

Original Research

Post-Combustion CO₂ Capture from an Industrial Power Plant Using Five Chemical Solvents: A Comparative TEA

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Abstract

CO₂ capture processes using five chemical solvents were modeled in Aspen Plus V.12.1 for the capture of over 90% CO₂ from a 456 ton/hour split flue gas stream containing 12.02 mol% CO₂ emitted by the Longview 780 MW power plant (West Virginia, USA). Since the flue gas contained 33.10 ppmv SO₂ and 35.47 ppmv NO₂, a gas polishing process, using deionized water (DIW), was included in the model for complete scrubbing of SO₂ and NO₂ from the raw flue gas before the CO₂ capture process. The five chemicals used for CO₂ capture included three amine-based solvents (ABs) (monoethanolamine (MEA), 2-amino-2-methyl-1-propanol (AMP), and (piperazine/methyldiethanolamine (PZ/MDEA)), and two amino acid-based solvents (AAs) (sodium glycinate (SGS) and potassium glycinate (PGS)). Since SGS and PGS exhibit phase separation, the CO₂ capture processes followed two distinct pathways: Pathway (i) involved direct CO₂ capture using all five solvents, and Pathway (ii) focused on bicarbonate nanomaterials production using only SGS and PGS. A Techno-economic assessment (TEA) of



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the CO₂ capture processes was conducted and the corresponding process hydraulics and mass transfer characteristics were calculated. The simulation results revealed the following: (1) for Pathway (i), the levelized cost of CO₂ capture (LCOC) for PGS was lower than that for SGS, MEA, AMP, and PZ/MDEA; (2) for Pathway (ii), PGS had a lower LCOC than SGS; (3) Pathway (ii) was more economically more favorable than Pathway (i); and (4) under the operating conditions used, the two-phase pressure drop values were negligible, and the liquid-side mass transfer coefficients (k_L) were an order of magnitude smaller than gas-side mass transfer coefficients (k_G), suggesting that the gas-liquid mass transfer resistance ($1/k_L$) was in the liquid-side. Our techno-economic analysis (TEA) underscores the uniqueness of using AAs solvents in industrial CO₂ capture, offering significant cost savings through the production of valuable bicarbonate nanomaterials.

Keywords

Post-combustion CO₂ capture; sodium glycinate; potassium glycinate; MEA; AMP; MDEA/PZ; Aspen Plus; techno-economic analysis

1. Introduction and Background

Under the Kyoto Protocol in 1997, the Greenhouse Gas (GHG) inventory covers the following: CO₂ (Carbon dioxide), CH₄ (Methane), HFCs (Hydrofluorocarbons), SF₆ (Sulphur hexafluoride), PFCs (Perfluorocarbons), N₂O (Nitrous oxide), and NF₃ (Nitrogen trifluoride) [1]. In 2023, the global GHG emissions were 58.79 GT (Giga-ton CO₂ equivalent), where the energy systems sector contributed 36% (21.27 GT), followed by the industrial sector with 24% (14.40 GT), the agriculture sector with 20% (11.9 GT), the transportation sector with 14% (7.98 GT), and the buildings sector with 6% (3.24 GT) [2].

The steady increase of GHG emissions into the atmosphere is leading to a global temperature rise and evident climate changes, with detrimental socio-economic, political, and environmental consequences [3]. These consequences include: (i) Increasing frequency and intensity of extreme heatwaves, droughts, hurricanes and floods, causing widespread damage and loss of life and infrastructure; (ii) Changing the precipitation patterns, with water scarcity in some regions and increased flooding in others, leading to disruption of food production; (iii) Rising sea levels, resulting in coastal erosion, inundation of low-lying areas, and displacement of communities affecting both human settlements and natural ecosystems; (iv) Increasing potential conflicts among humans arising from resource scarcity and environmental degradation; (v) Losing biodiversity and ecosystems, leading to declines in species populations and shifts in ecosystem dynamics; and (vi) Deteriorating human health, including increased rates of respiratory illness, heat-related illness, and the spread of disease-carrying insects, as well as mental health problems, such as anxiety and depression. Therefore, reducing GHG emissions is the most crucial step to alleviate the catastrophic outcomes of the global climate change.

As a GHG, CO₂ has become one of the chief drivers of climate change due primarily to fossil fuels combustion. Prior to the industrial revolution there was an equilibrium where naturally produced CO₂ was absorbed by natural sinks, including plants and trees, maintaining a healthy balance of

atmospheric CO₂. Industrialization, however, led to a substantial increase in deforestation, exacerbating the GHG effect by eliminating the CO₂ natural sinks. In addition, the warming oceans, dissolving much of atmospheric CO₂, have become less able to absorb CO₂ [4]. In response to these challenges, CO₂ capture technologies have been developed to mitigate emissions from fossil energy sources, including pre-combustion CO₂ capture, post-combustion CO₂ capture, and oxy-combustion [5].

The present study is focusing on the post-combustion CO₂ capture because of its wide industrial applications [6, 7]. The CO₂ in flue gas is about 11-13 mol% with a total pressure of one atmosphere [8], and accordingly CO₂ is often captured using chemical solvents. The reacted CO₂ is stripped from the products by heating and is then collected and conditioned for subsequent sequestration or use in other applications. The chemical solvents employed for CO₂ capture in this technology are either aqueous amine-based solvents (ABs) or Amino acid-based solvents (AAs).

ABs, such as MEA [9], AMP [10], and PZ/MDEA [11] were employed to capture CO₂. Since MEA is readily available [12] and exhibits rapid reaction with CO₂, it is the most commonly used chemical solvent [13]. Garcia et al. [14] used 30 wt% MEA in modeling a pilot-scale plant for CO₂ capture in Aspen Plus V.8.6, then validated their model with actual experimental data. Mandal et al. [13] and Osagie et al. [15] used AMP for CO₂ capture. Osagie et al. [15] simulated in Aspen Plus V.8.4 a pilot-scale process using AMP and validated their modeling with experimental data from Gabrielsen et al. [16]. The validated model was further extended to a 400 MWe NGCC where the LCOC was \$69.3/ton [15]. Also, Zhao et al. [17] used a blend of (20/30 wt% of PZ/MDEA) to capture CO₂ in a 650 MW PP, and PZ was identified as a promoter for MDEA [18].

AAs, such as glycine and alanine, were suggested as possible AAs for CO₂ capture due to their advantages over amine-based (ABs) solvents, such as: (i) AAs have significantly lower vapor pressures than ABs, which greatly minimize the solvent loss [19], (ii) AAs are more environmentally friendly and more resistant to oxidative degradation than ABs [20], (iii) AAs have high resistance to degradation [21], and (iv) the unique phase separation characteristics of SGS and PGS for CO₂ capture enables the solution to separate into distinct phases allowing two-pathways processes [22-26]. AAs have been commercialized for CO₂ capture by BASF and Siemens Co. [27, 28], who installed a pilot-plant in Germany. The pilot plant has been using AAs for CO₂ capture from 140 Nm³/s flue gas since 2009 [28]. In addition, BASF employed sodium or potassium salts of AAs (alanine, and diethyl-glycine or dimethyl-glycine) for removing CO₂ and H₂S from flue gas [29].

The AA (glycine) reacts with aqueous sodium hydroxide (NaOH) to produce sodium glycinate solutions (SGS) and with aqueous potassium hydroxide (KOH) to produce potassium glycinate solutions (PGS). Li et al. [23] showed the reactions between CO₂ and SGS or PGS led to the formation of regenerable NaHCO₃ (sodium bicarbonate) or KHCO₃ (potassium bicarbonate) nanomaterials having an average diameter of 45 nm. Bao et al. [22] reacted glycine and alanine with KOH to obtain deprotonated AAs (potassium glycinate or potassium alaninate). These deprotonated AAs absorbed CO₂ and formed carbamate, which underwent hydrolysis to yield bicarbonate and AAs. Wickramasinghe et al. [26] obtained sodium bicarbonate nanofibers and nanoflowers from the CO₂ reaction with glycine and alanine and reported the existence of a phase separation.

This unique phase separation allowed Wang et al. [24, 25] to model in Aspen Plus V.12.1 a process using SGS to capture CO₂ from a 45 ton/h raw flue gas split stream from the Wolverine coal-fired PP (MI, USA). They developed two process pathways: Pathway (i) for CO₂ capture and compression for subsequent sequestration, and Pathway (ii) for bicarbonate nanomaterials

production. They also performed TEA and calculated the process hydraulics and mass transfer characteristics for the two pathways.

The goal of this study was to model in Aspen Plus V.12.1 processes to capture more than 90% CO₂ from a 456 ton/h raw flue gas split stream from the 780 MW Longview coal-fired power plant (PP) (WV, USA) using three ABs solvents (MEA, AMP, and PZ/MDEA) and two AAs solvents (SGS and PGS). Since Table 1 shows that the raw flue gas used contains 0.003 mol% SO₂ and 0.004% mol% NO₂, a gas polishing process using deionized water (DIW) was also modeled in Aspen Plus V.12.1 to completely scrub these gases before the CO₂ capture. The raw flue gas scrubbing and CO₂ capture processes were carried out in adiabatic counter-current fixed-beds packed with Mellapak 250Y. The TEA of the two process Pathways (i) and (ii) were conducted and the hydraulics and mass transfer characteristics of the flue gas scrubbing and CO₂ capture processes were calculated. Figure 1 depicts a block diagram of the entire process.

Table 1 Comparison between the Longview and Wolverine Power Plants [30, 31].

	Longview Power Plant	Wolverine Power Plant
Capacity, MW	780	600
Gas Mass flow, ton/h	3,039	2,685
Temperature, °C	51.67	80
Pressure, bar	1	1
Split stream used, ton/h	456	45
Composition		
Component	mol%	mol%
CO ₂	12.022	13.330
O ₂	4.790	4.000
N ₂	79.198	70.358
Ar	0.980	-
H ₂ O	3.000	12.310
CO	0.003	-
SO ₂	0.003	0.002
NO ₂	0.004	-

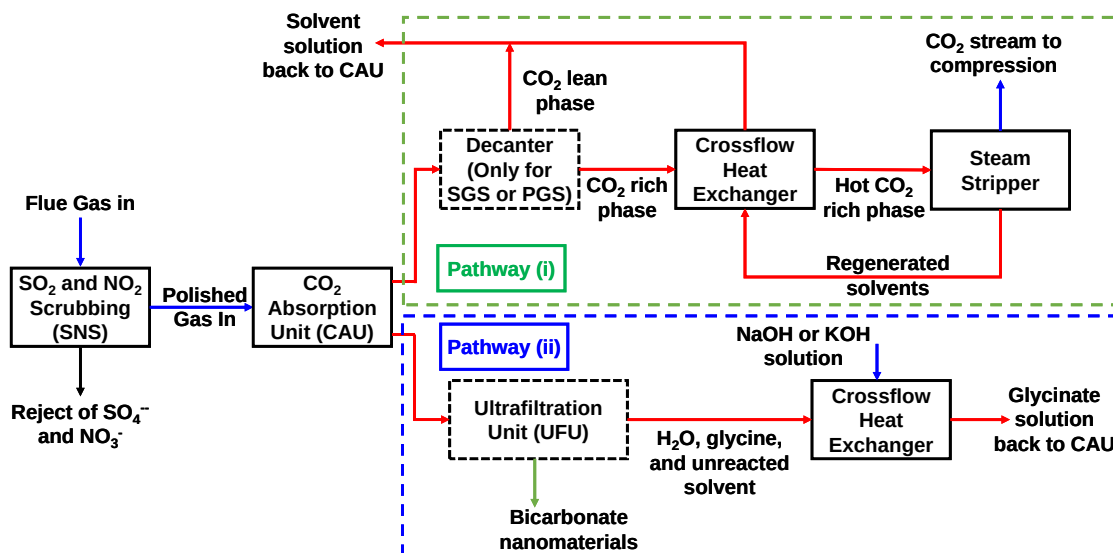


Figure 1 Block diagram of the overall process.

