# Direct Air Carbon Capture Using Metal-Organic Frameworks (MOFs): Techno-Economic Performance of Temperature Vacuum Swing Adsorption (TVSA) Systems

# *Captura directa de carbono en el aire mediante estructuras metalorgánicas (MOF): Rendimiento técnico-económico de los sistemas de adsorción por oscilación de temperatura y vacío (TVSA)*

# *Captura direta de carbono no ar usando estruturas metal-orgânicas (MOFs): desempenho técnico-econômico de sistemas de adsorção por oscilação de temperatura e vácuo (TVSA)*

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Recibido: 20/11/2024 Aceptado: 02/03/2025

**Summary. -** Direct Air Carbon Capture (DACC) technology is used to remove $CO_2$ directly from the atmosphere, helping tackle climate change and excessive greenhouse gas emissions efficiently. In this study, a techno-economic analysis of DACC has been carried out, including its working mechanisms, energy needs, and costs, as well as a summary of the current research status. This research compares two leading metal-organic frameworks (MOFs) — MIL-101(Cr)-PEI-800 and mmen-$Mg_2$(dobpdc) — focusing on their energy consumption, $CO_2$ adsorption, and cost. This study investigates the performance of these MOFs in a temperature vacuum swing adsorption (TVSA) process, which cyclically varies temperature and pressure to capture $CO_2$ and regenerate adsorbents. Among all materials, mmen-$Mg_2$(dobpdc) achieves the best performance with a much higher capacity and a favourable nonlinear isotherm shape, indicating significantly improved efficiency and lower energy input. DACC systems based on advanced MOFs hold great promise for minimizing non-point source emissions and should thus be considered essential components of a climate change mitigation strategy. This study contributes to direct future research and development toward more efficient and cost-effective MOFs in DACC applications.

***Keywords:*** Direct Air Carbon Capture, Temperature Vacuum Swing Adsorption, Metal-Organic Framework.

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Memoria Investigaciones en Ingeniería, núm. 28 (2025). pp. 269-286
https://doi.org/10.36561/ING.28.16
ISSN 2301-1092 • ISSN (en línea) 2301-1106 – Universidad de Montevideo, Uruguay

***Resumen. -*** *La tecnología de Captura Directa de Carbono en el Aire (DACC) se utiliza para eliminar* $CO_2$ *directamente de la atmósfera, lo que contribuye a combatir eficientemente el cambio climático y las emisiones excesivas de gases de efecto invernadero. En este estudio, se realizó un análisis tecnoeconómico de la DACC, incluyendo sus mecanismos de funcionamiento, necesidades energéticas y costes, así como un resumen del estado actual de la investigación. Esta investigación compara dos estructuras metalorgánicas (MOF) líderes —MIL-101(Cr)-PEI-800 y mmen-*$Mg_2$*(dobpdc)—, centrándose en su consumo energético, adsorción de* $CO_2$ *y coste. Este estudio investiga el rendimiento de estas MOF en un proceso de adsorción por oscilación de temperatura y vacío (TVSA), que varía cíclicamente la temperatura y la presión para capturar* $CO_2$ *y regenerar los adsorbentes. Entre todos los materiales, mmen-*$Mg_2$*(dobpdc) alcanza el mejor rendimiento, con una capacidad mucho mayor y una forma de isoterma no lineal favorable, lo que indica una eficiencia significativamente mejorada y un menor consumo de energía. Los sistemas DACC basados en MOF avanzados son muy prometedores para minimizar las emisiones de fuentes no puntuales y, por lo tanto, deberían considerarse componentes esenciales de una estrategia de mitigación del cambio climático. Este estudio contribuye a orientar la investigación y el desarrollo futuros hacia MOF más eficientes y rentables en aplicaciones DACC.*

***Palabras clave:*** *Captura directa de carbono en aire, adsorción por oscilación de temperatura y vacío, estructura metalorgánica.*

