

Performance Evaluation of Amine-Infused Resin (AIR) for LNG and Process Optimization through Simulation

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1 Introduction

2 Experiment

- 1) Experimental setting
- 2) Experimental result

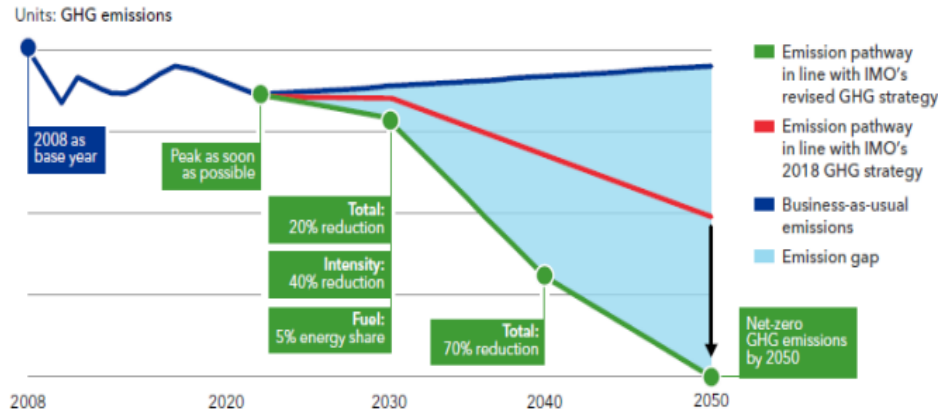
3 Process Simulation

- 1) Model description
- 2) Simulation result

4 Conclusion

Introduction

Background

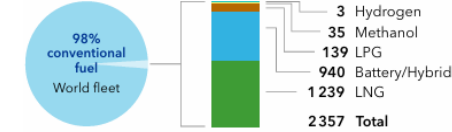


Source: DNV Maritime Forecast to 2050

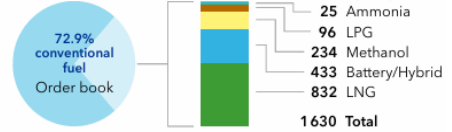
Alternative fuel uptake in the world fleet in number of ships (upper) and gross tonnage (lower), as of June 2024

NUMBER OF SHIPS

Ships in operation

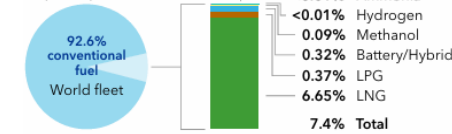


Ships on order

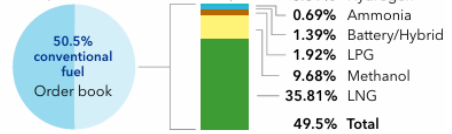


GROSS TONNAGE

Ships in operation



Ships on order



Sources: IHSMarkit (ihsmarkit.com) and DNV's Alternative Fuels Insights for the shipping industry - AFI platform (afi.dnv.com)

* Maritime Forecast to 2050, DNV(2024)

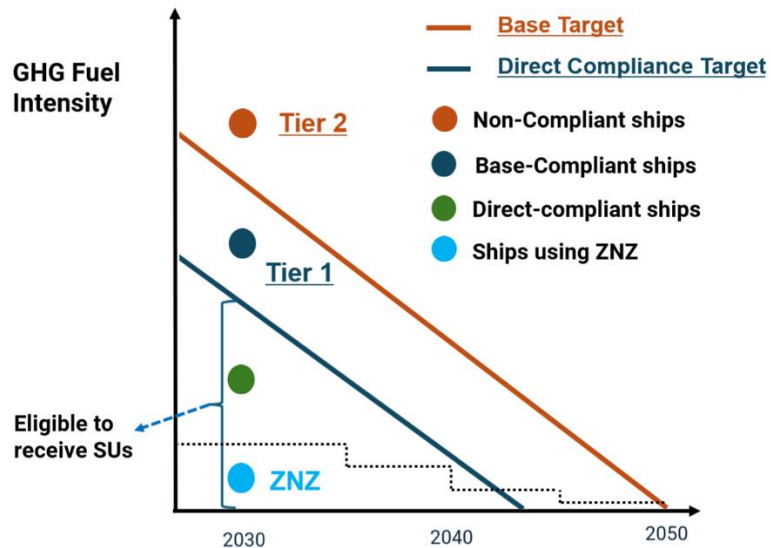
- Since the Industrial Revolution, the rapid increase in carbon dioxide emissions has accelerated global warming.
- Globally, there is a growing movement to reduce carbon emissions.
- In line with this trend, the shipping industry has set a target to achieve net-zero emissions by 2050.
- Accordingly, various studies are being conducted to reduce the use of fossil fuels, the primary source of carbon dioxide emissions.

- The use of low-carbon and carbon-free fuels is emerging as a promising alternative.
- Among orders for eco-friendly fuel-powered vessels, liquefied natural gas (LNG) accounts for approximately 50%, representing a significant proportion.

Introduction

Background

- LNG produces about 20% less CO₂ compared with conventional fossil fuels, which is why it is considered a relatively eco-friendly fuel.
- However, the shipping industry is now facing strict carbon emission regulations.
- At the 83rd session of the Marine Environment Protection Committee (MEPC), incentives for low-emission vessels were considered.



* Korean Register, IMO NEWS Flash(2025)



Figure 4. Conditioning and Capture equipment locations for 1 ton per hour capacity.

