34**

It should be noted that if the SO_2 and NO_2 scrubbing process costs are included in the TEA calculations, the CAPEX, OPEX, and LCOC of Pathway (II) will be 37,565,247 USD, 2,499.24 USD/h, and 43.50 USD/ton of CO_2 captured, respectively.

In summary, Table 22 shows the CAPEX, OPEX and LCOC for Pathways (I) and (II) with and without the including the cost of the SO_2 and NO_2 scrubbing process. These results indicate the Pathway (I) is more cost-effective than Pathway (II) whether the costs of the scrubbing process are considered or not.

Table 22: Sumary of TEA of the CO_2 capture process in Pathways (I) and (II)
With and without the SO_2 and NO_2 scrubbing process

	Pathway (I)	**Pathway (II)**	**Pathway (I)**	**Pathway (II)**
	With the Scrubbing process		Without the Scrubbing process	
CAPEX (2020-USD/ton.CO_2 captured)	3.60	9.43	2.97	8.67
OPEX (2020-USD/ton.CO_2 captured)	28.05	34.07	27.65	33.67
LCOC (2020-USD/ton.CO_2 captured)	**31.65**	**43.5**	**30.62**	**42.34**

6. Nomenclature

C	Market cost of $NaHCO_3$ or NaOH, USD/ton
CAPEX	Total capital costs, USD
E	Cost of electricity, USD/MWh
fc	Capacity factor
f_{CR}	Capital recovery factor
$f_{O\&M}$	4% of the Total CAPEX, USD/year
i	Annual discount rate, %
LCOC	Levelized Cost of CO_2 capture, USD/ton.CO_2
$\dot{m}_{NaHCO3}$	$NaHCO_3$ production rate, ton/h
$\dot{m}_{NaOH}$	NaOH makeup rate, ton/h
m	Mass flow rate, kg/s
Mwt	Molecular weight, kg/kmol
N	Plant lifetime, years
OPEX	Total operating cost, USD/h
P	Pressure, bar
Q	Volumetric flow rate, m^3/s
SGS	Sodium glycinate salt
T	Temperature, K
W	Total power required, Watt
Greek Symbols	
ρ	Mass density, kg/m^3
Subscripts	
G	Gas
S	Solvent
L	Liquid

7. Disclaimer

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LIFE CYCLE ASSESSMENT OF AN INNOVATIVE AMINO-ACID-BASED CO2 CAPTURE AND UTILIZATION TECHNOLOGY

FE0031707:Unique nanotechnology converts carbon dioxide to valuable products

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LIST OF EXHIBITS

ACRONYMS AND ABBREVIATIONS

AR5	Fifth Assessment Report
CCUS	Carbon capture utilization and storage
CFC-11	Trichlorofluoromethane
CH_4	Methane
CO_2	Carbon dioxide
CO_2e	Carbon dioxide equivalent
DOE	Department of Energy
EPA	Environmental Protection Agency
FOA	Funding Opportunity Announcement
GHG	Greenhouse gas
GWP	Global warming potential
g	Gram
H_2O	Water
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
kg	Kilogram
LCA	Life cycle analysis
LCI	Life cycle inventory
M	Thousand
MEA	Monoethanolamine
MW, MWe	Megawatt electric
N_2	Nitrogen
N_2O	Nitrous oxide
$NaHCO_3$	Sodium bicarbonate
NaOH	Sodium hydroxide
NETL	National Energy Technology Laboratory
NOx	Oxides of nitrogen
O_2	Oxygen
O3	ozone
PI	Principal investigator
PM	Particulate matter
SO_2	Sulfur dioxide
SO3	Sulfur trioxide
SOx	Oxides of sulfur
TRACI	Tool for the reduction and assessment of chemicals and other environmental impacts
TEA	Techno-economic analysis
U.S.	United States
VOCs	volatile organic compounds

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EXECUTIVE SUMMARY

This life cycle assessment (LCA) is being commissioned for the United States (U.S.) Department of Energy (DOE) National Energy Technology Laboratory (NETL) to satisfy the award requirements for Funding Opportunity Announcement (FOA) FE0031707: Unique nanotechnology converts carbon dioxide to valuable products. The Principal investigator (PI) for this project is Dr. Bingyun Li, professor and director of Nanomedicine Laboratory at WVU. This LCA report has been prepared in accordance with ISO 14040/14044 requirements for public release of comparative assessments for third parties.