***Resumo. -*** *A tecnologia de Captura Direta de Carbono no Ar (DACC) é usada para remover* $CO_2$ *diretamente da atmosfera, ajudando a combater as mudanças climáticas e as emissões excessivas de gases de efeito estufa de forma eficiente. Neste estudo, foi realizada uma análise técnico-econômica do DACC, incluindo seus mecanismos de funcionamento, necessidades energéticas e custos, bem como um resumo do status atual da pesquisa. Esta pesquisa compara duas estruturas metal-orgânicas (MOFs) líderes — MIL-101(Cr)-PEI-800 e mmen-*$Mg_2$*(dobpdc) — com foco em seu consumo de energia, adsorção de* $CO_2$ *e custo. Este estudo investiga o desempenho dessas MOFs em um processo de adsorção por oscilação de temperatura e vácuo (TVSA), que varia ciclicamente a temperatura e a pressão para capturar* $CO_2$ *e regenerar adsorventes. Entre todos os materiais, o mmen-*$Mg_2$*(dobpdc) atinge o melhor desempenho com uma capacidade muito maior e uma forma isotérmica não linear favorável, indicando eficiência significativamente melhorada e menor consumo de energia. Os sistemas DACC baseados em MOFs avançados são bastante promissores para minimizar as emissões de fontes difusas e, portanto, devem ser considerados componentes essenciais de uma estratégia de mitigação das mudanças climáticas. Este estudo contribui para direcionar futuras pesquisas e desenvolvimentos em direção a MOFs mais eficientes e econômicos em aplicações DACC.*

***Palavras-chave:*** *Captura direta de carbono no ar, adsorção por oscilação de temperatura e vácuo, estrutura metal-orgânica.*

## 1. Introduction.

- In recent years, there has been a continuous debate about humanity's contribution to the rise of atmospheric greenhouse gases and the resulting global warming. While the exact causal relationship is still under discussion, it is now widely accepted that human activities have significantly increased these gases in the atmosphere [1]. Human activities generate greenhouse gases (GHGs) in the atmosphere, primarily carbon dioxide ($CO_2$), methane ($CH_4$), chlorofluorocarbons (CFCs), and nitrous oxide ($N_2O$). These gases significantly contribute to global warming, which is one of the most pressing environmental threats facing humanity today. Among these GHGs, $CO_2$ has the largest impact, accounting for about 55% of the observed greenhouse effect and global warming. The emissions from thermal power plants (TPPs) are a major source of $CO_2$, as approximately 30% of the world's fossil fuel consumption is dedicated to power generation, leading to substantial $CO_2$ emissions [2]. The ongoing rise in atmospheric GHGs concentrations is the most significant factor driving global warming. Since the onset of industrialization, the substantial release of $CO_2$ from human activities has played a major role in enhancing the greenhouse effect, becoming a pressing environmental issue that requires urgent attention. Additionally, other gases, such as methane ($CH_4$), nitrous oxide ($N_2O$), and ozone-depleting substances (ODSs), including fluorinated gases, also contribute to climate change [3], [4]. The current level of $CO_2$ in the atmosphere is over 400 ppm and rising by about 2 ppm per year, mainly due to burning fossil fuels [5]. The International Energy Agency reports that more than two-thirds of greenhouse gas emissions and over 80% of carbon dioxide emissions stem from energy-related activities. The global $CO_2$ emissions grew by an average of 2.6% annually. Many studies have documented the statistics and detrimental effects of global warming, revealing that around 60% of the planet is now facing unprecedented high temperatures each year [6].

Currently, the most prevalent techniques for capturing $CO_2$ from gas mixtures include absorption, membrane separation, and low-temperature $CO_2$ capture. Absorption typically involves using solvents that selectively absorb $CO_2$ from flue gases, making it effective for large-scale industrial applications. Membrane separation utilizes selective permeability to separate $CO_2$ from other gases, offering a more energy-efficient and compact alternative. Low-temperature $CO_2$ capture, on the other hand, leverages cryogenic processes to condense and separate $CO_2$ from gas streams, which can be particularly advantageous in high-purity applications. Each of these methods presents unique advantages and challenges, making them suitable for different operational contexts and carbon capture goals [7].