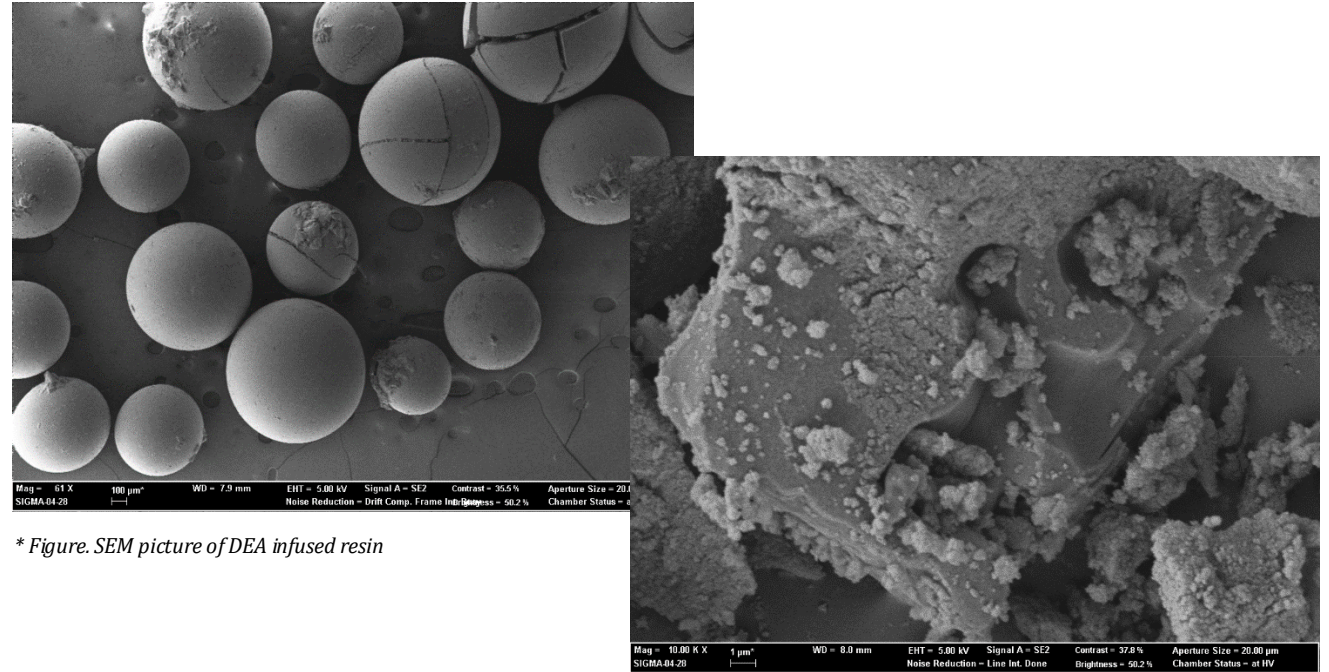
- Even small amounts of carbon dioxide generated during vessel operation need to be addressed.
- Consequently, the demand for on-board CO₂ capture is increasing.
- However, ships have limited space and energy, more research is required to develop practical solutions.

Introduction

Objective



* Figure. SHI's Ship with OCC system



* Figure. SEM picture of DEA infused resin

- SHI(Samsung Heavy Industries) successfully demonstrated the first amine-based onboard CO₂ capture technology in Korea.
- However, chemical absorbents have inherent challenges such as high regeneration energy requirements.
- To overcome these limitations, adsorbents are being considered as alternatives.
- Adsorbents offer lower regeneration energy demand and higher durability, making them more suitable for onboard CO₂ capture systems.
- In fact, Jung et al. (in progress, 2025) evaluated the performance of an amine infused resin, showing promising results under CO₂ 15 % condition.
- Experiments were conducted using amine-infused resin capable of both chemical absorption and physical adsorption.

Find the optimal operating condition of Adsorbent for OCC and Optimization through Simulation

Experiment

MEA / DEA Infused Resin Experiment – Experimental Apparatus



* Table. Specification of Experimental Setting

	Specification
Reactor	• Tubular • Size : ½” (id 13.1 mm) * 200 mmL • DP/DT : 5 bar/ 120 °C • Material : 316SS
Heat	• Range : ~ 150 °C • Band
Pressure	• Back Pressure Regulator
Mass Flow Controller	• Placed at inlet and outlet of the reactor • Range : ~500 sccm
Gas Chromatography	• Column : Porapak-N

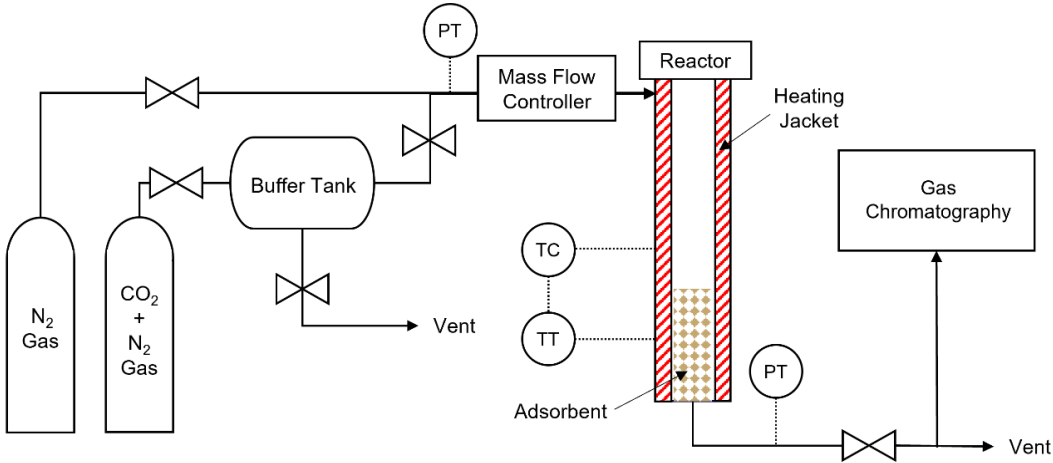
* Figure. Experimental Apparatus

Experiment

DEA Infused Resin Experiment

Experimental Procedure

- The reactor is packed with adsorbent.
- Reaction gas is stored in a buffer tank and controlled by an MFC before entering the reactor.
- The pressure of the reaction gas is regulated by a BPR located at the outlet of the reactor.
- After passing through the adsorbent, the reaction gas exits the reactor and is analyzed by GC.
- During regeneration, nitrogen controlled by the MFC is purged while the reactor temperature is increased.