The environmental impacts of the innovative amino acid-based carbon dioxide (CO_2) capture, utilization, and storage (CCUS) technology were quantitatively assessed using LCA model. The scope for CO_2 utilization process included the unit processes of flue gas washing, reverse osmosis, CO_2 absorption, ultrafiltration, and sodium hydroxide (NaOH) make-up. The products were considered to be 100% avoided burden. The scope for CO_2 capture process included the unit processes of flue gas washing, reverse osmosis, CO_2 absorption, and CO_2 regeneration. The results indicated that the CO_2 utilization process could achieve carbon negative, with the overall life-cycle global warming potential (GWP) impact of (-2,367.61) Mg CO_2e /1000 Mg CO_2 utilized. While for the CO_2 capture process, the life-cycle GWP impact are 303.47 Mg CO_2e /1000 Mg CO_2 captured. In addition, considering the comparison system, from the perspective of sodium bicarbonate ($NaHCO_3$) production, this AA-based technology resulted in a much lower GWP impact (0.0054 kg CO_2e/kg $NaHCO_3$) than the conventional Solvay process (1.2700 kg CO_2e/kg $NaHCO_3$). For the CO_2 capture process, the proposed AA-based CO_2 capture processes could yield less carbon emission than the current MEA-based process: 303.47 Mg CO_2e (AA-based) vs. 522.27 Mg CO_2e (MEA-based)/1000 Mg CO_2 captured.

1. GOAL AND SCOPE

1.1 STUDY GOAL

The intended application of this LCA is to evaluate the life-cycle environmental impact of global warming potential and other impacts of the proposed amino-acid-based CO_2 capture and utilization technology. Moreover, the life-cycle environmental impacts of this proposed technology are compared with the identified and defined comparison system as described in Section 1.2.1.

The major reason we take this LCA study is, though the proposed amino-acid-based CO_2 capture and utilization technology could capture and utilize CO_2, we are unaware of the life-cycle carbon balance. The other reason is that we would like to understand how this proposed technology is advantageous over comparable systems.

The intended audience for the LCA described herein is the U.S. DOE Carbon Utilization Program and the scientific peers.

This report could be disclosed to the public.