Fossil fuels will continue to be a major energy source, so we need technologies to capture and store $CO_2$ directly from the air, which is known as Direct Air Capture (DAC). Traditional carbon capture methods target specific sources like power plants, but DAC can capture $CO_2$ from any location, making it more versatile. There has been research into various DAC methods, including using solutions like sodium hydroxide [8]. However, these can be expensive and energy intensive.

More recent studies have focused on using solid materials called Metal-Organic Frameworks (MOFs), which are more efficient in capturing $CO_2$. Metal-organic frameworks (MOFs) offer numerous significant benefits that make them highly attractive for a range of applications, particularly in gas separation, storage, and catalysis. One of their standout features is their exceptionally high surface area, which enhances their capacity for gas adsorption and storage, making them efficient materials for capturing gases like $CO_2$ and hydrogen. Additionally, the tunability of MOFs allows for easy modification of their structural and chemical properties by altering the metal ions or organic linkers used in synthesis, enabling the design of materials tailored to specific applications, such as selective gas separation. Their highly porous structure facilitates efficient gas diffusion and adsorption, which is crucial for processes like carbon capture and air purification. Furthermore, their lightweight nature is advantageous in applications where weight is a concern, such as gas storage for transportation [7], [9]. Two promising MOFs are MIL-101(Cr)-PEI-800 and mmen-Mg2(dobpdc), which are known for their high capacity to adsorb $CO_2$ and their stability [8].

Solid adsorbents like MOFs can capture $CO_2$ through processes that use temperature and pressure changes. Studies have shown that these materials can be effective and potentially less costly than liquid solutions [10]. The research also explores different designs to improve efficiency, such as using monolith structures, which reduce pressure drops and increase mass transfer rates. Steam can be used as a stripping agent to regenerate the adsorbents, and some experiments have shown that certain adsorbents can withstand repeated cycles of adsorption and desorption using steam [11].

This paper evaluates the economic and energy performance of DAC using MIL-101(Cr)-PEI-800 and mmen-Mg2(dobpdc) in a temperature vacuum swing adsorption (TVSA) process. The study aims to optimize the conditions for DAC and guide future materials development to improve performance. Numerical models are used to analyze the effect of air and steam velocity on the system's $CO_2$ capture efficiency.

**2. Methodology. -** The study focuses on Direct Air Carbon Capture (DACC) technology using solid adsorbents and emphasizes the importance of material selection in its performance and cost-effectiveness, as illustrated in Figure I. Two metal-organic frameworks (MOFs), MIL-101(Cr)-PEI-800 and mmen-Mg2(dobpdc), are evaluated for their $CO_2$ capture capabilities. These MOFs are crucial because they offer high surface areas and tunable pore structures that enhance $CO_2$ adsorption, making them suitable for DACC applications. The study explores how these materials are used in monolithic contactors, structures designed to maximize the contact surface between the adsorbent and air. These contactors play a vital role in improving $CO_2$ capture efficiency by reducing pressure drops and increasing the adsorption rate, which leads to better overall performance in capturing atmospheric $CO_2$.