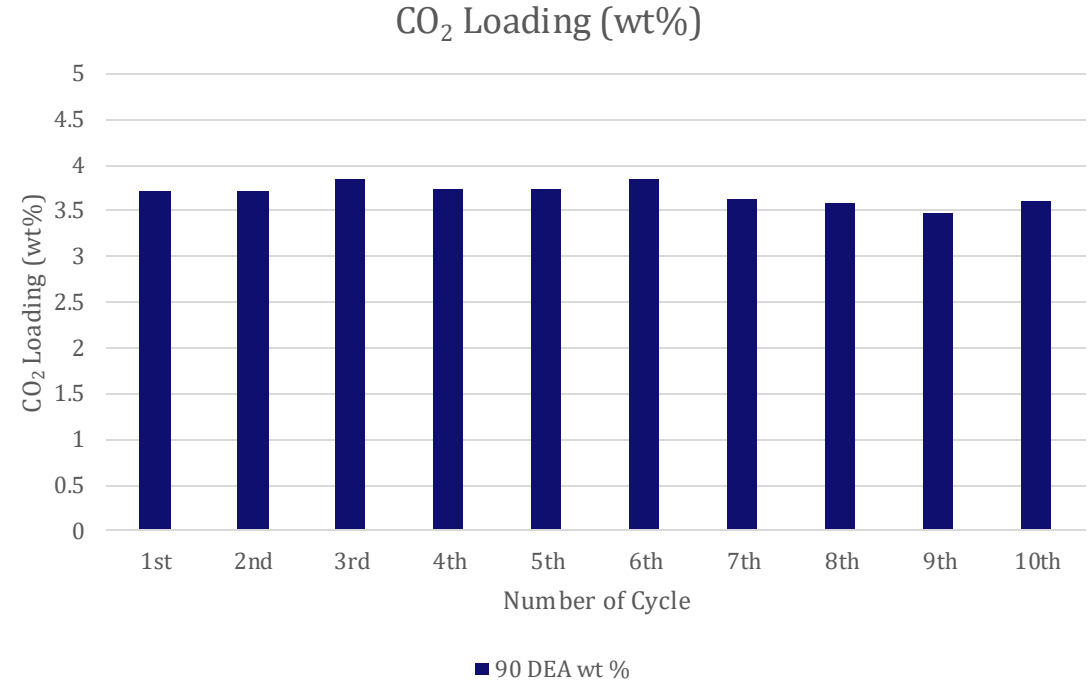
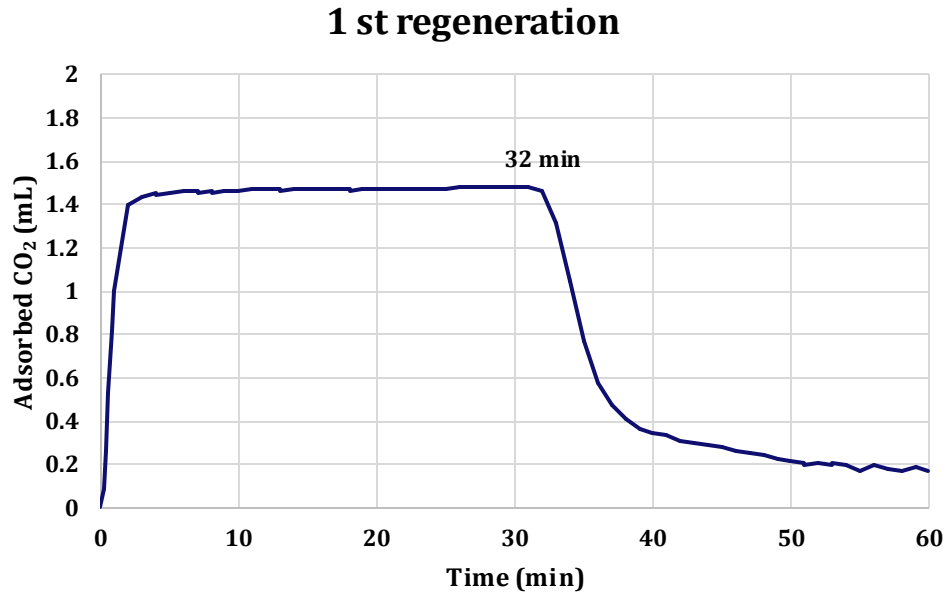
* Figure. Schematic of Experimental Setting

* Table. Detail of Experimental Condition

	Composition of Flue gas	Pressure	Mass	Adsorption			Regeneration			# of Cycle
				Temperature	Flow rate	Adsorption Time	Temperature	Flow rate (N ₂)	Regeneration Time	
DEA-Resin	CO ₂ 5 % N ₂ Balance	3.5 bara	3 g	30 °C	30 sccm	1 hour	90 °C	100 sccm	2 hours	10

Experiment

DEA Infused Resin Experiment



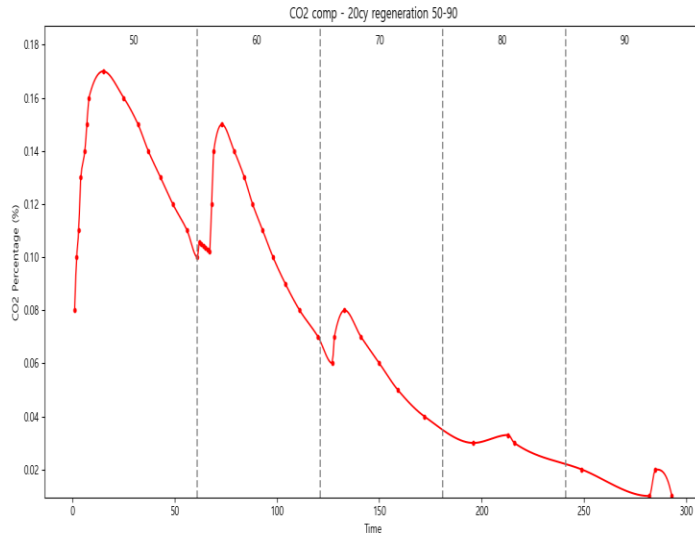
$$CO_2 \text{ Loading (wt\%)} = \frac{\text{Adsorbed } CO_2 \text{ (g)}}{\text{Amount of Adsorbent (g)}}$$

DEA infused Resin Adsorption Performance

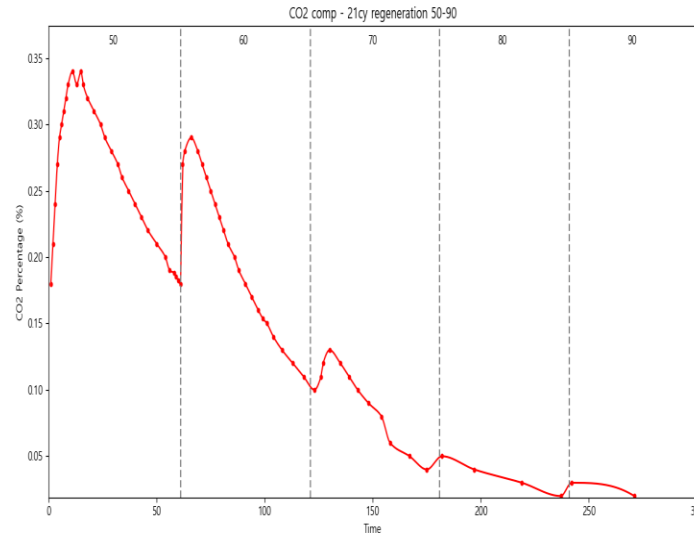
- Across all cycles, the maximum adsorption time remained similar, at approximately 30 minutes.
- CO₂ Loading (wt%) was calculated by adsorbed CO₂ which is accumulated by GC over amount of adsorbent.
- The average CO₂ Loading was 3.69 wt%.
- No significant performance degradation was observed.