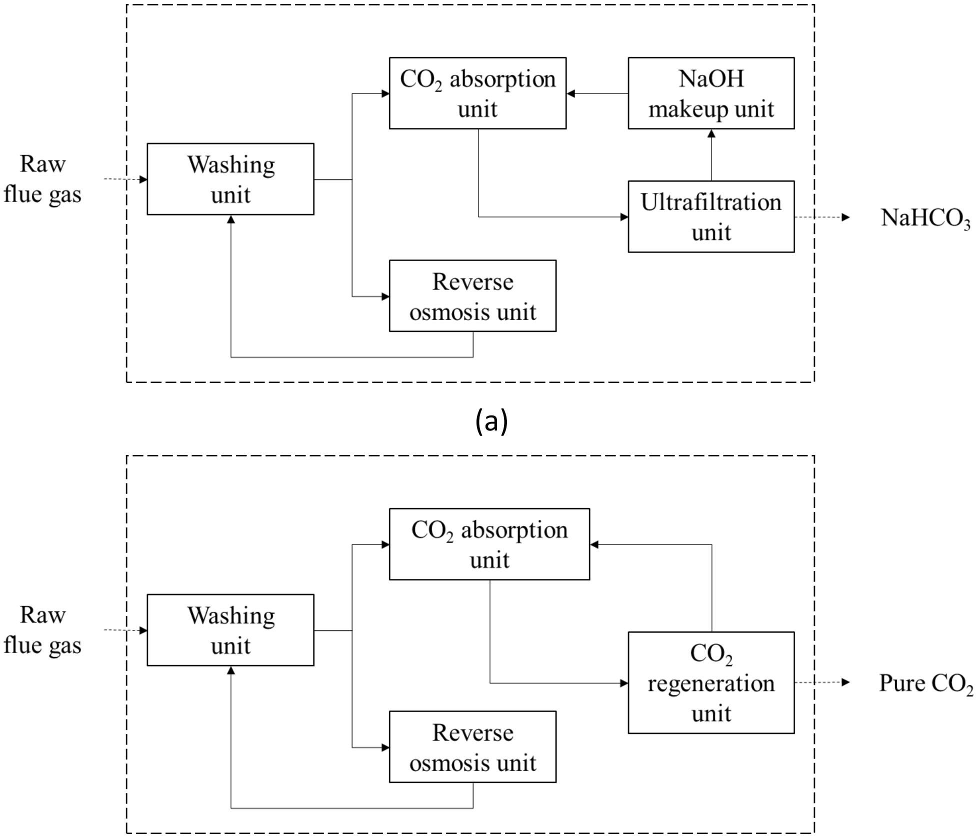
1.2 STUDY SCOPE

1.2.1 Functional Unit of the Study

For both the CO_2 utilization process and CO_2 capture process, the primary functional unit is 1000 Mg CO_2 converted or utilized, for being consistent between both and with the literature. In addition, we also used the functional unit of the production of 1 kg $NaHCO_3$ as the secondary functional unit to compare this proposed technology with the comparison system, which is the conventional system to produce $NaHCO_3$. And used the functional unit of the capture of 1000 Mg CO_2 to compare this AA-based process with MEA-based process.

1.2.2 System Boundary

In this study, we set the system boundary for both the CO_2 utilization process and CO_2 capture process, as illustrated in Figure 1. In specific, for the CO_2 utilization process, the raw flue gas was first processed via a washing unit with deionized water to remove the impurities such as sulfur dioxide (SO_2), sulfur trioxide (SO_3). As the result, the impurities dissolved in the water were removed via a reverse osmosis unit while the clean water was recycled back to the washing unit. The impurity-free flue gas was then put into a CO_2 absorption unit for the reaction to generate $NaHCO_3$ nanoparticles. Then these nanoparticles were separated with the glycine via an ultrafiltration unit. Finally, the separated nanoparticles were collected as the product, while glycine was mixed with added NaOH to recycle into the CO_2 absorption unit. The CO_2 capture process was generally similar to the CO_2 utilization process. The major difference is that, after the CO_2 absorption unit, the CO_2-rich phase was separated and heated to regenerate the pure CO_2 for sequestration. The CO_2 conversion rate is set as 90% to keep consistent with other studies, and the lifetime of the CCUS facilities is set as 30 years. The details of these chemical process modeling using Aspen Plus 10 can be found in our techno-economic analysis (TEA) modeling report.



(a)

(b)

Figure 1. The system boundary illustrated by the block flow diagram: (a) CO_2 utilization for $NaHCO_3$ production, and (b) CO_2 capture for pure CO_2 generation.

1.2.3 Carbon Dioxide Source

The CO_2 source in this study is set as the flue gas diversion. In specific, the compositions of 600 MW Wolverine power flue gas by Hoffman et al. (2010) was used here as the CO_2 source. The specific composition is reported in the accompany TEA report including the chemical process modeling.

1.2.4 Technology Representativeness

The Technology Readiness Level of this study is consistent with that’s stated in the overall report and TEA report. No additional adjustment for LCA part.

1.2.5 Geographical Representativeness

The geographical representativeness of this LCA study is national-level, without the site-specific information disclosed.

1.2.6 Temporal Representativeness

The product of the proposed CO_2 utilization process is $NaHCO_3$, which will be consumed once they are sold. That means, the CO_2 will be released after the product is consumed, but it has an "avoided burden" effect with substituting the current $NaHCO_3$ production.

1.2.7 Life Cycle Impact Assessment Methods for Results Interpretation

This study utilizes the Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts (TRACI) 2.1 method developed by US EPA, combined with the latest GWP factors included in the Intergovernmental Panel on Climate Change (IPCC) Fifth Assessment Report (AR5) report. In addition to the primary concern of the environmental impacts of Global Warming Potential, other related life-cycle environmental impacts are also evaluated. The details are as follow:

1. Global Warming Potential-GWP (kg CO_2e), based on IPCC AR5, 100-year time horizon; accounting for carbon climate feedback; abbreviation: GWP-100
2. Non-GHG impact assessment method
    a. acidification potential (kg SO_2e); abbreviation: AP
    b. particulate matter formation potential (kg $PM_{2.5}$e); abbreviation: PMFP
    c. photochemical smog formation potential (kg O_3e); abbreviation: PSFP
    d. eutrophication potential (kg Ne); abbreviation: EP
    e. ozone depletion potential (kg CFC-11e); abbreviation: ODP
    f. carcinogenics potential (CTUh); abbreviation: CP
    g. non carcinogenics potential (CTUh); abbreviation: NCP
    h. ecotoxicity potential (CTUe); abbreviation: ETP
    i. fossil fuel depletion (MJ surplus); abbreviation: FFD

1.2.8 Completeness Requirements

The inputs and outputs of carbon and energy within the system boundary were derived from the energy and material balance of chemical process modeling which has been reported in the accompany TEA report.