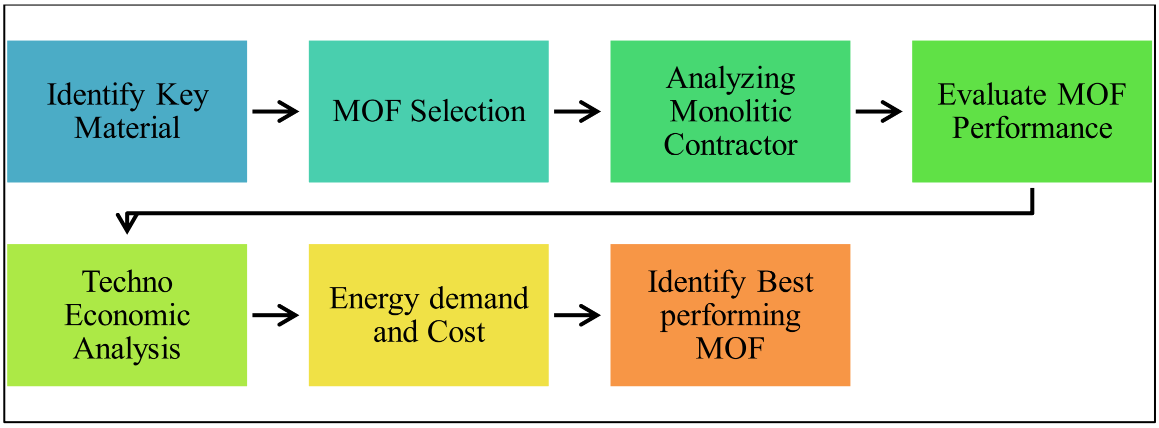

*Figure I. Methodology of Study*

The effectiveness of monolithic contactors is highlighted, as they allow for more efficient airflow and $CO_2$ adsorption, making them a viable option for large-scale DACC operations. In terms of cost evaluation, the study examines the energy demands and overall expenses of implementing these MOFs in a DACC system. mmen-Mg2(dobpdc) emerges as the more effective and cost-efficient material due to its higher $CO_2$ adsorption capacity and favorable non-linear isotherm behavior, which allows it to perform better under varying conditions. This material also requires less energy for regeneration compared to MIL-101(Cr)-PEI-800, making it a superior option for reducing $CO_2$ emissions. Overall, mmen-$Mg_2$(dobpdc) demonstrates better performance and economic viability, positioning it as a promising material for future DACC applications.

*A TVSA-based DAC system is presented by Sinah [12] to compare the performance of two MOF sorbents, namely, MIL-101-(Cr)-PEI800 and mmen-$Mg_2$(dobpdc). The monolith channel/ as shown in Figure II, through which the reactant, i.e., air flow, is assumed to be cylindrical for analysis. Each of these channels is coated with an absorbent film. The characteristics of the monolith channel are presented in Table I.*

**Table 1: Parameters of Monolith Channel**

| **Parameters of Monolith Channel** [12] | |
|---|---|
| **Absorbent film Thickness** | 60 microns |
| **Diameter of Monolith Channel** | 1270 microns |
| **Cell Density** | 400 cpsi |

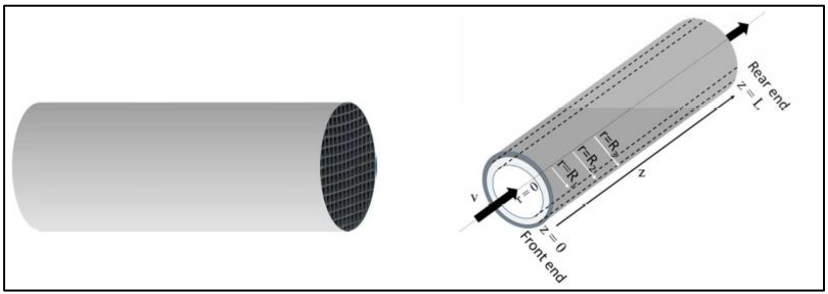

*Figure II. Monolith channel [12]*

The process (as illustrated in Figure 3) consists of the following five steps.