Experiment

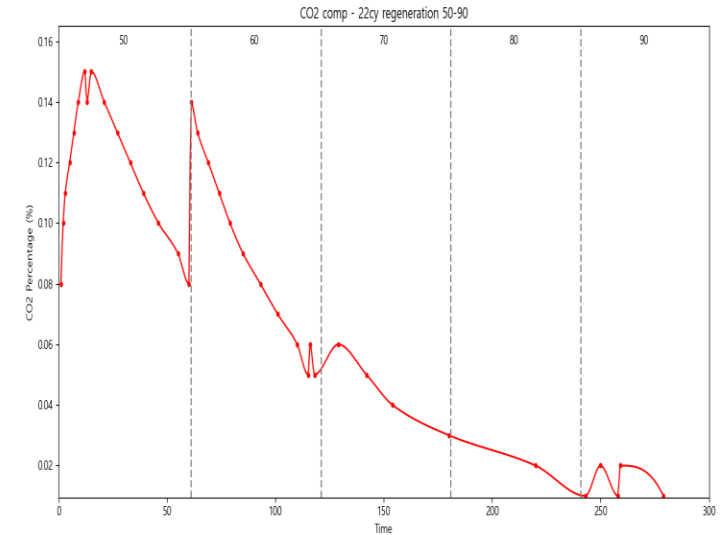
DEA Infused Resin Experiment - Regeneration Temperature Assessment for DEA Resin



CO₂ Desorption by Regeneration Temperature (20th Cycle)



CO₂ Desorption by Regeneration Temperature (21st Cycle)



CO₂ Desorption by Regeneration Temperature (22nd Cycle)

Experimental Procedure

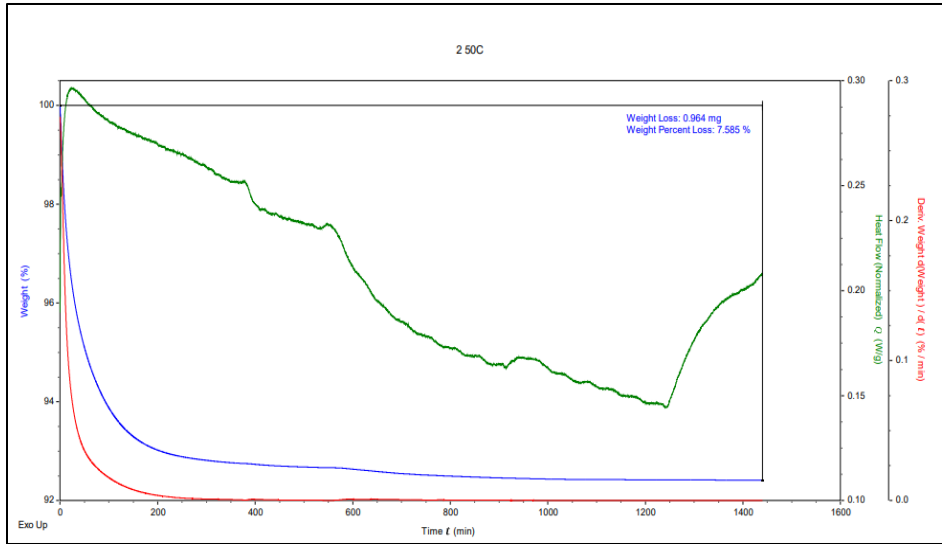
- To identify the optimal regeneration temperature for DEA.
- Purged with N₂ at 100 sccm, identical to the regeneration process.
- Measured the CO₂ released from the DEA resin as the temperature was increased from 50 to 90 °C, in increments of 10 °C per hour.

Results

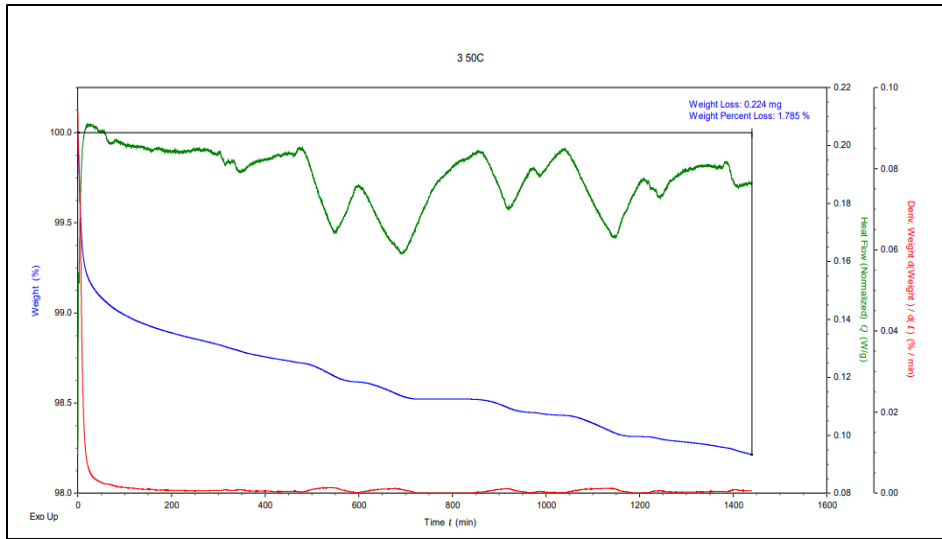
- The highest CO₂ desorption was observed at 50 °C and 60 °C, with an initial desorption peak also appearing at 70 °C.
- The highest CO₂ desorption was observed at 50 °C.

Experiment

DEA Infused Resin Experiment - TGA/DTA Analysis at 50°C



* CO₂ Loaded DEA Resin



* DEA Resin

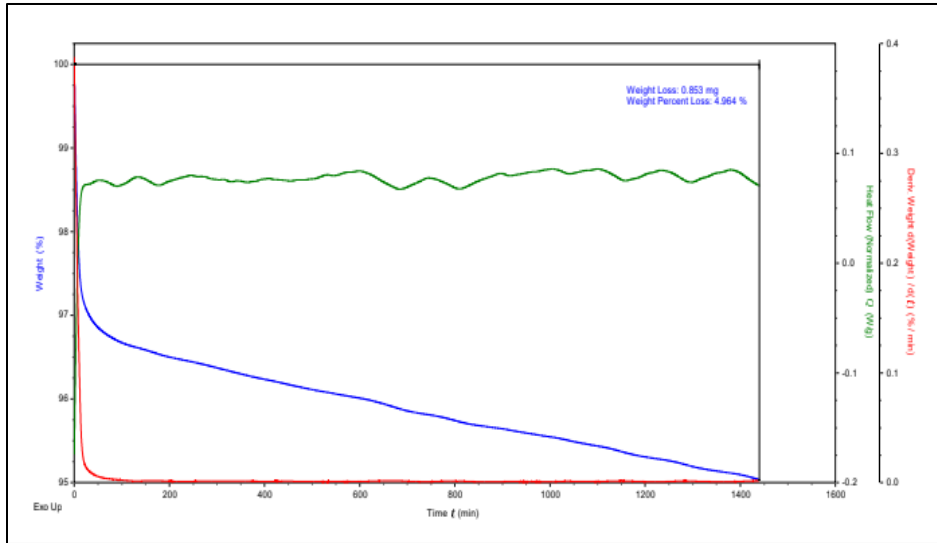
	CO ₂ Loaded DEA Resin	DEA Resin
Heat Flow	Exo up	
Derivation of Weight	7.585 %	1.785 %
Weight Loss	0.964 mg	0.224 mg