It should be emphasized that the Longview and Wolverine power plants [28, 29] are different as given in Table 1. For instance the raw flue gas in the Longview PP is at 51.67°C and contains 0.003 mol% SO₂ and 0.004 mol% NO₂ whereas that from the Wolverine is at 80°C and contains 0.002 mol% SO₂. The split flue gas stream flow rate from the Longview used in this study was 456 ton/h whereas that from the Wolverine used by Wang et al. [24, 31] was only 45 ton/h. Thus, the data published for the Wolverine power plant using only SGS are different when compared with those presented in this study for the five solvents, including SGS.

2. Research Approach

The steps of the research approach followed in this study are given in Figure 2, and as can be seen all the five solvents were used in Pathway (i), whereas only the two amino-acid-based solvents (SGS and PGS) were used in Pathway (ii).

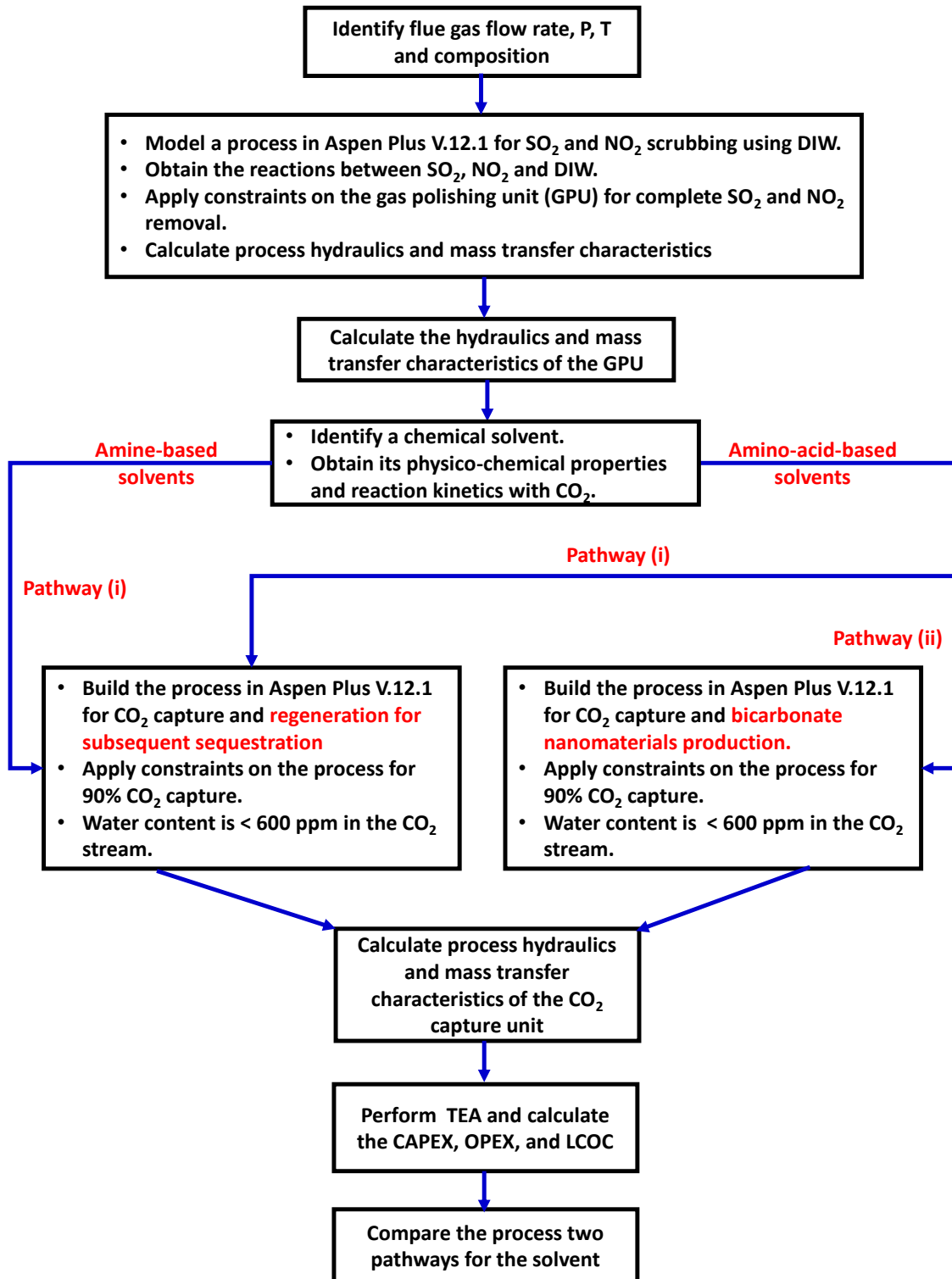


Figure 2 Research approach for SO₂ and NO₂ scrubbing and CO₂ capture process two pathways.

3. Required Parameters for Aspen Plus Models

3.1 Properties of the Flue Gas and Solvents Used

Table 2 gives the properties of the raw flue gas components from the Longview 780 MW PP, which were obtained from Aspen Plus v.12.1.

Table 2 Properties of the flue gas components of the Longview PP [25, 32, 33].

Property	CO ₂	O ₂	N ₂	Ar	H ₂ O	CO	SO ₂	NO ₂
MWt, kg/kmol	44.01	32.00	28.01	39.95	18.02	28.01	64.06	46.01
NBP, K	194.70	90.19	77.34	87.30	373.20	81.70	263.00	294.30
T _c , K	304.21	154.58	126.20	150.80	647.30	132.92	430.80	431.40
P _c , MPa	7.38	5.04	3.40	4.87	22.05	3.50	7.88	10.13
V _c , m ³ /kmol	0.09	0.07	0.09	0.07	0.06	0.09	0.12	0.17
ω, --	0.22	0.02	0.04	0.00	0.34	0.05	0.25	0.86
ΔH _f ^o , kJ/kmol	-393.51	0.00	0.00	0.00	-242.0	-110.5	-297.1	33.9
ΔG _f ^o , kJ/kmol	-394.37	0.00	0.00	0.00	-228.8	-137.2	-300.4	52.0

3.2 Properties of the Solvents Used

Also, the experimental density, viscosity and surface tension for aqueous MEA, AMP and PZ/MDEA solutions were calculated using Aspen technical reports [33-35], respectively. On the other hand, the experimental density, surface tension, viscosity, and heat capacity for SGS and PGS were obtained from the literature [36-38]. The Electrolyte Non-Random-Two-Liquid (ELEC-NRTL) Equation-of-State (EOS) was employed to model the CO₂ density in Aspen Plus V.12.1 [24].

The physico-chemical properties for SGS and PGS were found in reference [39]. The density and viscosity of 1-50 wt% SGS at 298-353 K are available in the literature [13, 21, 36, 40]. The density and viscosity of 0.1-2.98 kmol/m³ PGS at 293-313 K were measured by Portugal et al. [37]. The surface tension of SGS and PGS were reported by Matubayasi et al. [41] and Park et al. [38], respectively.

3.3 Henry's Law Constants (He') and Diffusivities (D_{iB}) of CO₂ in the Five Solvents

The He' for the non-reactive flue gas species (N₂, Ar, CO, H₂O, and O₂) in the five solvents were found in the literature [42]. Since CO₂ reacts with the five solvents, the He' and D_{iB} of CO₂ cannot be directly measured, however, using N₂O as a surrogate for CO₂, the He' and D_{iB} values were estimated by analogy. To conduct N₂O analogy, the He' and D_{iB} of CO₂ and N₂O in H₂O were published by Versteeg and Van Swaaij [43]. The He' values for CO₂ in MEA, AMP and PZ/MDEA were estimated by N₂O analogy and are available in Aspen reports [33-35]. Also, He' values for CO₂ in SGS and PGS were estimated by N₂O analogy as given in the literature [37, 44]. Those estimated CO₂ He' values in the five solvents were then implemented in Aspen Plus V.12.1 for process simulation.

The diffusivity of CO₂ (component *i*) into an aqueous solution of component (*B*) which is a mixture (solvent + water) was calculated using Equation (1) by Wilke and Chang [45]. The properties of B were predicted using the mixing rule expressed in Equation (2).

$$D_{iB} = 1.17282 \times 10^{-16} \frac{T(\varphi MWt_B)^{1/2}}{\mu_B v_i^{0.6}} \quad (1)$$

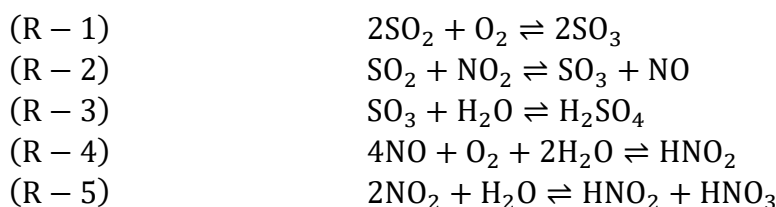
$$MWt_B = \frac{\sum_{j \neq i} x_j \varphi_j MWt_j}{\sum_{j \neq i} x_j} \quad (2)$$

In these equations, D_{iB} is the diffusivity of the i^{th} component into B (m^2/s), MWt_B and μ_B are the molecular weight ($kg/kmol$) and viscosity ($Pa \cdot s$) of B , v_i is the molar volume ($m^3/kmol$) of the i^{th} component at its boiling point. Also, x_j and φ_j are the mole fraction and association parameter of the j^{th} component in B , respectively. For MEA, AMP, MDEA, PZ, SGS and PGS, $\varphi = 1.0$ and for water, $\varphi = 2.26$.

4. Chemical Reactions in the Overall Process

4.1 SO_2 and NO_2 Reactions with DIW

SO_2 and NO_2 reactions with water (H_2O) take place in the gas polishing unit (GPU). Aspen Plus model considers reactions (R-1) through (R-5) as equilibrium reactions. In these reactions, SO_2 is oxidized by O_2 and NO_2 to become SO_3 , as in reactions (R-1) and (R-2). Also, in reaction (R-2), NO_2 is reduced NO. SO_3 then reacts with H_2O to form H_2SO_4 as in reaction (R-3). Also, NO and NO_2 react with H_2O to produce HNO_2 and HNO_3 as in reactions (R-4) and (R-5), respectively.



4.2 CO_2 Reactions with MEA and AMP

CO_2 reactions and kinetics with MEA and AMP can be found in reference [32, 35, 46], respectively.

4.3 CO_2 Reactions with and PZ/MDEA

The structures of MDEA and PZ are depicted in Figure 3 (a) and (c). MDEA and PZ are protonated to become MDEAH⁺ Figure 3 (b) and PZH⁺ following reactions (R-6) and (R-7). Also, since H_3O^+ is used for MDEA and PZ protonation, OH^- concentration becomes greater than that of H_3O^+ leading to a basic solution. When CO_2 comes in contact with the MDEA/PZ basic solution, reaction (R-15) occurs to produce bicarbonate ions. Also, MDEA reacts with CO_2 to form protonated MDEA (MDEAH⁺) and bicarbonate [47] as shown in reaction (R-9). As a cyclic amine, PZ reacts with CO_2 to produce carbamate ion PZCOO⁻ (Figure 3 (d)), as described in reaction (R-10). Since PZ has two amino groups, the formed carbamate PZCOO⁻ can be protonated as HPZCOO (Figure 3 (e)) using reaction (R-8) and can react with CO_2 to produce dicarbamate (Figure 3 (f)) according to (R-11). The forward and backward directions of reactions (R-9), (R-10), and (R-11) are for CO_2 absorption and desorption, respectively.