1. Air at ambient conditions (298K, 1 atm., 25% Relative Humidity) enters the channel. The $CO_2$ concentration in the air is assumed to be 400 ppm. Adsorption of $CO_2$ by the film begins in this step.
2. The second step involves the evacuation of air from the channel. This is done mainly to prevent the amine groups in the MOFs from being oxidized at high temperatures. The channel at the front end is closed and is evacuated by the use of a vacuum pump. The step continues until the oxygen concentration falls below 4%.
3. The third step involves pressurizing the channel to prevent any backflow of air (oxygen) from the rear end. This is done by closing the rear end and passing saturated steam at 1 atm through the front end.
4. Desorption occurs in step four by temperature swing. The rear end of the channel is opened, and saturated steam at 1 atm is fed to the channel from the front end. The steam condenses on the surface of the absorbent, increasing its temperature.
5. The last step involves cooling the system down to 348K from the desorption temperature of 373K. This is done to prevent the oxidative degeneration of the amine groups in the MOF. The vacuum pump is used for cooling using evaporating the water vapours out of the channel. As in the evacuation step, the front of the channel is closed, and pressure is dropped at the rear.

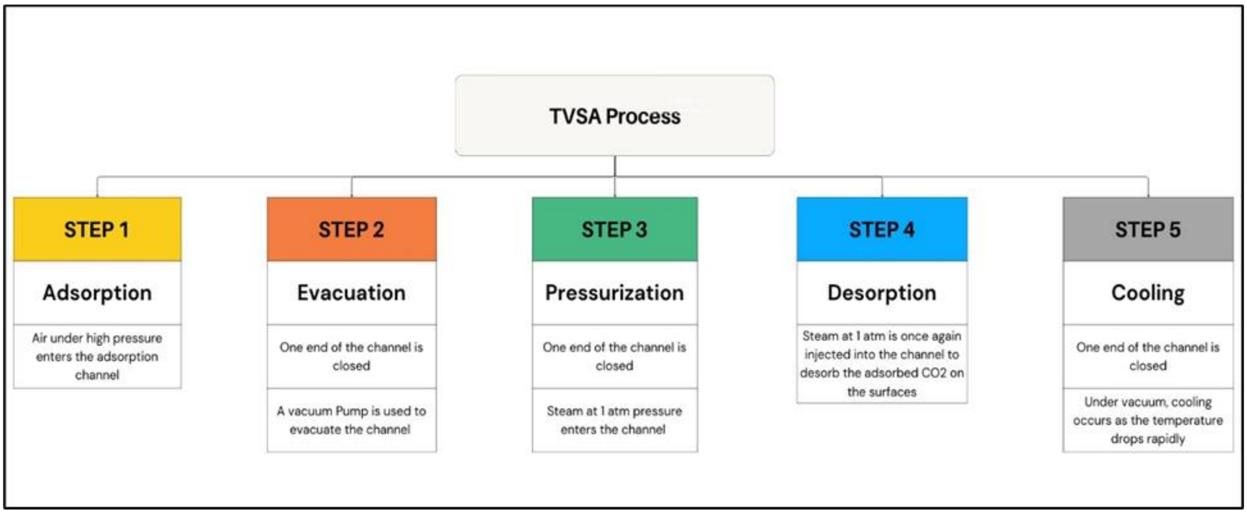

*Figure III. Process Flow of TVSA.*

## 3. Background. -

**3.1 Air Capture System. -** The research by J. K. Stolaroff et al. [13] explores the feasibility of capturing carbon dioxide ($CO_2$) directly from ambient air using a sodium hydroxide (NaOH) spray-based system. This approach is distinct from traditional methods that capture $CO_2$ from large, stationary sources such as power plants. The primary advantage of capturing $CO_2$ from ambient air is the potential to address emissions from diffuse sources and even past emissions. This can be particularly useful in achieving significant reductions in atmospheric $CO_2$ levels to mitigate climate change effects [14].

### 3.1.1 Process Overview. -

**System Description. -** The system involves spraying a solution of NaOH into the air, where it reacts with $CO_2$ to form sodium carbonate ($Na_2CO_3$). The $CO_2$-laden solution is then processed to regenerate NaOH and capture pure $CO_2$, which can be sequestered or utilized in various applications.