Time-Dependent SDT Results at 50 °C

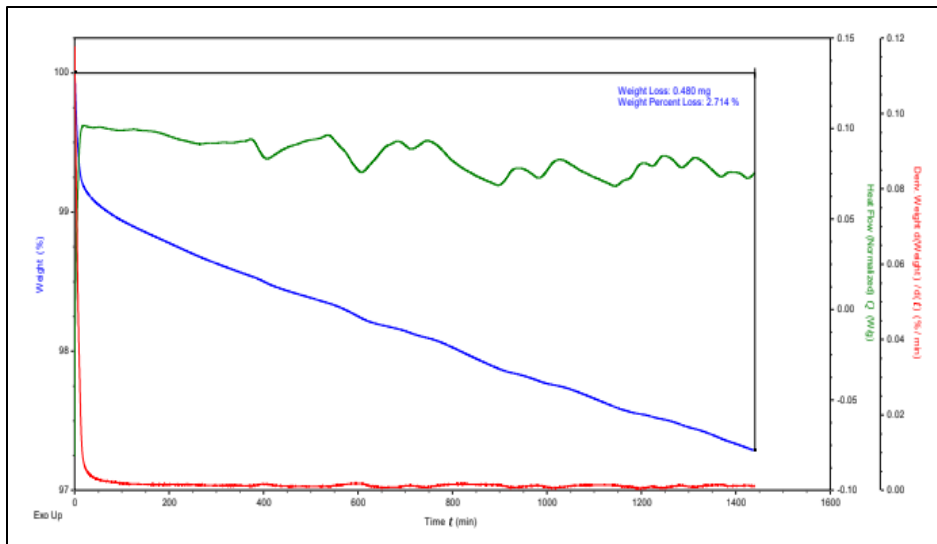
- The sample were kept at 50 °C for 24 hours resulted in substantially greater weight loss in CO₂ loaded DEA resin than in the unloaded sample, due to CO₂ desorption.
- The optimal regeneration time was approximately 30 minutes.

Experiment

DEA Infused Resin Experiment - TGA/DTA Analysis at 60°C



* CO₂ Loaded DEA Resin



* DEA Resin

	CO ₂ Loaded DEA Resin	DEA Resin
Heat Flow	Exo up	
Derivation of Weight	4.963 %	2.714 %
Weight Loss	0.853 mg	0.480 mg

Time-Dependent SDT Results at 60 °C

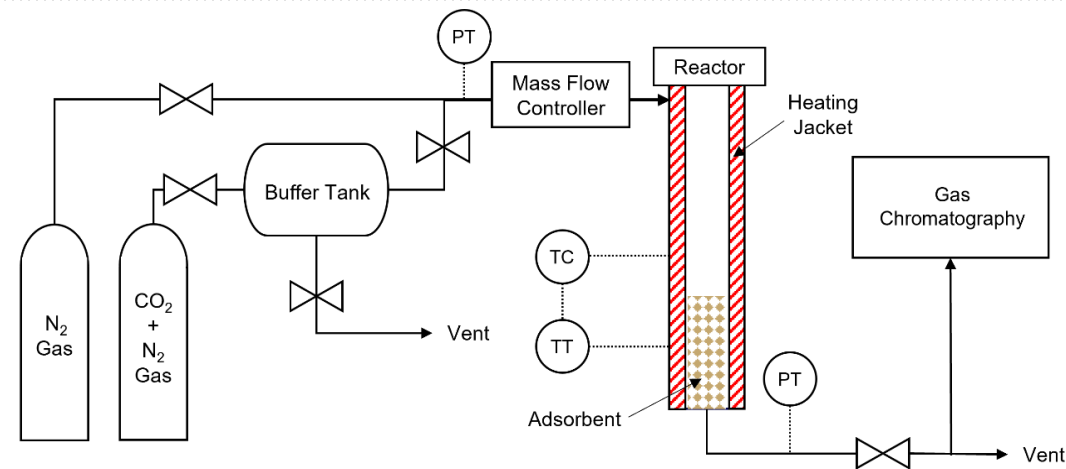
- Both CO₂ loaded and unloaded samples showed rapid initial weight loss, followed by a gradual decrease.
- As observed at 50 °C, CO₂ loaded DEA resin exhibited greater weight loss than the unloaded resin.
- At 60 °C, DEA resin showed even higher weight loss compared to 50 °C.

Experiment

DEA Infused Resin Experiment - Regeneration Temperature as an Operational Variable

Experimental Procedure

- Adsorption method applied consistently across experiments.
- Regeneration experiments conducted at 50°C, 60°C, and 90°C.