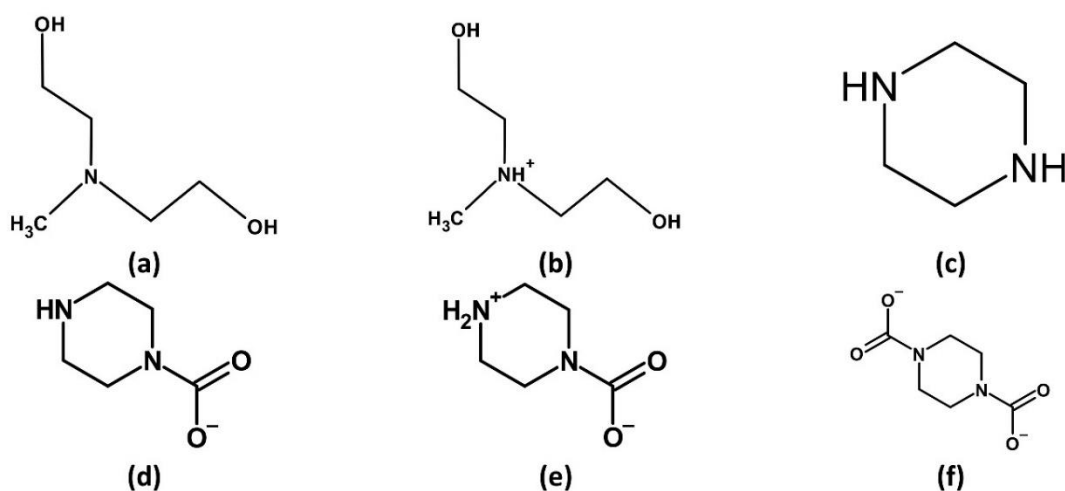
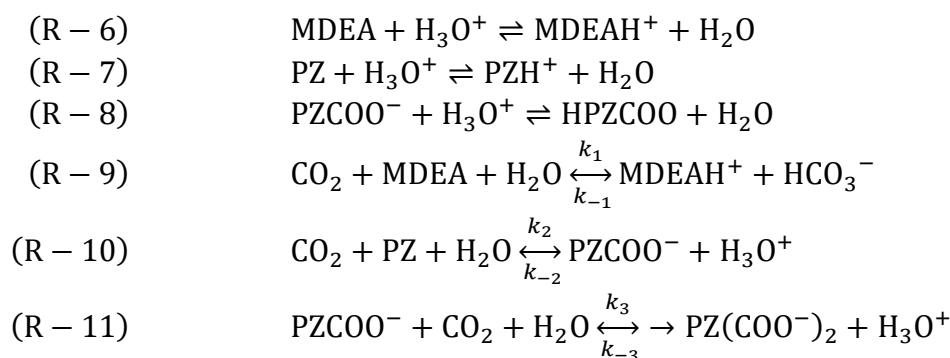


Figure 3 Structure of (a) MDEA, (b) MDEAH⁺, (c) PZ, (d) PZCOO⁻, (e) HPZCOO⁻, and (f) PZ(COO⁻)₂.



Reactions (R-6), (R-7), and (R-8) are equilibrium reactions and the standard Gibbs free energy change (ΔG°) was used to determine their corresponding equilibrium constants. On the other hand, reactions (R-9), (R-10), and (R-11) are kinetic reactions and their k_1 , k_{-1} , k_2 , k_{-2} , k_3 and k_{-3} were required. For reaction (R-9), k_1 and k_{-1} were provided by Rinker et al. [48], as expressed in Equations (3) and (4). Bishnoi and Rochelle [18] reported Equations (5) through (8) to calculate (k_2 and k_{-2}) and (k_3 and k_{-3}) for reactions (R-10) and (R-11), respectively. These k values were also available in the Aspen technical report [33].

$$k_1 = 2.22 \times 10^7 \exp\left(\frac{-4,543.57}{T}\right) \quad (3)$$

$$k_{-1} = 1.06 \times 10^{16} \exp\left(\frac{-12,793.85}{T}\right) \quad (4)$$

$$k_2 = 4.14 \times 10^{10} \exp\left(\frac{-4,045.03}{T}\right) \quad (5)$$

$$k_{-2} = 7.94 \times 10^{21} \exp\left(\frac{-7,929.73}{T}\right) \quad (6)$$

$$k_3 = 3.62 \times 10^{10} \exp \left(\frac{-4,045.03}{T} \right) \quad (7)$$

$$k_{-3} = 5.56 \times 10^{25} \exp \left(\frac{-9,245.15}{T} \right) \quad (8)$$

4.4 CO₂ Reactions with SGS and PGS

Zhang et al. [49] reported that glycine (Figure 4 (a)) forms a zwitterion according to reaction (R-12), to protonate the amino group as shown in Figure 4 (b) rendering it entirely unreactive towards CO₂ [50]. When the acidic group is neutralized and deprotonated by NaOH, forming SGS, it restores its reactivity. Details of the CO₂ reaction with SGS can be found elsewhere [24].

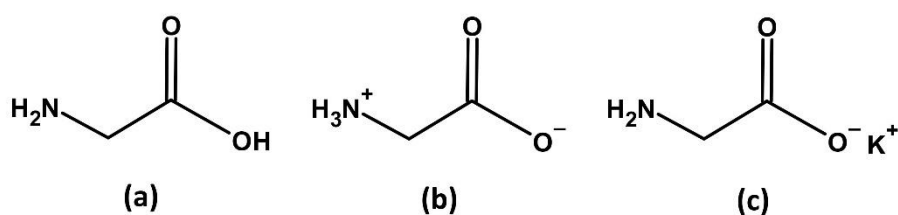
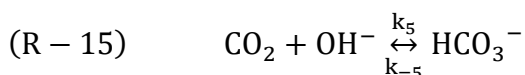
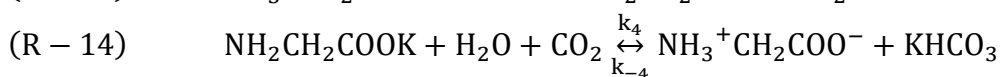
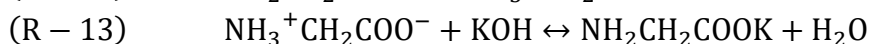
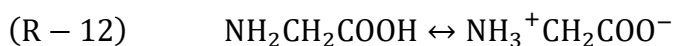


Figure 4 Structure of (a) Glycine, (b) Glycine zwitterion, (c) PGS [49].

Similarly, when KOH neutralizes the acidic group, the amino group (see Figure 4 (b)) is deprotonated according to reaction (R-13) to become PGS (Figure 4 (c)) and returns to the reactive state. The formed PGS will then react with CO₂ and forms carbamate intermediate, which undergoes hydrolysis to become bicarbonate, as shown in reaction (R-14) [37]. Also, because of the basic environment, bicarbonate is produced through reaction (R-15) between CO₂ and OH⁻. The forward direction of reaction (R-14) captures CO₂ and produce KHCO₃ nanomaterials which precipitate to form the CO₂-rich phase [22, 23, 26].



The k_4 and k_{-4} of reaction (R-14) are represented by Equations (9) and (10), proposed by Thee et al. [51]. Likewise, k_5 and k_{-5} of reaction (R-15) are expressed by Equations (11) and (12), respectively, which were obtained from Pinsent et al. [52] and Aspen technical report [32].

$$k_4 = 1.22 \times 10^{12} \exp \left(\frac{-5,434}{T} \right) \quad (9)$$

$$k_{-4} = 1.22 \times 10^{10} \exp \left(\frac{-7,754}{T} \right) \quad (10)$$

$$k_5 = 4.32 \times 10^{13} \exp \left(\frac{-6,667.5}{T} \right) \quad (11)$$

$$k_{-5} = 2.38 \times 10^{17} \exp\left(\frac{-14,821}{T}\right) \quad (12)$$

The units for the above reaction rate constants are in $\text{m}^3/\text{kmol}\cdot\text{s}$.

4.5 Reaction Rate Constants of CO_2 and the Solvents Used

The second order reaction rate constants (k') of CO_2 with SGS were measured in a wetted-wall column by Lee et al. [53]. Also, the k' of CO_2 reaction with PGS were provided by Portugal et al. [37], Guo et al. [19], and Khakharia et al. [54] in a stirred-cell reactor, a stopped-flow apparatus, and a wetted-wall column, respectively. The k' for CO_2 reactions with the solvents used is presented as a function of temperature in Figure 5. The figure shows that k' values follow the order: $\text{PZ} > \text{PGS} > \text{MEA} > \text{AMP} > \text{SGS} > \text{MDEA}$.

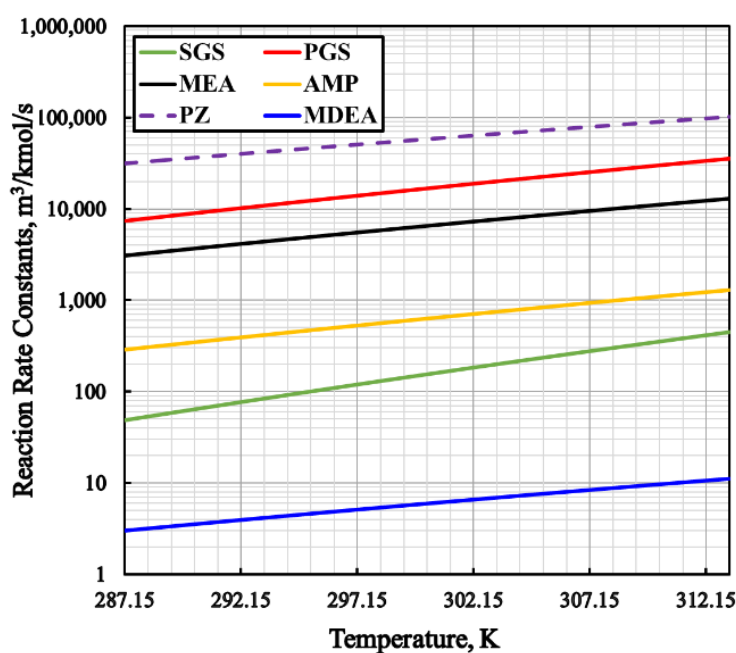


Figure 5 Reaction Rate Constants of CO_2 in the Solvents Used.

5. Process Flow Diagrams

Figure 6 shows the flow diagram of the raw flue gas scrubbing process. Figure 7 and Figure 8 depict Pathway (i) flow diagrams of the CO_2 capture process using ABs and AAs, respectively. Also, Figure 9 illustrates Pathway (ii) flow diagram of the CO_2 capture process to produce bicarbonate nanomaterials using AAs. Briefly, the raw flue gas enters the gas polishing process for complete removal of SO_2 and NO_2 using deionized water (DIW) in the gas polishing unit (GPU). The dissolved ions in the DIW were removed using a multistage reverse osmosis unit (ROU), and the polished gas was sent to the CO_2 capture process using five chemical solvents (MEA, AMP, PZ/MDEA, SGS and PGS). Since SGS and PGS exhibit phase separation, the CO_2 capture processes followed two distinct pathways. Pathway (i) involved direct CO_2 capture using all five solvents, and Pathway (ii) focused on bicarbonate nanomaterials production using only SGS and PGS. In both pathways, over 90% CO_2 was captured in the CO_2 absorption unit (CAU). Also, in pathway (i), the solvents were regenerated

using steam stripper and in Pathway (ii), an ultrafiltration unit (UFU) was used to separate the bicarbonate nanomaterials. Details of these process flow diagrams are given in the Supporting Materials.

