Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale,
Monika E. Polańska, Filip Logist (Eds.)

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Technoeconomic Analysis of a Novel Amine-Free Direct Air Capture System Integrated with HVAC

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ABSTRACT

The increasing need for Direct Air Capture (DAC) technologies is driven by the urgent global need to mitigate rising CO_2 levels due to climate change. In humid climates, DAC systems face challenges as high humidity increases the energy required for regeneration. This study introduces a novel DAC system integrated within an Air Handling Unit (AHU) that includes a silica gel wheel for air dehumidification before CO_2 capture, significantly enhancing physisorbent performance by optimizing conditions for CO_2 adsorption. This system, tailored for the AHU of Doha Tower, involves dehumidifying return air, subsequently cooling it for effective CO2 capture. The introduction of the silica gel wheel notably reduced the energy requirements by 81.5% for NbOFFIVE compared to configurations without dehumidification, and the thermal energy cost for NbOFFIVE when integrated with HVAC and silica gel is 70 USD/ ton_{CO2}, compared to 160 USD/ ton_{CO2} for SBA-15 + TEPA used alone. Additionally, the thermal energy cost for the HVAC system was reduced from 430 USD/ton_{CO2} to 303 USD/ ton_{CO2}. A technoeconomic analysis highlights these improvements as crucial for reducing operational costs and cutting capital expenditures by leveraging existing AHU infrastructure. Despite the higher initial cost of NbOFFIVE, the levelized cost for DAC using NbOFFIVE is estimated at 184 USD per ton of CO_2, making it economically advantageous compared to 208 USD per ton for SBA-15.

Keywords: DAC, HVAC, Dehumidification, Chemisorption, Physisorption

INTRODUCTION

Recent data shows a steady increase in global surface temperatures, with a notable 1°C rise since the pre-industrial period, making 2023 the hottest year to date [1]. These changes reflect broader climate shifts that manifest in altered weather patterns and varied precipitation across regions, contributing to environmental strain [2]. Within this context, the built environment emerges as a major energy consumer, responsible for substantial CO_2 emissions, particularly from systems like air conditioning that dominate building electricity usage [3, 4]. With projected temperature increases, the demand for cooling is expected to surge, potentially creating a feedback loop that could exacerbate global warming [5].

Direct Air Capture (DAC) technologies represent a promising avenue for mitigating atmospheric CO_2 levels. Unlike conventional methods that target emissions at their source, DAC systems capture carbon directly from the air, highlighting their potential in comprehensive climate strategies [6]. However, DAC's effectiveness is tempered by current technological and economic limitations, as evidenced by the modest capacity of existing facilities like the Orca in Iceland [16]. Innovations in material science and system design remain pivotal for enhancing DAC's efficiency and affordability, with costs of carbon removal varying widely [7].

The effectiveness of DAC is heavily influenced by the choice of capture materials—adsorbents and absorbents [8]. Adsorbents, in particular, are advantageous due to their lower energy requirements for regeneration and significant CO2 adsorption capabilities [9]. Developments in materials such as MOFs and amine-functionalized silica have achieved notable CO_2 uptake efficiencies