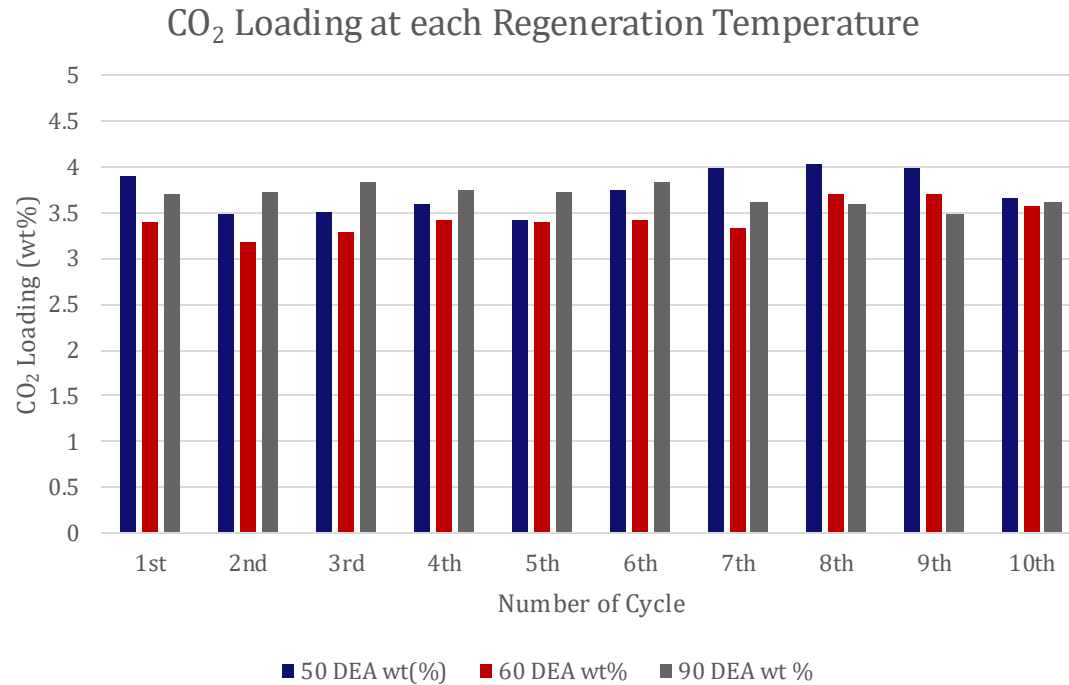


* Figure. Schematic of Experimental Setting

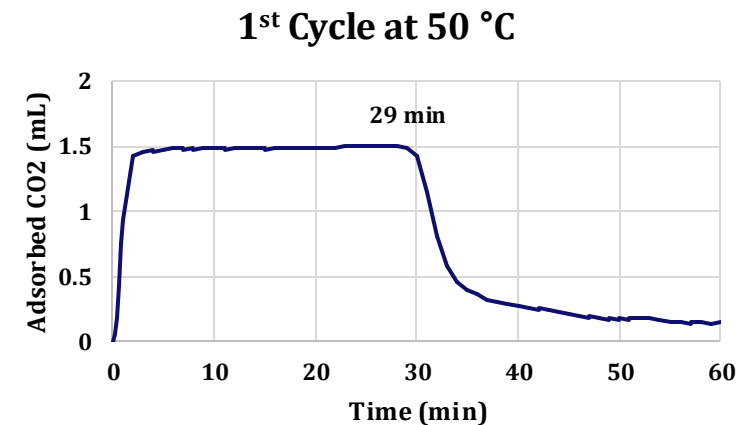
	Composition of Flue gas	Pressure	Mass	Adsorption			Regeneration			# of Cycle
				Temperature	Flow rate	Adsorption Time	Temperature	Flow rate (N ₂)	Regeneration Time	
DEA-Resin	CO ₂ 5 % N ₂ Balance	3.5 bara	3 g	30 °C	30 sccm	1 hour	90 °C	100 sccm	2 hours	10
							60 °C			
							50 °C			

Experiment

DEA Infused Resin Experiment - Adsorption Performance by Regeneration Temperature



Regeneration Temperature	Average CO ₂ Loading (wt %)
50 °C	3.73
60 °C	3.45
90 °C	3.69



Adsorption Performance by Regeneration Temperature

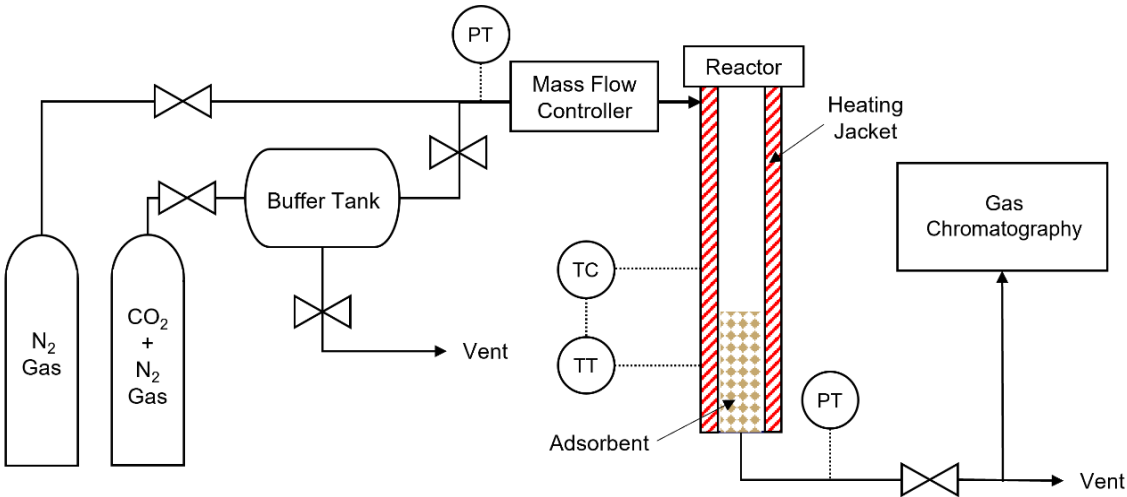
- Among the three regeneration temperatures, 50 °C yielded the highest average adsorption capacity.
- Across all cycles, the maximum adsorption time remained similar, at approximately 30 minutes.
- No significant performance degradation was observed at any regeneration temperature.

Experiment

DEA Infused Resin Experiment – Adsorption Pressure as an Operational Variable

Adsorption Pressure as an Operational Variable

- Adsorption method applied consistently across experiments except the pressure.
- The experiments were conducted under 3.5 bar and 1.3 bar.