Table 1. The life-cycle inventory for the material and energy flow of 1000 Mg CO_2 conversion for utilization and capture, respectively.

		Item	Unit	Quantity
CO_2 *Utilization*	*Output*			
	Products	$NaHCO_3$	Mg	1907.57
	Emission to water	H_2SO_4	Mg	0.40
	Input			
	Material	NaOH	Mg	908.28
	Energy	electricity	MWh	94.91
	Resources	CO_2	Mg	1000
CO_2 Capture	*Output*			
	Products	Pure CO_2	Mg	1000
	Emission to water	H_2SO_4	Mg	0.40
	Input			
	Energy	Electricity	MWh	94.91
		Steam heat	MWh_{th}	492.60

2 LIFE CYCLE INVENTORY ANALYSIS

2.1 MODELING PLATFORM

The modeling platform in this study is a third-party LCA software – SimaPro 9.1. We provide the accompany LCA data along with the report.

2.2 UNIT PROCESS DESCRIPTIONS

The CO_2 utilization process includes unit processes of flue gas washing, reverse osmosis, CO_2 absorption, ultrafiltration, and NaOH making-up. While the CO_2 capture process includes unit processes of flue gas washing, reverse osmosis, CO_2 absorption, and CO_2 regeneration.

Specifically, for the CO_2 utilization process, the original flue gas was first passed through a deionized water washing unit to remove impurities such as SO_2 and SO_3. A reverse osmosis unit filtered the impurities while recycling the clean water back into the washing unit. Next, the flue gas without impurities was fed into a CO_2 absorption unit, which reacted to generate $NaHCO_3$ nanofibers. Then, these nanofibers were separated from glycine by an ultrafiltration unit. Finally, the separated bicarbonate nanomaterials were collected as the final product, while the glycine was mixed with the NaOH and recycled to the CO_2 absorption unit.

The CO_2 capture process is essentially similar to the CO_2 utilization process. The main difference is that following the CO_2 absorption unit, the CO_2-rich phase was separated and heated to generate pure CO_2 for sequestration. The products were treated as the 100% avoided burden, i.e., the produced $NaHCO_3$ can avoid/substitute its current production. The Solvay process was used as the currently typical production process for $NaHCO_3$ (Steinhauser 2008).

2.3 DATA SOURCES AND QUALITY ASSESSMENT

All the foreground data related to the abovementioned unit processes are the PI-provided data, from the chemical process modeling which has been report in the accompany TEA report. As to the background data of the inputs, we refereed to the LCI database, USLCI and EcoInvent, after the examination of the experts. All the data used in this study has been well-examined and they meets the technical, geographical, and temporal representativeness requirements defined in the *Study Scope*.

Table 2. The data sources and reference processes.

		Item	Source	Assessment
CO_2 *Utilization*	Emission to water	H_2SO_4	Sulphuric acid, liquid, at plant/US- US-EI U	Satisfied
	Input			
	Material	NaOH	Sodium hydroxide, 50% in H_2O, diaphragm cell, at plant/US-US-EI U	Satisfied
	Energy	electricity	Electricity mix 2011/US US-EI U	Satisfied
	Resources	CO_2	Carbon dioxide liquid, at plant/US- US-EI U	Satisfied
CO_2 Capture	Emission to water	H_2SO_4	Sulphuric acid, liquid, at plant/US- US-EI U	Satisfied
	Input			
	Energy	Electricity	Electricity mix 2011/US US-EI U	Satisfied
		Steam heat	Steam, for chemical processes, at plant/US- US-EI U	Satisfied

2.4 RESULTS OF INVENTORY COMPLETENESS CHECK

With the energy and mass balance setting in the chemical process modeling, the models developed in this study meet the carbon and energy balance requirements of the completeness check.

3 LIFE CYCLE IMPACT ASSESSMENT

3.1 LIFE CYCLE IMPACT ASSESSMENT METHODS

The 100-year GWP factors for CO_2, CH_4, and N_2O utilized in this analysis are depicted in **Exhibit 3-1**.