https://doi.org/10.69997/sct.119305

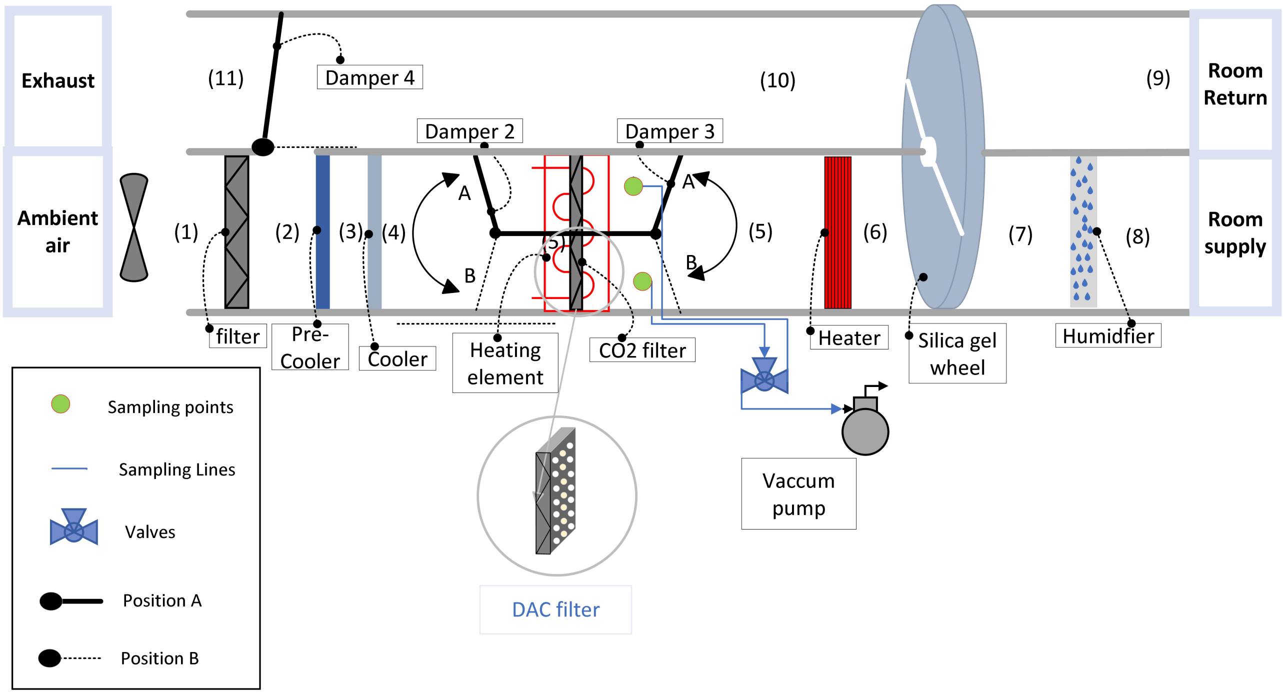

Figure 1: System diagram shows the Air handling unit compenents, DAC and silica gel wheel

under ambient conditions [10]. Yet, managing humidity remains a critical challenge, with innovations aimed at mitigating moisture to enhance system performance [11].

In advancing our previous investigations where the integration of DAC within HVAC systems to optimize energy use and CO_2 capture in buildings were investigated [12-15]. We examine the technoeconomic aspects of employing a novel physisorbent, NbOFFIVE with silica gel, and compare its performance and cost-effectiveness to a setup using SBA-15 alone, without silica gel. Both scenarios utilize integration within HVAC systems, aiming to establish a comparative understanding of their viability and scalability in urban structures like Doha Tower. This analysis seeks to identify the most efficient and economically feasible solution for large-scale implementation in modern buildings.

METHODOLGY

System description

In the configuration shown in Figure 1, return air is first dehumidified by passing through the silica gel wheel at Point 9, which was experimentally proven in our previous work to desorb water without heating, thereby reducing costs associated with water desorption. Following dehumidification, this air is mixed with the required fresh air at Point 2. The mixture is then cooled by the cooling coil to reach the supply temperature of 12°C at Point 3. After cooling, the dry, cooled air enters the Direct Air Capture (DAC) unit at Point 3, where CO_2 is captured using NbOFFIVE, a physisorbent free of amines. This material choice not only eliminates the cost of water desorption from DAC but also removes functionalization cost, enhances stability and avoids interactions of amines with air.