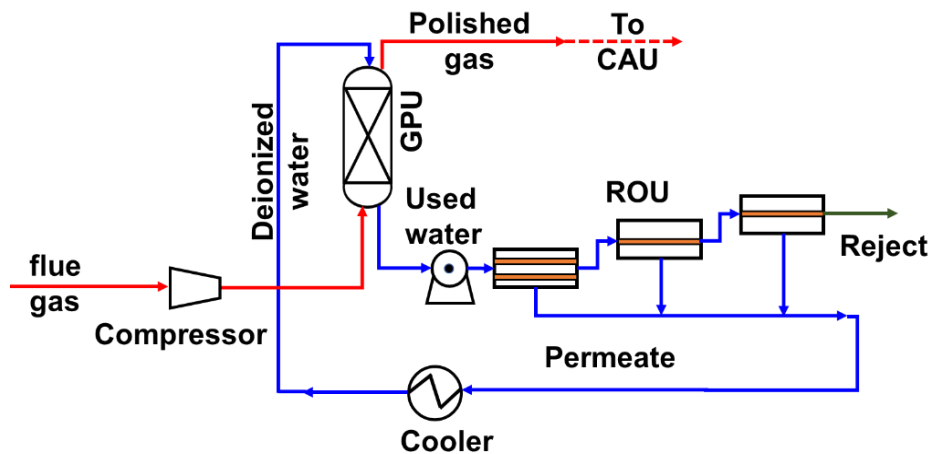


Figure 6 SO₂ and NO₂ Scrubbing Process.

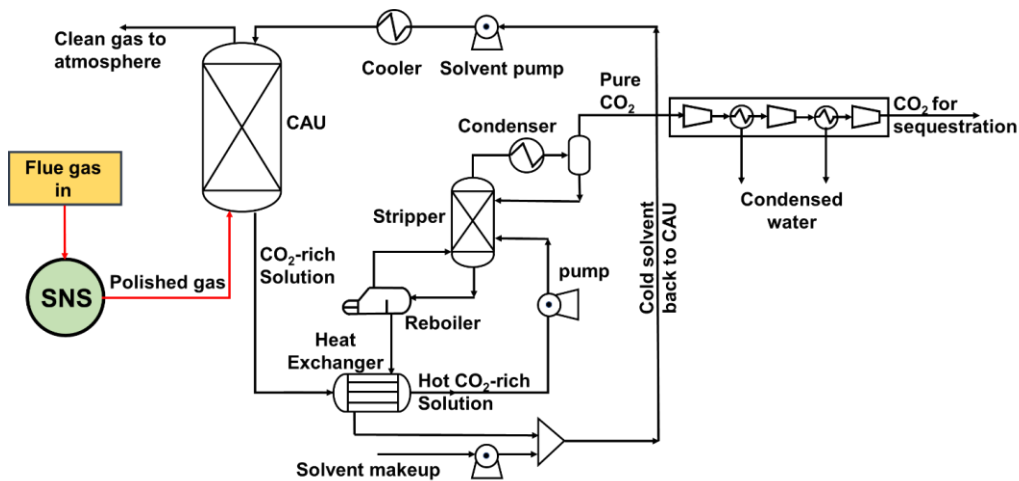


Figure 7 Pathway (i) for ABs Solvents.

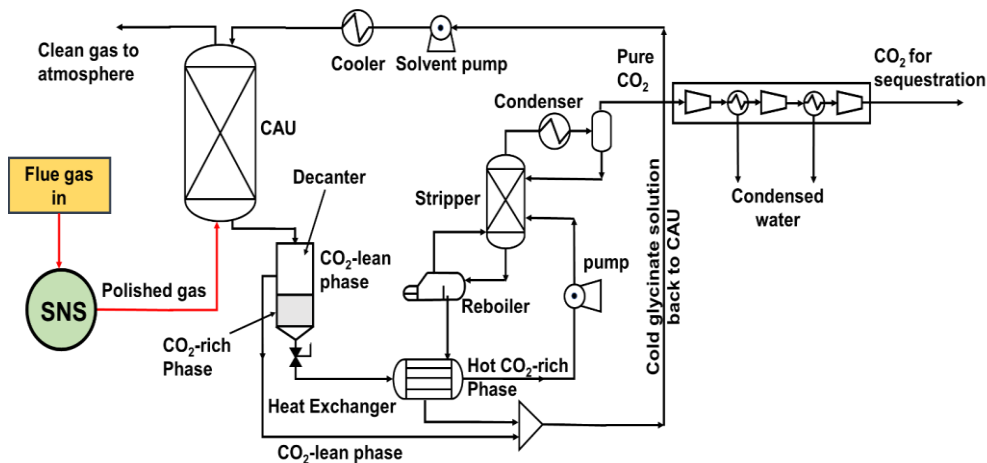


Figure 8 Pathway (i) for AAs Solvents.

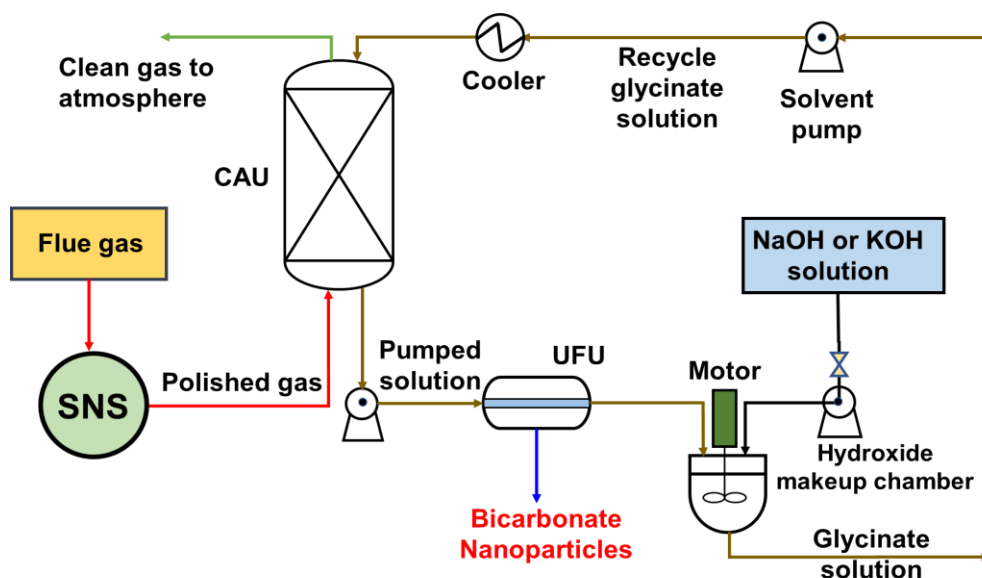


Figure 9 Pathway (ii) for AAs Solvents.

6. Hydraulics and Mass Transfer Characteristics of Packed-beds

The hydraulics of two-phase flow in counter-current packed-beds are required for proper design and scale-up of a continuous gas absorption process [55]. In this study, the Gas Polishing Unit (GPU) in the flue gas SO_2 and NO_2 scrubbing (SNS) system and the CO_2 absorption unit (CAU) in the CO_2 absorption system (CAS) are fixed-beds packed with Mellapak 250Y structured packing with a porosity (ϵ) of 0.987 and a specific surface area of 256 $1/\text{m}$. The correlations required for calculating the hydraulics and mass transfer characteristics in fixed-beds can be found in Wang et al. [24, 25].

7. Results and Discussion

7.1 SO_2 and NO_2 Scrubbing System (SNS)

The Longview power plant flue gas contains 33.2 and 35.5 ppmv of SO_2 and NO_2 , respectively. In this study, a DIW flow rate of $0.075 \text{ m}^3/\text{s}$ was utilized to polish a 112.63 m^3 split stream of flue gas stream (at 1.38 bar and 364.48 K) in the gas polishing unit (GPU), which an adiabatic fixed-bed absorber (4.2 m ID and 21.5 m packing height) using Mellapak 250Y.

7.1.1 Mole Fraction and Temperature Profiles in the GPU

The Aspen Plus V.12.1 simulation results indicated that the SO_2 and NO_2 mole fractions decrease with increasing the packing height of the GPU, reaching a null value at approximately 6 m height, as illustrated in Figure 10. Both SO_2 and NO_2 conversions within the GPU were 99.99 mol%. Also, Figure 11 shows that the gas temperature decreases from 364.48 to 304.43 K, whereas the DIW temperature increases from 298.15 to 312.17 K, which was attributed to the heat of absorption. The inlet raw flue gas and outlet polished gas stream conditions and compositions are given in Table 3.

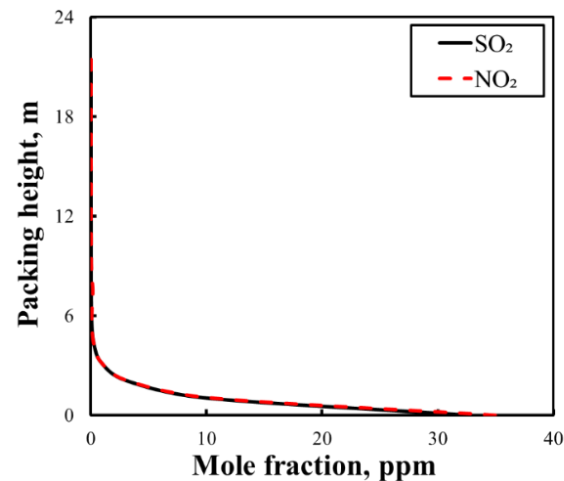


Figure 10 SO₂ and NO₂ Gas Mole Fraction Profiles in GPU.

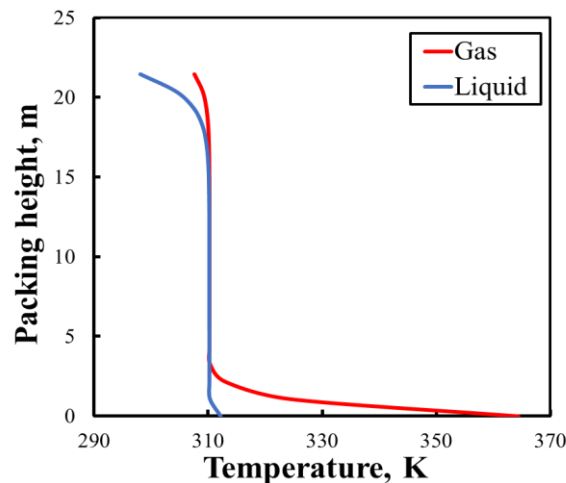


Figure 11 Liquid and Gas Temperature Profiles in GPU.

Table 3 Gas streams entering and exiting the GPU.