Exhibit 3-1. IPCC AR5 GWPs [1]

GHG	20-year	100-year	Units
CO_2	1	1	kg CO_2e
CH_4	87	36	kg CO_2e
N_2O	268	298	kg CO_2e
SF_6	17,500	23,500	kg CO_2e

This analysis utilizes the latest factors available in TRACI 2.1, with modified *characterization factors* for GWP to reflect the current state of science from the IPCC. The following describes the non-GWP midpoint impact assessment categories included in this analysis:

- **Acidification Potential (AP):** The increased concentration of hydrogen ions in a local environment. This can be from the direct addition of acids, or by indirect chemical reactions from the addition of substances such as ammonia. [14] Reporting units are kg SO_2-equivalent.

- **Eutrophication Potential (EP):** The "enrichment of an aquatic ecosystem with nutrients (nitrogen, phosphorus) that accelerate biological productivity (growth of algae and weeds) and an undesirable accumulation of algal biomass." [16] Reporting units are kg nitrogen (N)-equivalent.

- **Photochemical Smog Formation Potential (PSFP):** Ground-level ozone, formed by the reaction of NO_x and volatile organic compounds (VOCs) in the presence of sunlight. [14] Reporting units are kg trichlorofluoromethane (CFC-11)-equivalent.

- **Ozone Depletion Potential (ODP):** The deterioration of ozone within the stratosphere by chemicals such as CFCs. Stratospheric ozone provides protection for people, crops, and other plant life from radiation. [14] Reporting units are kg ozone (O_3)-equivalent.

- **Particulate Matter Formation Potential (PMFP):** Particulate matter (PM) includes "a mixture of solid particles and liquid droplets found in the air" that are smaller than 10 microns in diameter. [17] Smaller diameter particulate matter (2.5 microns or smaller) can be formed by chemical reactions in the atmosphere (e.g., SO_2 and NO_x). Almost all PM impacts are caused by PM 2.5 microns or smaller ($PM_{2.5}$). [18] Reporting units are kg $PM_{2.5}$-equivalent.

- **Carcinogenics Potential (CP):** Potential of a chemical released into an evaluative environment to cause human cancer effects (Bare 2002). Reporting units are CTUh.

- **Non Carcinogenics Potential (NCP):** Potential of a chemical released into an evaluative environment to cause human noncancer effects (Bare 2002). Reporting units are CTUh.
- **Ecotoxicity Potential (ETP):** Potential of a chemical released into an evaluative environment to cause ecological harm (Bare 2002). Reporting units are CTUe.
- **Fossil Fuel Depletion (FFD):** Potential to lead to the reduction of the availability of low cost/energy fossil fuel supplies (Bare 2002). Reporting units are MJ surplus.

3.2 DATA QUALITY ASSESSMENT

There are not any known data limitations or omissions of inventory data that may affect the interpretation of each impact categories result. The completeness was tested and determined not to affect the interpretation of results for each impact category is sufficient.

3.3 LIFE CYCLE IMPACT ASSESSMENT RESULTS

The overall GWP impact of the CO_2 utilization process is -2,367.61 Mg CO_2e/1000 Mg CO_2 utilization. The contribution of the NaOH making-up process to the overall GHG emissions is 97.93%. The electricity consumption of the entire process results in 5.51% of the GHG emissions. Other environmental impacts of the CO_2 utilization process show that eight out of ten impacts were negative, including global warming, smog, acidification, eutrophication, carcinogenics, non-carcinogenics, respiratory effects, and ecotoxicity.

The total GWP impact of the CO_2 capture process is 303.47 Mg CO_2e/1000 Mg CO_2 captured. For the unit processes, the CO_2 regeneration process contributes to an overall GHG emission impact of 95.36%. Of this, steam heat from the reboiler used to regenerate pure CO_2 accounts for 70%, while electricity used for other equipment accounts for 30% of the overall GWP impact. In addition, other environmental impacts of the CO_2 capture process are evaluated and summarized. Carcinogenics and ecotoxicity are the two impacts with the highest normalized values.

The details of the LCA results are listed in Tables 3 and 4.

Table 3. Life cycle environmental impacts of the CO_2 utilization process for coal power flue gas by impact and unit process on a 1000 Mg CO_2 basis.