This system does not employ full recirculation as studied in [13] which reduces the need for additional filtration to manage airborne particulates, as fresh air is continuously introduced. However, it captures about 50% of ambient CO_2 levels due to the filtering of recirculated CO_2, with only fresh air and emissions from indoor occupants and appliances contributing to the CO_2 load. This setup will be compared to an alternative where SBA-15-TEPA [15] is used without a silica gel wheel and positioned at the beginning of the return stream at Point 9, both integrated within an Air Handling Unit (AHU) in an HVAC system. The comparative analysis aims to evaluate the performance and economic aspects of using NbOFFIVE versus SBA-15.

Space and AHU design

In designing the AHU setup for a standard office space in Qatar, we considered a room volume of 800 m³ with 30 occupants, aligned with ASHRAE standards for space allocation and ventilation. The AHU is optimized to maintain thermal comfort and indoor air quality, addressing both sensible and latent cooling loads. Our calculations incorporated factors like occupant density, equipment heat gains, and external climatic conditions, with special consideration given to the interaction between one external wall and the conditioned space. The required supply flow rate was calculated to effectively manage these loads, ensuring stable indoor conditions of 23°C and a specific humidity ratio, by balancing the heat contributions from occupants, equipment, and infiltration.

Adsorbents analysis

The CO_2 and water uptake capacities for SBA-15 functionalized with TEPA were measured using a dynamic adsorption experiments. This chemisorbent, known for its high CO_2 capture capacity, was tested under both dry and humid direct air capture (DAC) conditions using a 3P mixSorb analyzer. The rigorous synthesis and detailed characterization of these materials are comprehensively documented in the literature [15]. In contrast, NbOFFIVE, a fluorine-functionalized physisorbent, demonstrates excellent thermal stability with a CO_2 capture capacity of 1.3 mmol/g at 298 K in dry conditions. However, under humid conditions, its performance is reduced. The CO_2 and water uptake for NbOFFIVE were calculated based on a model outlined in the referenced study, utilizing following equations [16]:

$$q^*_{CO2} = q_s . b . \frac{P_{CO2}}{[1+(b.P_{CO2})^{\omega}]^{\frac{1}{\omega}}} \qquad (1)$$

Where P_{CO2} is the CO_2 partial pressure. The parameters b and ω describe the affinity and heterogeneity which are function of adsorption temperature and reference temperature, respectively. q_s represents the saturation loading and expressed in temperature dependent form as shown in equation (2). The parameters b and ω describe the affinity and heterogeneity.

The water isotherm data under equilibrium conditions were fitted using Guggenheim - Anderson - de Boer (GAB) model [16]:

$$q^*_{H2O} = \frac{C_m C_G K_{ads} x}{(1-K_{ads}x)(1+(C_G-1)K_{ads}x)} \qquad (2)$$

Here, the relative humidity is represented by x, and Cm, Cg and Kads are fitting parameters.

Energy calculations

In this study, the energy required for the Thermal Swing Adsorption (TSA) process was estimated by building upon the methodology outlined in our previous work [17]. This involved considering the mechanical work needed for CO_2 compression, the heat necessary for desorbing CO_2 and H_2O, and the energy to facilitate the thermal swing of the sorbent and its adsorbed components. The analysis excluded parasitic losses such as pressure drops and heat dissipation. Energy consumption for sorbent regeneration was quantified, including the power for the vacuum pump operation, calculated as

$$\mathrm{W_{comp}} = \frac{\mathrm{R.T_{pump}}}{\eta_{\mathrm{pump}}} . \ln\left(\frac{P_{amb}}{P_{des}}\right) \qquad (3)$$

The sensible heat required to raise the sorbent to the desorption temperature was expressed as

$$\mathrm{Q_{sens}} = \left(\frac{\mathrm{c_{p_{sorb}}}}{\triangle \mathrm{q_{CO2}}} + \mathrm{c_{p_{CO2}}} + \mathrm{c_{p_{H2O}}} \left(\frac{\triangle \mathrm{q_{H2O}}}{\triangle \mathrm{q_{CO2}}}\right)\right) . (T_{des} - T_{ads}) \qquad (4)$$