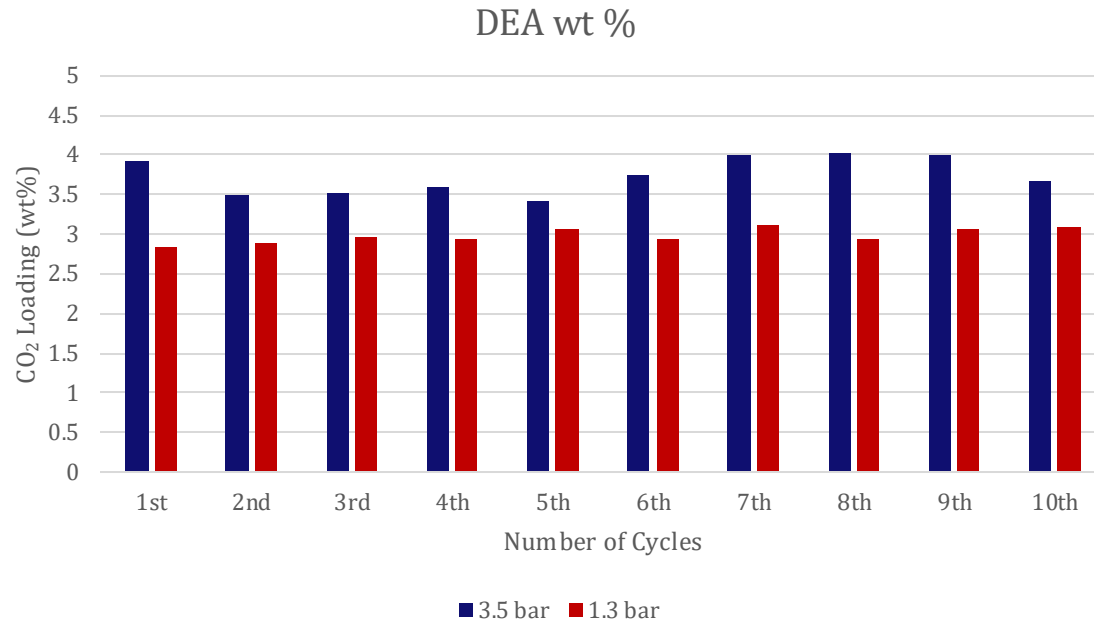


* Figure. Schematic of Experimental Setting

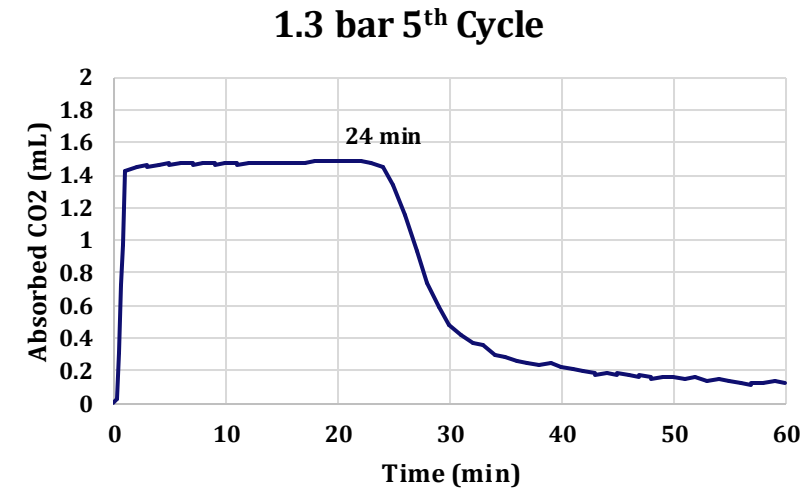
	Composition of Flue gas	Pressure	Mass	Adsorption			Regeneration			# of Cycle
				Temperature	Flow rate	Adsorption Time	Temperature	Flow rate (N ₂)	Regeneration Time	
DEA-Resin	CO ₂ 5 % N ₂ Balance	3.5 bar	3 g	30 °C	30 sccm	1 hour	50 °C	100 sccm	2 hours	10
		1.3 bar								

Experiment

DEA Infused Resin Experiment - Adsorption Performance by Adsorption Pressure



Adsorption Pressure	Average CO ₂ Loading (wt %)
1.3 bar	2.98
3.5 bar	3.45



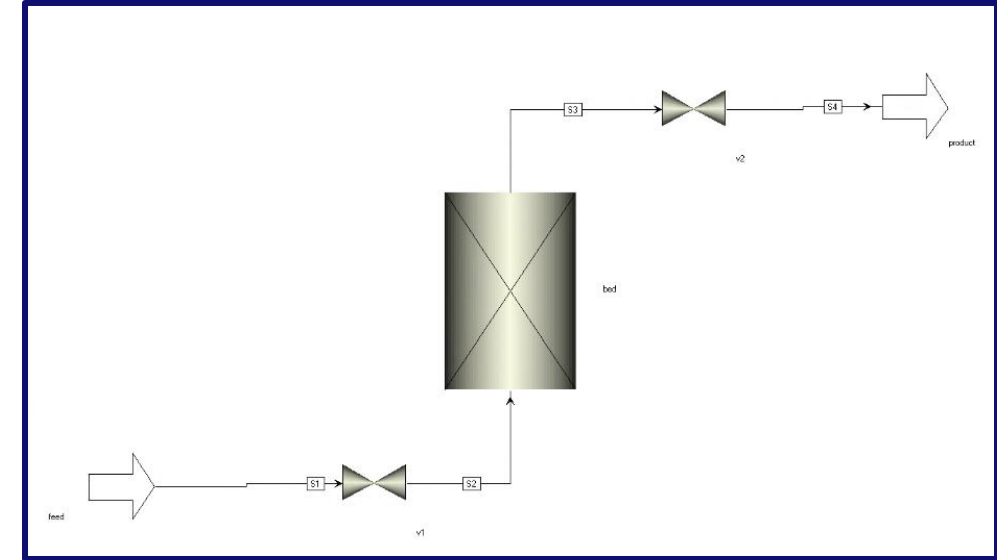
Adsorption Performance under different pressure

- Compared to 3.5 bar, the adsorption performance at 1.3 bar was about 0.5 points lower.
- The maximum adsorption time also decreased from 30 minutes to 24 minutes.
- Similar to the case at 3.5 bar, no noticeable degradation was observed.

Process Simulation

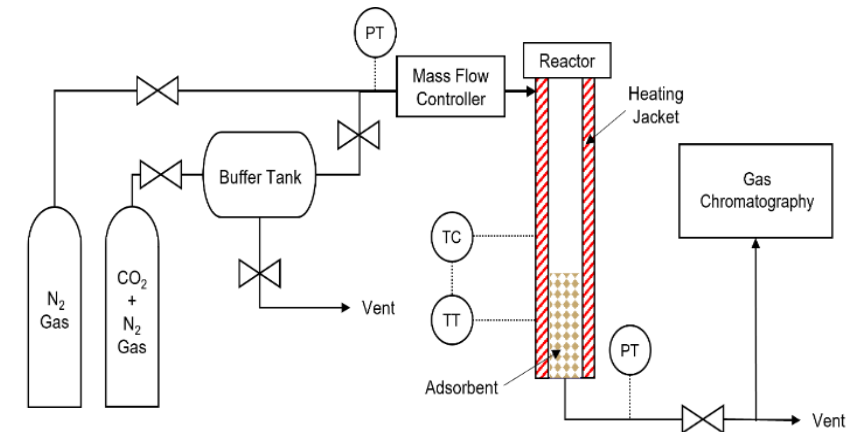
Model description

- Process simulation was performed using Aspen Adsorption, an adsorption process modeling tool.
- The simulation was based on the lab scale model.
- Only the adsorption phase of the adsorption-regeneration cycle was simulated.
- Model fitting was carried out using experimental conditions and parameters obtained from the experiments.



* Figure. Aspen Adsorption

	Composition of Flue gas	Pressure	Mass	Adsorption		
				Temperature	Flow rate	Adsorption Time
DEA-Resin	CO ₂ 5 % N ₂ Balance	3.5 bara	3 g	30 °C	30 sccm	1 hour



Process Simulation

Model description

* Table. Key Models in Simulation

Model	Method	Equation
Adsorption isotherm model	Langmuir 1	$w_i = \frac{IP_1P_i}{1 + IP_2P_i}$
Mass transfer model	Lumped resistance with a linear driving force	$\frac{\partial w_i}{\partial t} = MTC_{si}(w_i^* - w_i)$
Energy Balance	Non-isothermal with Gas & Solid Conduction	$\begin{aligned} &(\varepsilon_i \rho_g C_{p,g} + \rho_s C_{p,s}) \frac{\partial T}{\partial t} \\ &= \varepsilon_i \frac{\partial (v_g \rho_g C_{p,g} T)}{\partial z} - \rho_s \Delta H_{ads} \frac{dq}{dt} \end{aligned}$
Pressure drop, Gas velocity within the bed	Ergun equation	$\begin{aligned} &\frac{\partial p}{\partial z} \\ &= - \left(\frac{1.5 \times 10^{-3} (1 - \varepsilon_i)^2}{(2r_p \psi)^2 \varepsilon_i^3} \mu v_g \right. \\ &\quad \left. + 1.75 \times 10^{-5} \rho_g \frac{(1 - \varepsilon_i)}{2r_p \psi \varepsilon_i^3} v_g^2 \right) \end{aligned}$