	Compressed flue gas	Polished flue gas
Temperature, K	364.48	304.43
Pressure, bar	1.38	1.18
Mass flow rate, kg/s	126.63	127.12
Composition		
Component	mol%	
CO ₂	12.022	11.936
O ₂	4.79	4.756
N ₂	79.198	78.674
Ar	0.98	0.974
H ₂ O	3.00	3.657
CO	0.003	0.003
SO ₂	0.003	0.000
NO ₂	0.004	0.000

7.1.2 Hydraulics and Mass Transfer in the GPU

Figure 12 (a-d) presents profiles of the two-phase pressure distribution, liquid holdup (β_L), liquid-side (k_L) and gas-side (k_G) mass transfer coefficients, and the normalized specific packing wetted area (a_w/a) in the GPU calculated with Aspen Plus V.12.1 using the correlations by Billet and Schultes [56]. Figure 12 (a) shows the compressed flue gas enters at the bottom of GPU at 1.38 bar and exits as a polished gas at 1.18 bar, resulting in a 0.2 bar pressure drop over the 21.5 m packing height. Figure 12 (b) shows the average liquid holdup is the highest (5.85%) at the top and decreases to 5.67% at the end of the GPU. Figure 12 (c) shows the average k_G values to be much greater than k_L values, suggesting that the mass transfer resistance ($1/k_L$) resides in the liquid-side. Figure 12 (d) shows a_w/a values decreasing from 0.244 at the top to GPU to 0.241 at the bottom, displaying a similar trend to that of β_L . This finding is significant for industrial CO₂ capture applications because it suggests that improving the liquid-phase mass transfer (e.g., using different packing with larger specific surface area or introduce enhanced mixing) could improve the overall CO₂ capture process.

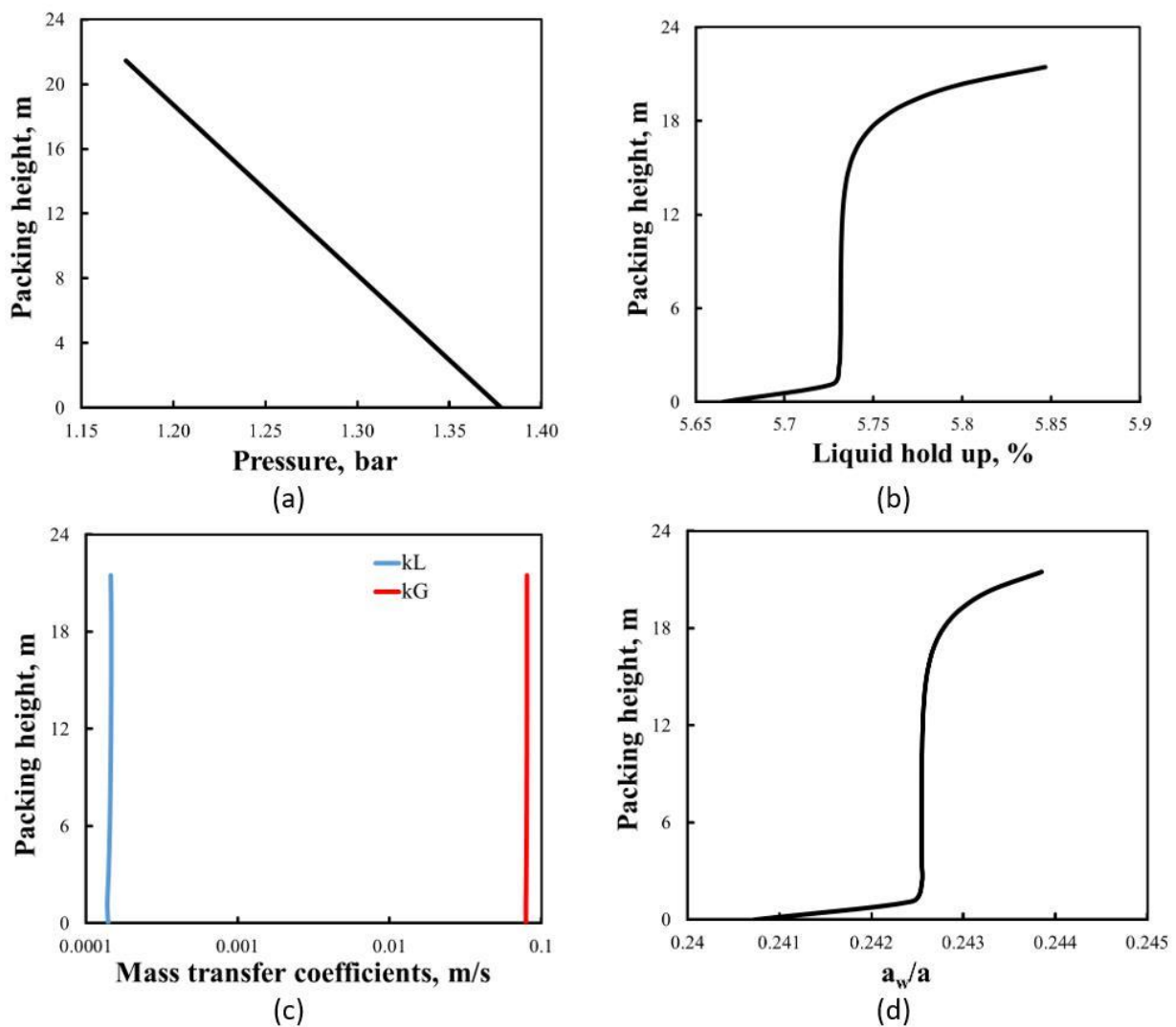


Figure 12 Pressure, liquid holdup, mass transfer coefficients, and normalized specific packing wetted area profiles in the GPU.

7.1.3 Reverse Osmosis Unit (ROU) of the SNS System

In a continuous CO₂ capture process operating under steady-state conditions, the sulfate (SO₄²⁻) and nitrate (NO₃⁻) ions present in the water exiting the GPU must be continuously removed using the Reverse Osmosis Unit (ROU). The ROU is a crossflow filtration system driven by pressure and employ a semipermeable membrane to separate salts from liquids [57]. The BW30-400 membrane, manufactured by Dow and described by in [24], was chosen to achieve a 99.5% rejection efficiency for both SO₄²⁻ and NO₃⁻ from the used DIW. Adhering to Dow's design guideline [58], the ROU employed in this study comprises three stages, each containing 17, 8, and 4 elements, respectively. A single element incorporates six BW30-400 membranes organized sequentially. Following the removal of 99.5% of SO₄²⁻ and NO₃⁻, the resulting permeate (cleaned water) is recycled back to the GPU for further removal of SO₂ and NO₂. Meanwhile, the reject stream containing water and dissolved acids can either be discarded or utilized in reactions with KOH to yield K₂SO₄ and KNO₃, which are valuable and marketable products.

7.2 Pathway (i): CO₂ Absorption System (CAS)

After the GPU, the polished flue gas flow rate was 127.12 kg/s at a pressure of 1.18 bar and a temperature of 304.43 K. In Pathway (i), the five solvents were used to capture CO₂ in the CO₂ absorption unit (CAU), which is adiabatic fixed-bed absorber. The solution exiting from the CAU went to the stripper for solvent regeneration and CO₂ release. The released CO₂ was compressed in a multistage compressor with intercooling to 152.7 bar in preparation for subsequent sequestration.

7.2.1 Pathway (i): Operating Conditions for the Five Solvents

The polished flue gas (containing N₂, CO₂, O₂, and H₂O) enters from the bottom of the CAU at a rate of 127.12 kg/s to react with 3 M aqueous solvents entering at the top of CAU. The required flow rate of each solvent to capture at least 90% CO₂ are given in Table 4.

Table 4 Operating conditions and CO₂ capture efficiency of the CAU.

	MEA	AMP	MDEA/PZ	SGS	PGS
Temperature, K	298.15				
Pressure, bar	1				
Solvent concentration, kmol/m ³	3				
Solvent flow rate, m ³ /s	0.31	0.37	0.24	0.45	0.26
Absorber diameter, m	8				
Packing height, m	48				
CO ₂ capture efficiency, %	90.58	90.15	91.66	91.12	92.54

This table indicates that the required solvent flow rates to capture over 90% CO₂ follow the order: PZ/MDEA < PGS < MEA < AMP < SGS.

7.2.2 Pathway (i): Liquid and Gas Temperature Profiles in the CAU

The polished gas enters at the bottom of CAU at 304.43 K and leaves at the top at higher temperatures of 325.49, 324.94, 324.82, 318.61, and 319.38 K for MEA, AMP, MDEA/PZ, SGS, and PGS, respectively. Also, the liquid-phase enters at the top of the CAU at 298.15 K and leaves at the bottom at higher temperatures of 309.79, 315.18, 314.41, 307.99, and 309.16 K for MEA, AMP, MDEA/PZ, SGS, and PGS, respectively. The behavior was due to the heat transfer between the gas and liquid phases in the CAU.

7.2.3 Pathway (i): CO₂ Mole Fraction and Absorption Efficiency Profiles in the CAU

The predicted CO₂ mole fraction profiles using Aspen Plus V.12.1 using the five solvents are shown in Figure 13. This figure shows that the polished flue gas enters at the bottom of CAU with 11.94 CO₂ mol% and exits at the top of the absorber with 1.14, 1.28, 1.01, 1.20, and 0.95 mol% CO₂ for MEA, AMP, MDEA/PZ, SGS, and PGS, respectively. Also, Figure 13 confirms that the CO₂ capture efficiency is greater than 90 mol%, set as one of the main process constraints.

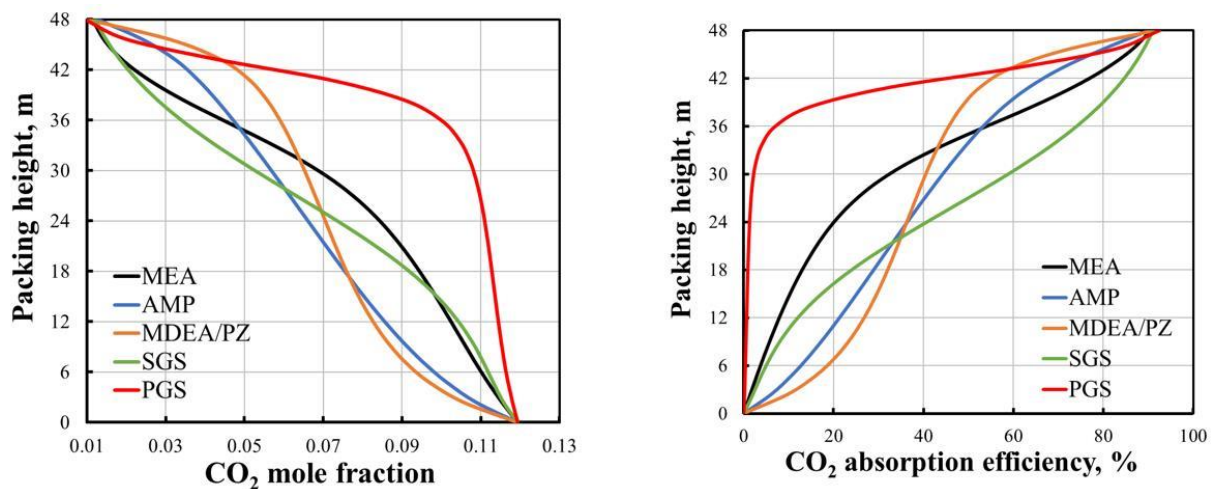


Figure 13 CO₂ mole fraction and absorption efficiency profiles in the CAU.