The heat inputs for desorption enthalpies of CO_2 and H2O were calculated and added to the total heat per mole of separated CO_2 (Equations 5 and 6).

$$Q_{des} = \Delta \mathrm{H_{H2O}} \left(\frac{\triangle \mathrm{q_{H2O}}}{\triangle \mathrm{q_{CO2}}}\right) + \Delta \mathrm{H_{CO2}} \qquad (5)$$

$$Q_{Total} = Q_{des} + \mathrm{Q_{sens}} + Q_{cooling} \qquad (6)$$

Furthermore, the main components of the AHU, including precooler, cooler, heater, and fan, were modeled using the mass balance equation, the first and second laws of thermodynamics, with the energy balance for each component detailed in [18], represented by

$$\dot{m}_i \times h_i + \dot{Q}_i + \dot{W}_i = \dot{m}_o \times h_o + \dot{Q}_o + \dot{W}_o \qquad (7)$$

Technoeconomic analysis

The levelized cost is calculated using Equation 8, which accounts for capital expenditures (CAPEX), fixed operating costs ($OPEX_{fix}$), variable operating costs ($OPEX_{var}$), and the amount of CO_2 captured ($CO_{2,captured}$). The CAPEX includes the base costs of equipment required for the TVSA process in the DAC system, such as the vacuum pump, heat exchanger, heat pump, and the adsorbent filters, as well as the costs associated with equipment delivery and installation. The variable OPEX accounts for utility costs, including electricity requirements for heating, cooling, and vacuum generation. The fixed OPEX covers maintenance, labor, insurance, administrative expenses, and filter replacement costs. The Capital Recovery Factor (CRF), which is used to annualize the capital investment over the project lifetime, is calculated using Equation 9. It is derived from the interest rate and project lifetime.

$$LC = \frac{CAPEX.CRF + OPEX_{fix}}{CO_{2,captured}} + OPEX_{var} \qquad (8)$$

$$CRF = \frac{i(1+i)^n}{(1+i)^n - 1} \qquad (9)$$

where i is the discount rate (7%) and n is the project lifetime (20 years) [19].

Moreover, a sensitivity analysis is performed to examine the impact of varying discount rates and utility prices, primarily electricity, on the levelized cost of the DAC system.

RESULTS

Figure 2a displays the thermal energy required for five different cases concerning HVAC and DAC systems. The first two bars (A and B) represent the cooling load consumption of an HVAC system when operating alone and within an integrated system incorporating DAC and silica gel (as outlined in Figure 1). The significant decrease in energy from A to B demonstrates the efficiency improvement when HVAC is combined with silica gel, which aids in moisture control.