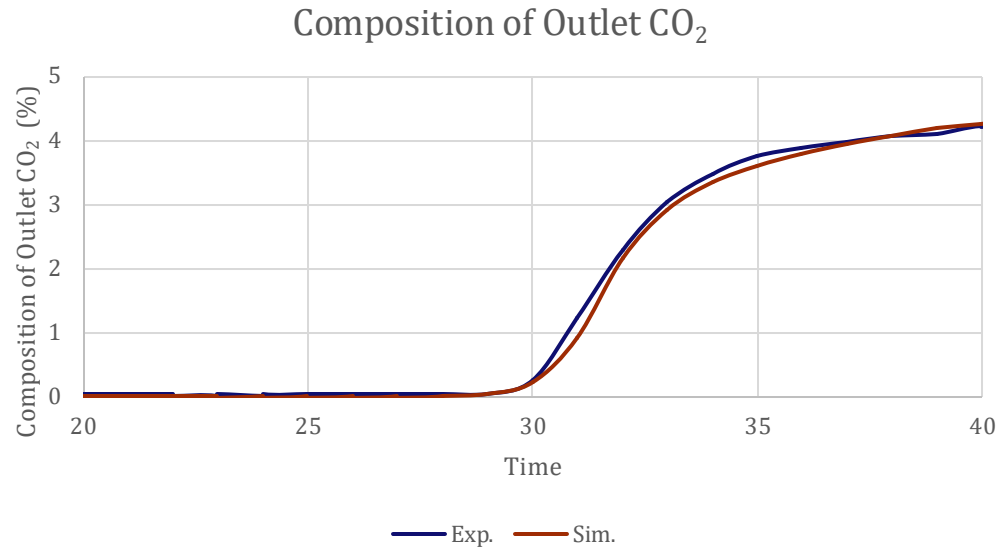
w_i : Adsorption capacity of adsorbent (mmol CO₂ / g of adsorbent)

ε_i : Inter-particle voidage
 $C_{p,(g,s)}$: Heat Capacity of gas and solid

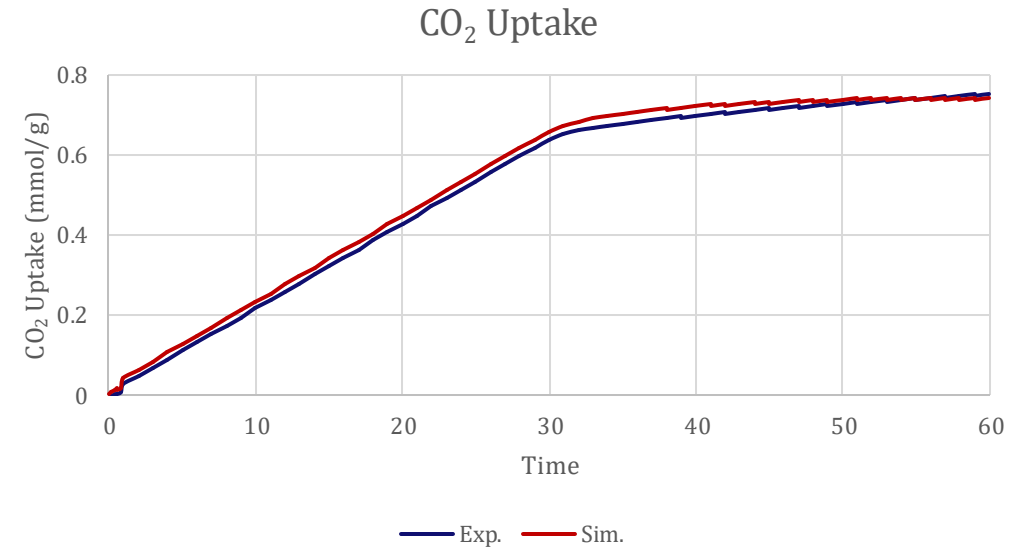
r_p : Particle radius
 ψ : Sphericity
 v_g : Gas Velocity

Process Simulation

Simulation Results



* Figure. Outlet CO₂ Concentration of Exp. and Sim.



* Figure. CO₂ Hold up in bed of Exp. and Sim.

- The breakthrough point and overall adsorption behavior were well simulated.
- Differences in adsorption rate were attributed to bed hold-up.

	Composition of Outlet CO ₂	CO ₂ Uptake
RMSE	0.1	0.017

1. The adsorption performance of DEA infused resin was evaluated
 1. When regenerated at 90 , the resin showed 3.69 wt% adsorption performance, and no degradation was observed even after 10 cycles.
 2. Regeneration temperature experiments were conducted from 50 °C to 90 °C, with 1-hour increments..
 1. The highest desorption was observed at 50 °C and 60 °C.
 2. At 50 °C, the resin exhibited the highest adsorption performance, with no degradation after 10 cycles.
 3. Pressure experiments indicated that adsorption performance decreased by about 0.5 wt% compared to near-atmospheric pressure. It did not affect stability.
 4. Aspen Adsorption simulations were carried out, successfully reproducing the adsorption process.
-

Future Work

- Further characterization of DEA-infused resins
 - Economic evaluation of the process
 - Desorption simulations
- Bed sizing and process design through simulation

Reference

- Hwang. S. J. et al (2017). Solubility of Carbon Dioxide in Aqueous Solutions of Three Secondary Amines: 2-(Butylamino)ethanol, 2-(Isopropylamino)ethanol, and 2-(ethylamino)ethanol Secondary Alkanolamine Solutions. *Journal of Chemical Engineering and engineering data*, 62, 2428-2433. DOI: 10.1021/acs.jced.7b00364
- Meng F. et al (2022). Research progress of aqueous amine solution for CO₂ Capture:A review. *Renewable and Sustainable Energy Reviews*. 168, 112902. <https://doi.org/10.1016/j.rser.2022.112902>
- Huertas J. et al (2015). CO₂ Absorbing Capacity of MEA. *Journal of Chemistry*. Volume 2015, 7. <http://dx.doi.org/10.1155/2015/965015>
- Xu X. et al (2018). CO₂ Capture by amine infused hydrogels (AIHs). *Journal of Materials Chemistry A*. Issue 11.
- Dutcher B. et al (2013). Amine-based CO₂ Capture Technology Development from the beginning of 2013 – A Review. *ACS Applied Materials & Interfaces*. Vol 7/Issue 4. <https://pubs.acs.org/doi/abs/10.1021/am507465f>
- Jung J. et al (2024). Application of amine infused hydrogels (AIHs) for selective capture of CO₂ from H₂/CO₂ and N₂/CO₂ gas mixture. *Chemical Engineering Science*. 288, 119799.
- Jung J. et al (2022). Onboard CO₂ Capture Process Design using Rigorous Rate-based Model. *Journal of Ocean Engineering and Technology* 36 (3), 168-180.
- Wood C. et al (2018). Carbon Capture with polyethylenimine hydrogel beads (PEI HBs). *Journal of Materials Chemistry A*, 2018, 6, 21468-21474.