7.2.4 Pathway (i): Hydraulics and Mass Transfer Characteristics in the CAU

Figure 14 (a-d) presents the profiles of the two-phase pressure distribution, liquid holdup (β_L), liquid-side (k_L) and gas-side (k_G) mass transfer coefficients, and the normalized specific packing wetted area (a_w/a) in the CAU calculated with Aspen Plus V.12.1 using the correlations by Billet and Schultes [56]. Figure 14 (a) shows the pressure distribution is almost linear with a maximum pressure drop of 0.15 bar over 48 m long packing, and Figure 14 (b) shows the liquid holdups followed the order $\beta_{L-SGS} > \beta_{L-AMP} > \beta_{L-PGS} \geq \beta_{L-MEA} > \beta_{L-MDEA/PZ}$, which implies that both liquid velocity and viscosity have a direct effect on the liquid holdup. Figure 14 (c) shows that the gas-side mass transfer coefficients (k_G) are orders of magnitude greater than liquid-side mass transfer coefficients (k_L) and hence the resistance to the overall mass transfer is mainly located in the liquid side. Figure 14 (d) follows the order $a_{w-AMP} > a_{w-SGS} > a_{w-PGS} > a_{w-MDEA/PZ} > a_{w-MEA}$, which indicated that the effects of liquid surface tension and density on the specific packing wetted area

were stronger than the effect of liquid velocity according to the correlation by Billet and Schultes [56].

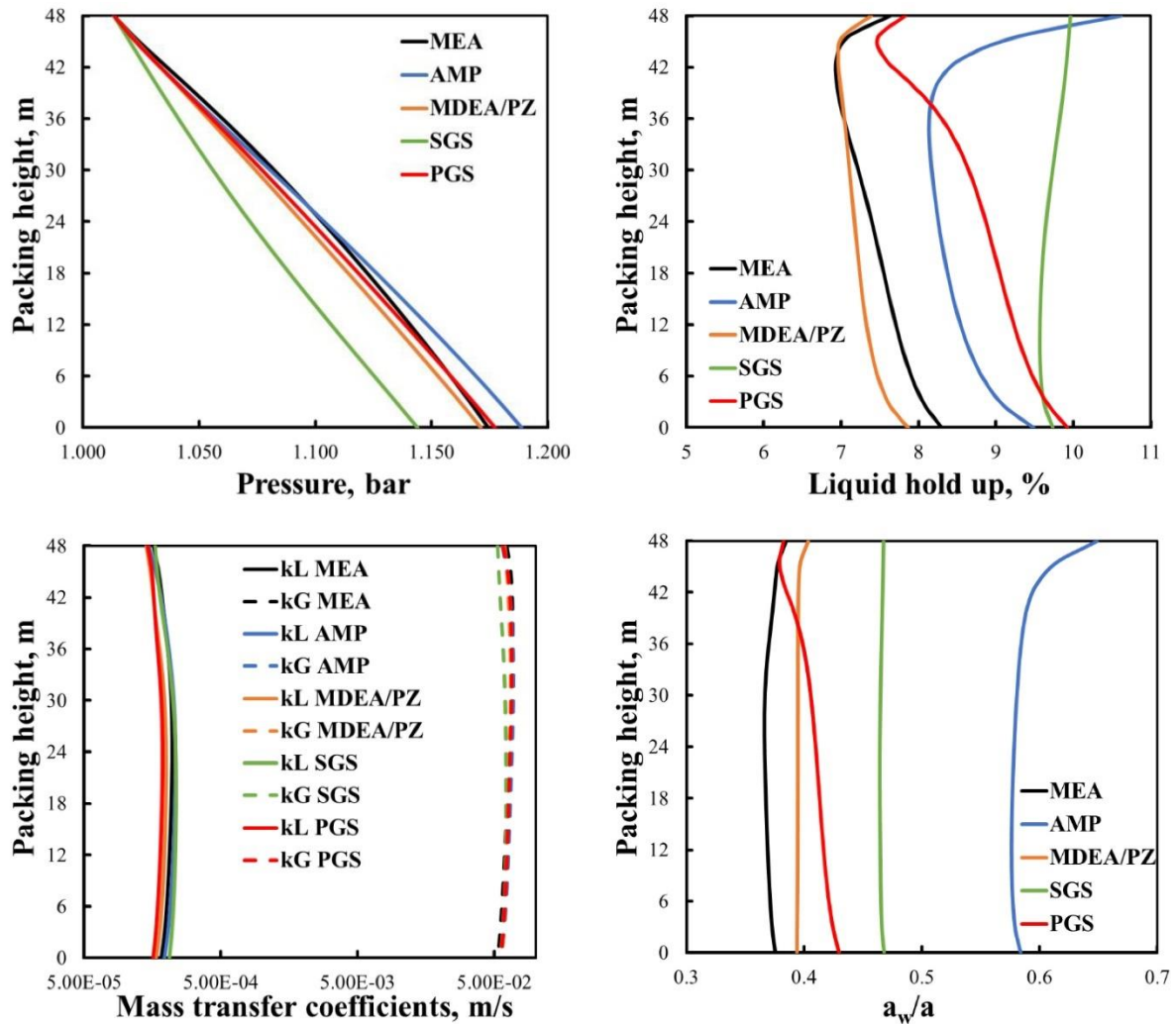


Figure 14 Pressure, liquid holdup, mass transfer coefficients, and packing specific wetted area profiles in CAU for five solvents (pathway (i)).

7.2.5 Pathway (i): Stripper Performance

For the processes using ABs, the CO₂-rich solution coming the bottom of the CAU does not exhibit phase separation, whereas the processes using AAs, the solutions exhibit a phase-separation into a CO₂-rich (lower) phase and a CO₂-lean (upper) phase as reported by [23]. The CO₂-rich phase primarily includes bicarbonate nanomaterials and water. Hence, for the regeneration step in the processes using MEA, AMP and MDEA/PZ, the entire CO₂-rich solution from the absorber is directed to the stripper, however, for the processes using SGS and PGS process, only the CO₂-rich phase is directed to the stripper. It is important to mention that preheating the solution stream sent to the stripper will lower the reboiler duty [59]. Therefore, a crossflow heat exchanger was used to preheat the CO₂-rich phase using CO₂-lean phase stream recovered from the stripper after regeneration. The inlet and outlet conditions of CO₂-rich and CO₂-lean phase streams and the heat exchanger duty are given in Table 5.

Table 5 Stream conditions of crossflow heat exchanger.

	MEA	AMP	MDEA/PZ	SGS	PGS
CO ₂ -rich phase flow rate, kg/s	329.34	386.33	251.25	127.69	95.77
CO ₂ -rich phase inlet temperature, K	312.96	315.18	314.48	308.59	309.13
CO ₂ -rich phase outlet temperature, K	398.15	398.15	392.10	372.33	382.51
CO ₂ -lean phase flow rate, kg/s	290.65	344.49	222.18	105.11	74.36
CO ₂ -lean phase inlet temperature, K	401.60	401.15	402.10	379.62	389.64
CO ₂ -lean phase outlet temperature, K	315.70	326.89	324.65	312.59	313.13
Heat exchanger duty, MW	96.04	100.70	61.40	26.10	17.16

The energy required for the CO₂-rich phase stream in the stripper includes the sensible heat to increase the temperature of liquid from the crossflow heat exchanger to the reboiler temperature, heat of evaporation in the reboiler to produce a gas phase composed of CO₂ and H₂O which is condensed in the overhead condenser, and the required heat for the endothermic CO₂ desorption reaction. It should be noted that in the case of SGS or PGS process, the CO₂ in the CO₂-rich phase is in the form of NaHCO₃ or KHCO₃ nanomaterials, and stripping CO₂ from them reduces the sensible heat as well as the heat of evaporation. Therefore, regenerating only the CO₂-rich phase instead of the entire CO₂-rich solution coming from the bottom of the CAU in the case of SGS and PGS process is an energy-saving strategy. Table 6 shows the size and packing of the stripper used for regenerating the five solvents, the CO₂-rich phase flow rate, the reboiler duty and the condenser duty.

Table 6 Operating conditions for the stripper.

	MEA	AMP	MDEA/PZ	SGS	PGS
Pressure, bar	2.4			1	
Stripper Inner diameter, m	6			4	
Packing height, m	36			24	
Packing type	Mellapak 250Y				
CO ₂ -rich phase flow rate, kg/s	329.34	386.33	251.25	127.69	95.77
Reboiler temperature, K	401.60	401.15	402.10	379.62	389.64
Reboiler heat duty, MW	103.83	115.10	71.68	41.01	40.31
Condenser temperature, K	293.15				
Condenser heat duty, MW	-63.72	-71.08	-32.19	-8.74	-4.47

In the stripper, the CO₂-rich solution is heated within the reboiler to generate CO₂ and water vapor moving upward through the stripper to reach the condenser, so that water vapor is partially condensed and the CO₂ stream is recovered. This CO₂ stream was further compressed in conditioning for subsequent sequestration. The mass flow rate and composition of the inlet and outlet streams of the stripper are given in Table 7.

Table 7 Flow rate and composition of the stripper streams.

	MEA		AMP		MDEA/PZ		SGS		PGS	
Inlet Rich-solution flow rate (kg/s)	329.34		386.33		251.25		127.69		95.77	
Composition (wt%)	MEA	1.28	AMP	15.23	MDEA	11.96	NaGly	0	KGly	0
	H ₂ O	74.51	H ₂ O	66.01	PZ	0.49	H ₂ O	69.54	H ₂ O	50.84
	MEAH ⁺	9.65	AMPH ⁺	11.13	H ₂ O	60.00	HGlyOH	0	HGlyOH	0
	MEACOO ⁻	11.02	AMPCOO ⁻	0.22	CO ₂	0.47	NaHCO ₃	30.45	KHCO ₃	49.15
	HCO ₃ ⁻	2.99	HCO ₃ ⁻	7.20	HCO ₃ ⁻	3.74	NaOH	0.00	KOH	0.00
	CO ₃ ²⁻	0.02	CO ₃ ²⁻	0.12	MDEAH ⁺	5.87	CO ₂	0.013	CO ₂	0.012
	CO ₂	0.53	CO ₂	0.09	PZH ⁺	2.20	-	-	-	-
	-	-	-	-	HPZCOO	13.70	-	-	-	-
	-	-	-	-	PZCOO ⁻	1.41	-	-	-	-
	-	-	-	-	PZCOO ²⁻	0.16	-	-	-	-
Outlet Lean-solution flow rate (kg/s)	290.65		344.49		222.18		105.11		74.36	
Composition (wt%)	MEA	15.95	AMP	29.11	MDEA	20.06	NaGly	0	KGly	0
	H ₂ O	79.13	H ₂ O	70.65	PZ	13.83	H ₂ O	82.38	H ₂ O	64.52
	MEAH ⁺	1.87	AMPH ⁺	0.15	H ₂ O	65.34	HGlyOH	0.00	KGlyOH	0.00
	MEACOO ⁻	0.00	AMPCOO ⁻	0.0056	HCO ₃ ⁻	0.05	NaHCO ₃	0.00	KHCO ₃	0.00
	HCO ₃ ⁻	0.31	HCO ₃ ⁻	0.08	MDEAH ⁺	0.05	NaOH	17.62	KOH	35.48
	CO ₃ ²⁻	0.00	CO ₃ ²⁻	0.0055	PZH ⁺	0.30	CO ₂	0.00	CO ₂	0.00
	CO ₂	0.40	CO ₂	0.0002	HPZCOO	0.02	-	-	-	-
Outlet CO₂ stream flow rate (kg/s)	20.37		20.26		20.66		20.58		20.90	
Composition	CO ₂	99.49	CO ₂	99.53	CO ₂	99.53	CO ₂	99.00	CO ₂	99.00

(wt%)	H ₂ O	0.51	H ₂ O	0.47	H ₂ O	0.47	H ₂ O	1.00	H ₂ O	1.00
Outlet H₂O stream flow rate (kg/s)	18.31		21.58		8.41		2.01		0.52	
Composition (wt%)	CO ₂	0.40	CO ₂	0.37	CO ₂	0.39	CO ₂	0.17	CO ₂	0.17
	H ₂ O	98.98	H ₂ O	90.72	H ₂ O	97.37	H ₂ O	99.83	H ₂ O	99.83
	MEA ⁺	0.31	AMP	0.015	MDEA ⁺	0.11	-	-	-	-
	HCO ₃ ⁻	0.31	AMPH ⁺	5.31	PZH ⁺	0.45	-	-	-	-
			HCO ₃ ⁻	3.58	HCO ₃ ⁻	0.37	-	-	-	-
	-	-	-	-	HPZCOO	1.31	-	-	-	-

7.3 Pathway (ii): Bicarbonate Nanomaterials Production

7.3.1 Pathway (ii): Operating Conditions for SGS and PGS

The polished flue gas from the SNS system with the composition given in Table 3, enters from the bottom of the CAU at a rate of 127.12 kg/s to react with 3 M (mol/L) of SGS or PGS solution which enters from the top of the CAU. The dimensions of the CAU are given in Table 8. To meet the process constraint (>90% CO₂ capture efficiency), the required SGS and PGS solvent flow rates were adjusted to 282 L/s and 158 L/s, respectively.