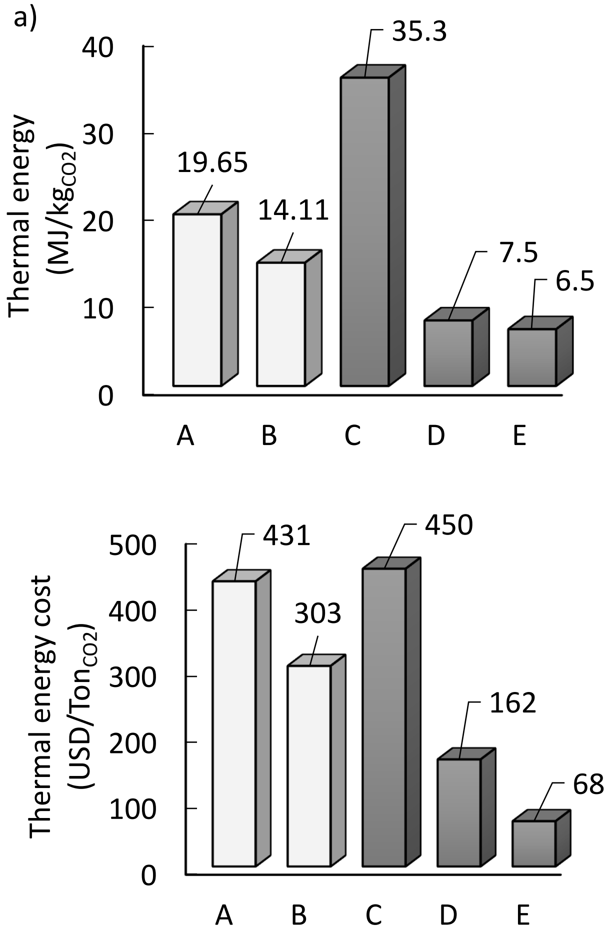

Figure 2: 2a) Thermal energy (MJ/kgCO2) and 2b) Thermal energy cost (USD/ $KgCO_2$) for (A) HVAC only, (B) HVAC within integration, (C) NbOFFIVE based DAC only, (D) SBA-15 + TEPA based DAC only, (E) NbOFFIVE based DAC within integration.

For bars C to E, it focus on DAC systems. The 'C' bar represents a DAC system using the physisorbent material NbOFFIVE, notable for its sensitivity to humidity, which explains its higher thermal energy consumption. Bar 'D' illustrates the thermal energy for a chemisorption-based DAC system using SBA-15 + TEPA, known for high CO_2 uptake efficiencies [15]. Finally, bar 'E' shows the reduced thermal energy consumption for an NbOFFIVE-based DAC system when integrated within the HVAC system incorporating silica gel wheel. This reduction highlights the effectiveness of integrating silica gel for moisture removal and leveraging the cooler air streams from the HVAC system, which significantly lowers thermal energy requirements, making it even more efficient than the SBA-15 + TEPA system.

Figure 2b correlates these thermal energies to their respective costs, normalized by the amount of CO_2 captured. The calculated costs incorporate the required electricity for a heat pump (assuming a COP of 2.6) and the local Qatari electricity rates (0.03 USD/kwh). This economic analysis further emphasizes the cost-effectiveness of integrated systems, particularly when using NbOFFIVE within an HVAC setup, due to the synergistic effects of reduced thermal loads and optimized energy use.

This detailed energy and cost analysis provides valuable insights into the selection of HVAC and DAC configurations, guiding towards choices that balance performance with economic feasibility in a climate-sensitive deployment scenario.

The levelized cost of the DAC system in this study is \$190 per ton of CO_2, which is within the range of \$88 to \$228 per ton of CO_2 estimated by the National Academy of Sciences (NAS) for DAC systems with solid adsorbents. Additionally, TVSA using a magnesium-based solid MOF sorbent has been reported to have a price range of \$60–\$190 per ton of CO_2[20].The sensitivity analysis indicates that the levelized cost of the DAC increases with a higher discount rate, reaching \$227 per ton of CO_2 at a 15% discount rate (Figure 3, a). Furthermore, utility prices significantly impact the levelized cost, with unsubsidized electricity prices in Qatar potentially driving the DAC's levelized cost up to \$306 per ton of CO_2 (Figure 3, b).

For SBA15 the levelized cost is 218 \$/ton CO_2. At a discount rate of 15% the cost gets higher to 251\$/ton CO_2 and at a high electricity cost of 0.14 \$/kWh the levelized becomes 438 \$/ton CO_2.