Impact	Unit	Total	Washing Unit	Reverse Osmosis Unit	CO_2 Absorption Unit	Ultrafiltration Unit	NaOH Makeup Unit	CO_2 Consumed Feedstock	Avoided Burden
Ozone depletion	kg CFC-11 eq	5.35E-02	7.24E-04	9.96E-05	3.55E-05	2.73E-05	1.30E-01	0.00	-7.76E-02
Global warming	kg CO_2 eq	-1.37E+06	1.79E+04	2.46E+03	8.77E+02	6.74E+02	1.03E+06	-1.00E+03	-2.42E+06
Smog	kg O3 eq	-1.08E+05	6.64E+02	9.14E+01	3.26E+01	2.51E+01	5.36E+04	0.00	-1.62E+05
Acidification	kg SO2 eq	-1.60E+04	7.48E+01	1.03E+01	3.67E+00	2.83E+00	8.76E+03	0.00	-2.48E+04
Eutrophication	kg N eq	-1.01E+04	3.91E+01	5.38E+00	1.92E+00	1.48E+00	2.10E+02	0.00	-1.03E+04
Carcinogenics	CTUh	-3.41E-01	6.57E-04	9.04E-05	3.23E-05	2.48E-05	5.01E-03	0.00	-3.47E-01
Non carcinogenics	CTUh	-1.29E+00	2.29E-03	3.16E-04	1.13E-04	8.66E-05	1.15E-01	0.00	-1.41E+00
Respiratory effects	kg PM2.5 eq	-2.49E+03	4.60E+00	6.34E-01	2.26E-01	1.74E-01	4.82E+02	0.00	-2.97E+03
Ecotoxicity	CTUe	-8.56E+07	5.24E+04	2.45E+05	2.57E+03	1.98E+03	9.72E+05	0.00	-8.69E+07
Fossil fuel depletion	MJ surplus	4.45E+05	2.05E+04	2.83E+03	1.01E+03	7.76E+02	1.62E+06	0.00	-1.20E+06

Table 4. Life cycle environmental impacts of the CO_2 capture process for coal power flue gas by impact and unit process on a 1000 Mg CO_2 basis.

Impact	Unit	Total	Washing Unit	Reverse Osmosis Unit	CO_2 Absorption	Regeneration Unit
Ozone depletion	kg CFC-11 eq	2.45E-02	3.16E-04	1.27E-04	1.27E-04	2.39E-02
Global warming	kg CO_2 eq	3.03E+05	7.80E+03	3.15E+03	3.14E+03	2.89E+05
Smog	kg O3 eq	1.02E+04	2.90E+02	1.17E+02	1.17E+02	9.69E+03
Acidification	kg SO2 eq	1.06E+03	3.27E+01	1.32E+01	1.32E+01	1.00E+03
Eutrophication	kg N eq	4.28E+02	1.71E+01	6.89E+00	6.88E+00	3.97E+02
Carcinogenics	CTUh	7.38E-03	2.87E-04	1.16E-04	1.16E-04	6.86E-03
Non carcinogenics	CTUh	3.71E-02	1.00E-03	4.04E-04	4.03E-04	3.53E-02
Respiratory effects	kg PM2.5 eq	1.04E+02	2.01E+00	8.11E-01	8.10E-01	1.00E+02
Ecotoxicity	CTUe	9.57E+05	2.29E+04	2.47E+05	9.22E+03	6.78E+05
Fossil fuel depletion	MJ surplus	4.55E+05	8.97E+03	3.62E+03	3.62E+03	4.39E+05

4 LIFE CYCLE INTERPRETATION

This study indicates that both the CO_2 utilization and capture processes could achieve carbon negative.

Considering the comparison system, from the perspective of sodium bicarbonate production, this AA-based technology has a much lower GWP impact (0.0054 kg CO_2e/kg $NaHCO_3$) than the conventional Solvay process (1.2700 kg CO_2e/kg $NaHCO_3$) to produce the same amount of products.

Regarding the CO_2 capture process, the MEA-based process to capture CO_2 from coal power flue gas was consistently modeled via Aspen Plus 10 platform. Our results indicate the proposed AA-based CO_2 capture processes could achieve less carbon emission than the MEA process: 303.47 Mg CO_2e Vs. 522.27 Mg CO_2e (MEA).

The limitation of the GWP impact evaluated in this study is, we take the product of $NaHCO_3$ as a 100% avoided burden in the LCA framework. However, in the reality, whether this can be realized depends on a lot of factors, mainly the global market. However, a preliminary market potential analysis was conducted by the team, which showed a possibility of this 100% consumption of the produced $NaHCO_3$.

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