Table 8 Operating conditions and CO₂ capture efficiency of the CAU.

	SGS	PGS
Temperature, K	298.15	
Pressure, bar	1	
Solvent concentration, kmol/m ³	3	
Solvent flow rate, L/s	282	158
Column diameter, m	8	
Packing height, m	48	
CO ₂ capture efficiency, %	90.20	90.95

7.3.2 Pathway (ii): CO₂ Mole Fraction and Absorption Efficiency Profile in the CAU

Because of the exothermic chemical reactions between CO₂ and SGS and PGS, both liquid and gas temperatures increased in the adiabatic CAU. The SGS and PGS solvents enter from the top of CAU at 298.15 K and exit from the bottom at 310.40 K and 304.60 K, respectively. Also, the polished gas enters from the bottom of the CAU at 304.43 K and leaves from the top 308.63 K and 324.96 K for SGS and PGS, respectively.

The predicted CO₂ mole fraction profiles in the CAU using Aspen Plus V.12.1 are shown in Figure 15; and as can be observed, the inlet polished flue gas has 11.94 CO₂ mol% and the outlet clean gas has 1.3 mol% and 1.1 mol% CO₂ for SGS and PGS, respectively. Also, Figure 15 confirms that the CO₂ capture efficiency is more than 90 mol%, set as one of the process constraints.

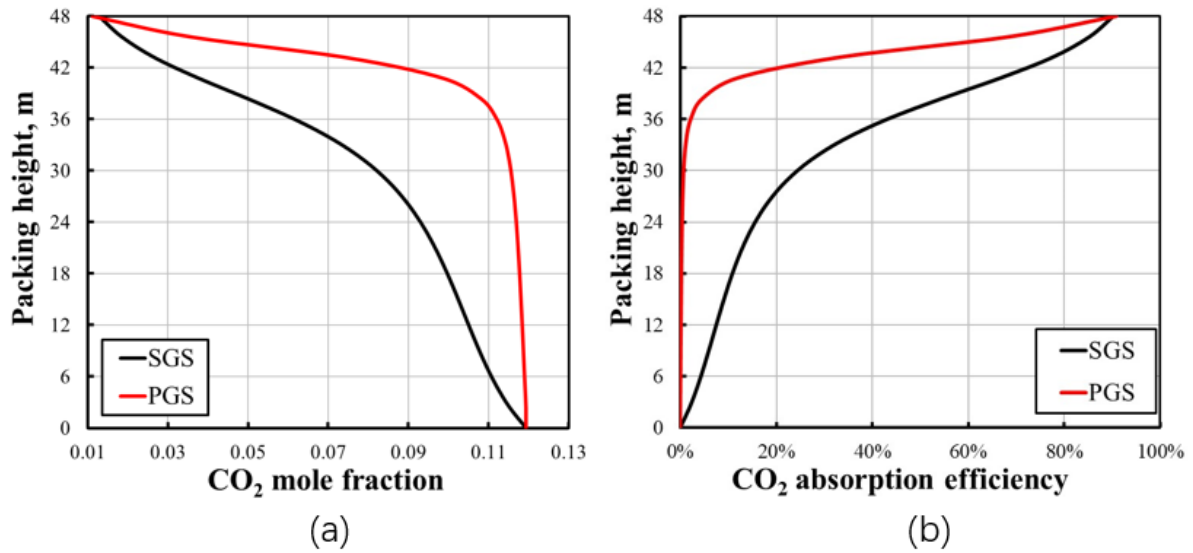


Figure 15 CO₂ mole fraction and absorption efficiency profiles in the absorber.

7.3.3 Pathway (ii) Hydraulics and Mass Transfer Characteristics in the CAU

Under the operating conditions used, the hydraulics of the CAU were calculated using Aspen Plus V.12.1, and Figure 16 (a)-(d) depicts the profiles of the pressure drop, liquid holdup (β_L), mass transfer coefficients (k_L and k_G), and normalized packing specific wetted area (a_w/a). The figure shows that the pressure drop is about 0.16 bar over the 48-meter packing height. The average liquid holdup ranges from 7.4% to 8.4% for SGS and from 5.5% to 5.8% for PGS. The (a_w/a) values vary from 0.375 to 0.389 for SGS and from 0.271 to 0.293 for PGS, and they follow a similar trend as (β_L). The higher values of (a_w/a) and (β_L) for SGS compared to PGS can be due to the higher required SGS solvent flow rate to meet the process constraints. Also, k_L values were significantly lower than k_G , emphasizing the importance of the resistance (i/k_L) in the liquid-side.

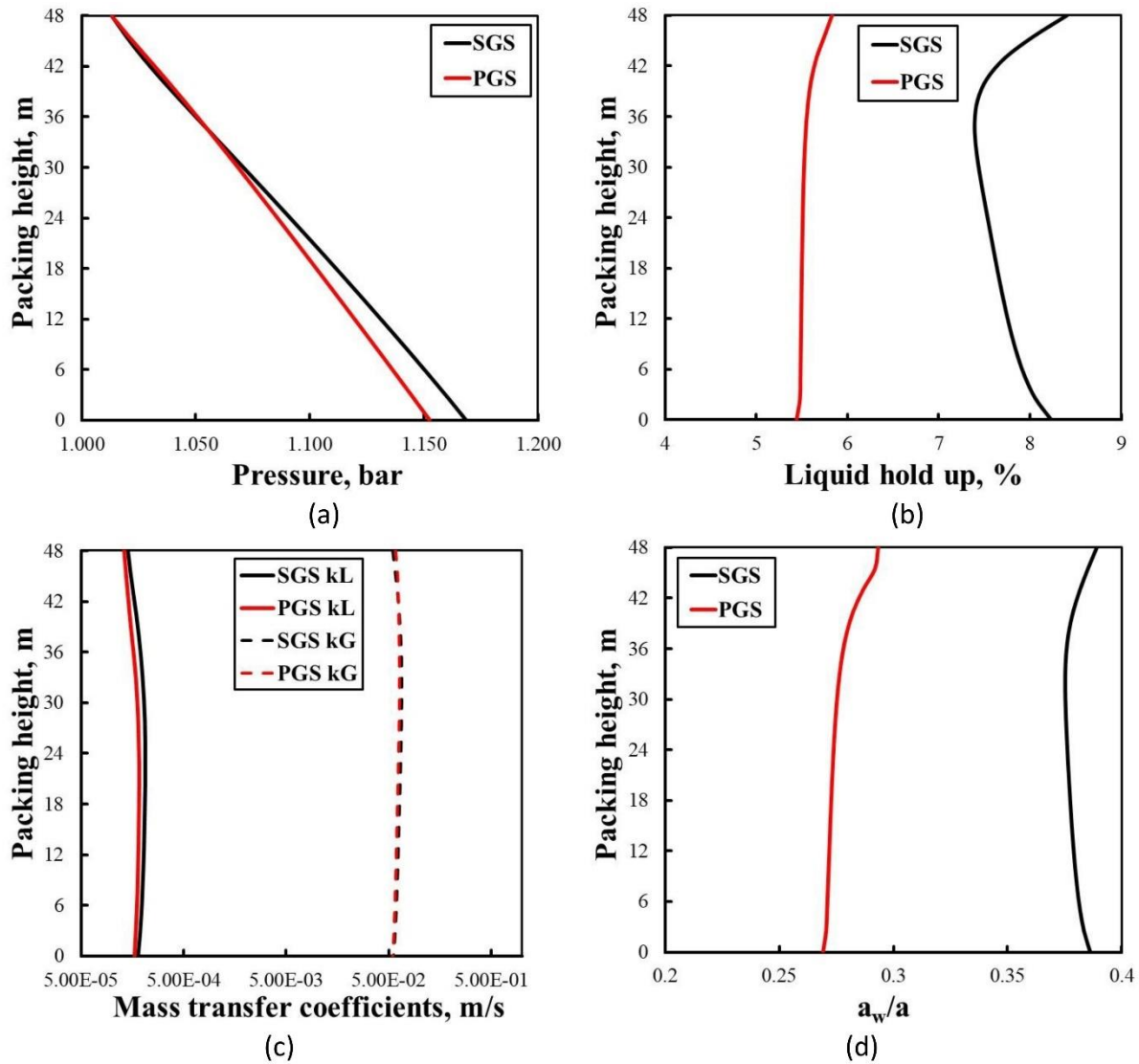


Figure 16 Profiles of (a) pressure, (b) liquid holdup, (c) mass transfer coefficients, and (d) normalized packing specific wetted area in the CAU for Pathway (ii).

7.3.4 Pathway (ii): Ultra-Filtration Unit (UFU)

The solution exiting from the bottom of the CAU contains glycine, unreacted SGS or PGS, water, and solid NaHCO_3 or KHCO_3 nanomaterials of about 25 nm [23]. These nanomaterials were separated from the solution with an Ultrafiltration Unit (UFU) employing DOW SFP-2860 membranes. The UFU operates based on the principle of pressure inequality across semipermeable membrane. The membrane separates the solid nanomaterials as retentate while allowing water, glycine, and unreacted SGS or PGS to pass through as permeate. The specifications of the SFP-2860 membrane can be found elsewhere are available in the literature [24]. Considering the average feed flow rate for a single membrane and the total liquid flow rate, it was determined that 454 or 253 membranes, operating with a differential pressure of 3.2 MPa, were necessary to separate sodium and potassium bicarbonate nanoparticles from the solution for SGS and PGS, respectively. Utilizing this specific semipermeable membrane, the process yield was 38.477 kg/s of NaHCO_3 and 46.255 kg/s of KHCO_3 solid nanomaterials.

7.3.5 Pathway (ii): Hydroxide Makeup Chamber

The UFU permeate includes a mix of H₂O, glycine, and unreacted SGS or PGS. The SGS permeate contains 75.43 wt% H₂O, 12.78 wt% NaGly, and 11.76 wt% glycine. The PGS permeate contains 76.04 wt% H₂O, 0.90 wt% KGly, and 23.05 wt% glycine. For converting the glycine in the permeate back into SGS or PGS, a highly concentrated NaOH or KOH solution was introduced into the NaOH or KOH makeup chamber, which is a CSTR equipped with an agitator and propeller. The CSTR volume required was 2.31 m³ for SGS and 1.29 m³ for PGS, with inside diameters of 1.38 m and 1.13 m, respectively. The agitator within the CSTR operates at 200 revolutions per minute (rpm), driven by a pitched blade turbine requiring 10.8 kW and 4.1 kW of power for SGS and PGS, respectively. In the CSTR, the highly exothermic reaction between the aqueous NaOH or KOH and glycine, generated heat that raised the resulting aqueous SGS or PGS solution temperature to 335.3 K and 333.3 K, respectively. Consequently, the hot aqueous SGS or PGS solution was cooled to 298.15 K before sending it back to CAU for the capture of more CO₂.