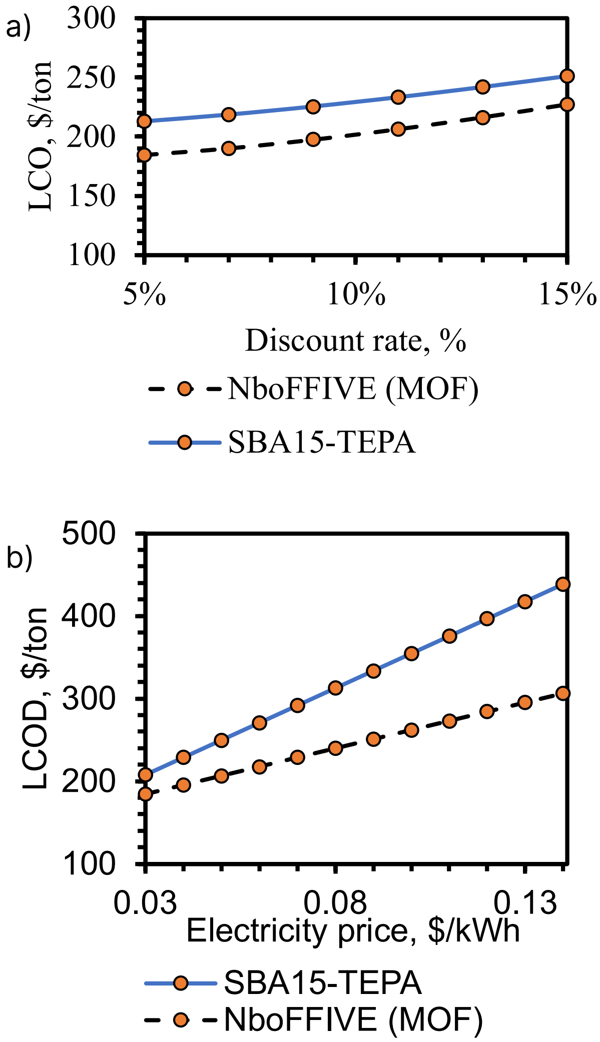

Figure 3: Effect of discount rate (a) and electricity price (b) on levelized cost of DAC.

ACKNOWLEDGEMENTS

Authors acknowledge the financial support from Qatar Environment and Energy Research institute (QEERI), Hamad bin Khalifa University (HBKU) (member of Qatar Foundation). The authors also would like to acknowledge the Core Labs and Hamad Bin Khalifa University for their contribution in the material characterization. This publication was made possible by NPRP 12 grant # (NPRP12C-0821-190017), GSRA8-L-1-0506-21032 from the Qatar National Research Fund (a member of the Qatar Foundation). The findings herein reflect the work and are solely the responsibility of the authors. Open Access funding provided by the Qatar National Library.

Conclusion

In conclusion, this study demonstrates the significant potential of integrating Direct Air Capture (DAC) technology within an Air Handling Unit (AHU) to effectively mitigate the challenges posed by high humidity in DAC systems. By incorporating a silica gel wheel for air dehumidification before CO_2 capture, the system tailored for the AHU of Doha Tower significantly enhances the performance of physisorbents like NbOFFIVE, reducing their energy requirements by 81.5% compared to traditional configurations. This integration not only leads to a substantial decrease in thermal energy costs—from 430 USD/tonCO2 to 303 USD/tonCO$_2$ for the HVAC system and from 160 USD/tonCO$_2$ to 70 USD/tonCO$_2$ for NbOFFIVE—but also notably lowers the levelized cost of DAC to 184 USD per ton of CO_2, offering an economic advantage over systems using SBA-15 + TEPA. Furthermore, this innovative integration allows for the utilization of an amine-free system, marking a significant advancement, particularly for indoor applications where health concerns are paramount. The technoeconomic analysis underscores the crucial role of leveraging existing AHU infrastructure to cut operational costs and capital expenditures, making this integrated DAC system a highly attractive solution for large-scale CO_2 capture in building environments.

REFERENCES

1. Esper, J., et al., *The IPCC's reductive Common Era temperature history*. Communications Earth & Environment, 2024. **5**(1): p. 222.
2. Trancoso, R., et al., *Significantly wetter or drier future conditions for one to two thirds of the world's population*. Nature Communications, 2024. **15**(1): p. 483.
3. González-Torres, M., et al., *A review on buildings energy information: Trends, end-uses, fuels and drivers*. Energy Reports, 2022. **8**: p. 626-637.
4. Abdullatif, Y.M., et al., *Thermodynamic analysis of gravity assisted solar-powered reverse osmosis unit for greenhouses situated in a depleted zone*. Case Studies in Thermal Engineering, 2021. **25**: p. 100990.
5. Ghazi, B., R. Przybylak, and A. Pospieszyńska, *Projection of climate change impacts on extreme temperature and precipitation in Central Poland*. Scientific Reports, 2023. **13**(1): p. 18772.
6. McQueen, N., et al., *A review of direct air capture (DAC): scaling up commercial technologies and innovating for the future*. Progress in Energy, 2021. **3**(3): p. 032001.
7. You, T., *Research on the Current Situation and Future Development Trends of Direct Air Capture Technology*. Highlights in Science, Engineering and Technology, 2024. **83**: p. 349-353.
8. Essehli, R., et al., *Single crystal structure, vibrational spectroscopy, gas sorption and antimicrobial properties of a new inorganic acidic*

diphosphates material (NH4)2Mg(H2P2O7)2•2H2O. Scientific Reports, 2020. **10**(1): p. 8909.

9. Zavahir, S., et al., *Fluorescent Zn(II)-Based Metal-Organic Framework: Interaction with Organic Solvents and CO2 and Methane Capture.* Molecules, 2022. **27**(12): p. 3845.
10. Lai, J.Y., L.H. Ngu, and S.S. Hashim, *A review of CO2 adsorbents performance for different carbon capture technology processes conditions.* Greenhouse Gases: Science and Technology, 2021. **11**(5): p. 1076-1117.
11. Wilson, S.M. and F.H. Tezel, *Direct dry air capture of CO2 using VTSA with faujasite zeolites.* Industrial & Engineering Chemistry Research, 2020. **59**(18): p. 8783-8794.
12. Abdullatif, Y., et al., *Emerging trends in direct air capture of CO 2: a review of technology options targeting net-zero emissions.* RSC advances, 2023. **13**(9): p. 5687-5722.
13. Abdullatif, Y.M., et al., *Optimizing chemisorption based direct air capture unit efficiency in HVAC systems: A study on the impact of DAC location and adsorption conditions as a response to the climate crisis and indoor air quality.* Energy Conversion and Management, 2023. **291**: p. 117280.
14. Sodiq, A., et al., *A review on progress made in direct air capture of CO2.* Environmental Technology & Innovation, 2023. **29**: p. 102991.
15. Surkatti, R., et al., *Comparative analysis of amine-functionalized silica for direct air capture (DAC): Material characterization, performance, and thermodynamic efficiency.* Separation and Purification Technology, 2025. **354**: p. 128641.
16. Balasubramaniam, B.M., et al., *Process-performance of solid sorbents for Direct Air Capture (DAC) of CO2 in optimized temperature-vacuum swing adsorption (TVSA) cycles.* Chemical Engineering Journal, 2024. **485**: p. 149568.
17. Abdullatif, Y.M., et al., *Optimizing chemisorption based direct air capture unit efficiency in HVAC systems: A study on the impact of DAC location and adsorption conditions as a response to the climate crisis and indoor air quality.* Energy Conversion and Management, 2023. **291**.
18. Abdullatif, Y.M., et al., *Thermodynamic analysis of gravity assisted solar-powered reverse osmosis unit for greenhouses situated in a depleted zone.* Case Studies in Thermal Engineering, 2021. **25**.
19. Fasihi, M., O. Efimova, and C. Breyer, *Techno-economic assessment of CO2 direct air capture plants.* Journal of Cleaner Production, 2019. **224**: p. 957-980.
20. Azarabadi, H. and K.S. Lackner, *A sorbent-focused techno-economic analysis of direct air capture.* Applied Energy, 2019. **250**: p. 959-975.