8. Techno-Economic Analysis (TEA)

The CAPEX of the CO₂ capture process includes the cost of all equipment and installation and material factors. Table 9 presents a breakdown of the costs associated with solvents, packing materials, and membranes utilized in this TEA. These are in 2023-USD.

Table 9 Costs of materials used in TEA calculations (2023-USD).

Material	Cost
Mellapak 250Y [60]	178 \$/m ³
SFP-2860 membrane [61]	1,650 \$/module
NaHCO ₃ [62]	203 \$/ton
Cost of 3M SGS solution [63]	1.15 \$/L
NaOH [64]	450 \$/ton
KHCO ₃ [65]	555 \$/ton
Cost of 3M PGS solution [63]	1.18 \$/L
KOH [66]	1000 \$/ton
BW30-400 membrane [67]	900 \$/module
Cost of 3M MEA	1.4 \$/L
Cost of 3M MDEA/PZ	1.95 \$/L
Cost of 3M AMP	2.6 \$/L

The equations used for calculating the CAPEX are available elsewhere [68-71]. The installation factors to account for the expenditure incurred during plant construction, including equipment, equipment erection, piping and buildings, are also available in the literature [69]. Also, the equations used to calculate the OPEX are available in the literature [70, 71]. In addition, the equations required for calculating LCOC are available in literature [70, 71], and the required parameters are summarized in Table 10.

Table 10 Utility prices in 2023-USD and parameters to calculate LCOC.

Parameter	Value
Cost of electricity	75.4 USD/MWh
Cost of steam [72]	6.33 USD/ton
CEPCI for 2023	797.9
i	10%/yr
N	30 years
fc	0.8
f _{O&M}	4% of the Total CAPEX, USD/year
f _{CR}	0.10608

8.1 Pathway (i): TEA for the Five Solvents

The CAPEX, OPEX, and LCOC for the five solvents used to capture CO₂ following Pathway (i) are given in Table 11, Table 12 and Table 13, respectively. These tables show that the values calculated for PGS are lower than those obtained for the other four solvents. This could be attributed to the lowest regeneration duty for this solvent. Also, since PGS exhibited the lowest LCOC, it was the best candidate for Pathway (i) among the five solvents used.

Table 11 Total CAPEX of pathway (i) in 2023-USD.

	MEA	AMP	MDEA/PZ	SGS	PGS
Stripper	\$3,294,537	\$3,294,537	\$3,294,537	\$1,342,407	\$1,342,407
Heat exchangers	\$56,747,376	\$44,862,278	\$29,608,291	\$22,819,692	\$14,971,880
Packing cost	\$811,792	\$811,792	\$811,792	\$642,297	\$642,297
Absorber	\$5,580,203	\$5,580,203	\$5,580,203	\$5,580,203	\$5,580,203
GPU	\$2,476,284	\$2,476,284	\$2,476,284	\$2,476,284	\$2,476,284
Initial solvent	\$871,417	\$850,403	\$1,170,741	\$780,601	\$792,009
Rotating equipment	\$8,560,102	\$8,541,503	\$8,957,958	\$10,310,074	\$10,458,710
Total CAPEX	\$78,341,713	\$66,417,001	\$51,899,807	\$43,951,558	\$36,263,790

Table 12 Total OPEX of pathway (i) in 2023-USD.

	MEA	AMP	MDEA/PZ	SGS	PGS
Heat Exchanger, MW	7.65	9.46	5.51	6.89	3.25
Rotating equipment, MW	12.00	11.96	12.20	14.01	15.00
Steam cost, \$/h	1,093.82	1,276.13	729.22	432.97	410.18
Makeup solvent cost, \$/h	0.01	133.51	0.02	-	-
O&M, \$/hr	447.16	379.09	296.23	250.87	201.47
Total OPEX, \$/h	3,022.22	3,403.56	2,360.79	2,259.10	1,987.99

Table 13 Total LCOC of pathway (i) in 2023-USD.

	MEA	AMP	MDEA/PZ	SGS	PGS
CO ₂ capture rate, ton/h	72.97	72.62	74.02	73.36	74.50
CAPEX Contribution to LCOC, \$/ton CO ₂	16.25	13.84	10.61	9.07	7.37
OPEX Contribution to LCOC, \$/ton CO ₂	41.42	46.87	31.89	30.80	26.69
Total LCOC, \$/ton CO ₂	57.67	60.71	42.51	39.87	34.06

8.2 Pathway (ii): TEA for SGS and PGS

The CAPEX, OPEX and LCOC for using SGS and PGS for the CO₂ capture process following Pathway (ii) are given in Table 14, Table 15, and Table 16, respectively. These tables indicate that the values calculated for PGS are lower than those for SGS. This could be attributed to the PGS faster reaction kinetics with CO₂ than SGS, which led to using smaller solvent flow rate, and hence lower pumping duty and smaller heat exchanger size. Also, PGS captured 73.21 ton of CO₂ per hour and produced 46.26 ton of KHCO₃ nanomaterials per hour, whereas SGS captured 72.61 ton of CO₂ per hour and produce 38.48 ton of NaHCO₃ nanomaterials per hour. Thus, once again, the PGS solvent appeared to be favorable than SGS for Pathway (ii).

Table 14 Total CAPEX of Pathway (ii) in 2023-USD.

	SGS	PGS
Heat Exchangers	\$7,747,941	\$8,476,634
Packing Cost	\$570,931	\$570,931
Absorber	\$5,580,203	\$5,580,203
Ultrafiltration unit	\$1,242,440	\$719,643
Reaction chamber	\$952,887	\$808,559
GPU	\$2,476,284	\$2,476,284
Initial solvent	\$780,601	\$792,009
Rotating equipment	\$3,618,114	\$2,776,887
Total CAPEX	\$22,969,402	\$22,201,148

Table 15 Total OPEX of Pathway (ii) in 2023-USD.

	SGS	PGS
Heat exchanger, MW	4.92	4.40
Rotating equipment, MW	5.41	3.3270
Ultrafiltration power, MW	0.08	0.05
NaOH makeup, MW	0.01	0.01
Polishing unit power, MW	0.13	0.13
O&M, \$/h	127.608	\$123.34
Hydroxide cost, \$/h	29,677.69	93,319.18
Bicarbonate price, \$/h	28,119.01	92,418.40
Total OPEX, \$/h	\$2,464.93	1,606.41

Table 16 Total LCOC of Pathway (ii) in 2023-USD.

	SGS	PGS
CO ₂ capture rate, ton/h	72.61	73.21
CAPEX Contribution to LCOC, \$/ton CO ₂	4.79	4.59
OPEX contribution to LCOC, \$/ton CO ₂	33.95	21.94
Total LCOC, \$/ton.CO ₂	38.73	26.53

Lower LCOC values for PGS suggest that it is the most cost-effective solvent for capturing one ton of CO₂, as it demonstrates the lowest Capital Expenditure (CAPEX) and Operational Expenditure (OPEX) among the solvents tested. This behavior means that selecting PGS could allow CO₂ capture at a lower overall cost for large-scale industrial applications.

9. Conclusions

Five different chemical solvents (SGS, and PGS, MEA, AMP, and MDEA/PZ) were used to capture CO₂ from a split flue gas stream (456 ton/h) of the Longview 780 MW power plant (West Viginia, USA). Before CO₂ capture, SO₂ and NO₂ in the flue gas were scrubbed with DIW in a gas polishing process. The flue gas polishing and CO₂ capture processes were modeled in Aspen Plus V.12.1. Using SGS and PGS to capture CO₂ led to phase separation and subsequently two process pathways. In Pathways (i), the five solvents were used to capture CO₂ for subsequent sequestration, and in Pathway (ii), only SGS and PGS were used to produce valuable sodium and potassium bicarbonate nanomaterials. For both pathways, the CO₂ capture process TEA was conducted, and the process hydraulics and gas-liquid mass transfer were calculated.

The Aspen Plus V.12.1 simulation results revealed the flowing: (1) for Pathway (i) the LCOC for PGS were lower than those of SGS, MEA, AMP, and MDEA/PZ; (2) for Pathway (ii), the LCOC values of PGS were lower than those of SGS; (3) comparing LCOC values of the two pathways, pathway (ii) was more economically favorable than pathway (i); and (4) under the operating conditions used, the two-phase pressure drop values were negligible, and k_L values were order of magnitude smaller than k_G values, suggesting that gas-liquid mass transfer resistance ($1/k_L$) was in the liquid-side.

Despite these promising results, the current study has some limitations, particularly in predicting the process hydraulic and mass transfer using the 1999 correlations by Billet and Schultes [56], which might not be fully adequate for use in industrial-scale processes. Future work could focus on pilot-scale experiments with different packing and presentative solvents under actual process operating conditions to build accurate and scalable correlations to be implemented in Aspen Plus simulations. Also, exploring additional AAs solvent could further improves the cost-effectiveness of the post-combustion CO₂ capture process. Such efforts could improve Aspen Plus modeling, optimization and scale up of industrial processes.

Abbreviations

Notations

a	Specific packing area, 1/m
a_w	Specific packing wetted area, 1/m
AMP	2-Amino-2-methyl-1-propanol
CAPEX	Capital expenditure, 2023-USD
CAU	CO ₂ absorption unit
CAS	CO ₂ absorption system
CSTR	Continuous stirred tank reactor
c_p	Heat capacity, J/mol/K
D_{CO_2}	Diffusivity of CO ₂ , m ² /s
g	Acceleration due to gravity, 9.81 m/s ²
GPU	Gas polishing unit
ΔG_f°	Standard Gibbs free energy of formation (1 bar and 298.15 K), kJ/kmol
H	Height of packing, m
He'	Henry's Law constant of CO ₂ , Pa·m ³ /mol
ΔH_f°	Standard heat of formation (1 bar and 298.15 K), kJ/kmol
k_G	Gas-side mass transfer coefficient, m/s
k_{-i}	Backward second-order reaction rate constant of i th component, m ³ /kmol/s
k_i	Forward second-order reaction rate constant of i th component, m ³ /kmol/s
k_L	Liquid-side mass transfer coefficient, m/s
LCOC	Levelized cost of CO ₂ capture, 2023-USD/ton of CO ₂ captured
MEA	Monoethanolamine
MWt	Molecular weight, kg/kmol
NBP	Normal boiling point, K
O&M	Operating and maintenance cost, 2023-USD/h
OPEX	Total operating cost, 2023-USD/h
P	Pressure, bar
P_c	Critical pressure, MPa
PGS	Potassium glycinate salt
PZ/MDEA	Blend of piperazine/methyldiethanolamine
SGS	Sodium glycinate salt
SNS	SO ₂ and NO ₂ scrubbing system
T	Temperature, K
T_c	Critical temperature, K
TEA	Techno-economic analysis
UFU	Ultrafiltration unit
V_c	Critical molar volume, m ³ /kmol

Greek Symbols

β_L	Liquid holdup
ω	Acentric factor

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Competing Interests

The authors have declared that no competing interests exist.

Additional Materials

The following additional materials are uploaded at the page of this paper.

1. Supporting Materials: Process Flow Diagrams.

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