**Contractor Design. -** The contactor is the component where air interacts with the NaOH solution to absorb $CO_2$. Different designs for contactors include convection towers, open pools, and packed scrubbing towers [15]. This study focuses on a spray-based contractor.

- **Spray-Based Contactor:** The system utilizes fine spray nozzles to create a mist of NaOH solution that increases the contact surface area between the air and the absorbing liquid. A critical aspect of the design is managing drop coalescence, which can reduce the efficiency of $CO_2$ absorption [16].

The description of Direct Air Capture using the wet scrubbing method is given in Table II.

| Aspect | Details |
|---|---|
| $CO_2$ Capture Method | Direct capture from ambient air using wet scrubbing |
| Absorbent Used | Sodium hydroxide (NaOH) |
| Recovery Process | Two-step precipitation and crystallization followed by customization with sodium tri-titanate |
| Energy Requirement | Approximately 50% less high-grade heat than conventional; lower maximum temperature required |
| Contactor Design | Packed scrubbing towers or open towers with NaOH spray |
| Advantages | Reduces $CO_2$ systematically from dispersed emissions, substantial cost reduction, pure $CO_2$ stream generated |

*Table II. DAC using wet scrubbing method [17]*

**3.1.2 Temperature Swing Adsorption. -** Temperature Vacuum Swing Adsorption (TVSA) combines temperature and vacuum swings, which significantly lowers the energy required for the desorption process compared to TSA, which relies solely on heating. This makes TVSA more energy efficient. The comparison of different $CO_2$ capture methods is given in Table IV.

| Method | Process Description | Efficiency | Advantages | Disadvantages | Key References |
|---|---|---|---|---|---|
| **TVSA (Temperature Vacuum Swing Adsorption)** | Involves the adsorption of $CO_2$ at lower temperatures and desorption at higher temperatures under vacuum conditions. | High | High working capacity, lower energy consumption compared to TSA. | Requires precise temperature control and vacuum systems. | [18], [19] |
| **TSA (Temperature Swing Adsorption)** | Adsorption of $CO_2$ occurs at ambient temperature and desorption at elevated temperatures. | Moderate to High | Simple setup, effective for large-scale applications. | Higher energy consumption due to heating requirements. | [20], [21] |
| **Capture from Ambient Air Using Sodium Hydroxide Spray** | Involves spraying a sodium hydroxide solution to capture $CO_2$ from ambient air, forming sodium carbonate. | Variable | Effective for low $CO_2$ concentrations, can be integrated with existing systems. | Chemical handling and disposal issues, lower efficiency for high $CO_2$ concentrations. | [13] |
| **Electrochemical Conversion** | Electrochemical reduction of $CO_2$ to valuable products using electrical energy | Moderate to high | Produces high-value chemicals and fuels, potential for integration with renewable energy sources | Complex catalyst development, high energy consumption, scalability challenges | [22] |

*Table III. Different $CO_2$ Capture Methods.*

The addition of vacuum swing in TSA reduces the desorption time, leading to shorter cycle times and higher throughput. This efficiency can result in lower operational costs and improved overall process economics. TVSA systems typically produce high-purity $CO_2$ streams due to the effective desorption facilitated by vacuum. This high purity can be advantageous for subsequent $CO_2$ utilization or sequestration. It has a lower environmental impact as it requires less water compared to the NaOH spray method, which involves significant water use and potential chemical handling issues. This makes the process more sustainable and environmentally friendly. TVSA is more cost-effective, especially for large-scale applications, due to its lower energy requirements and efficient operation. While initial capital costs for vacuum equipment may be higher, the long-term savings in operational costs make it a better economic choice.

Temperature Swing Adsorption (TSA) is a cyclic process used for the capture of $CO_2$ and other gases; details are given in Table 5. It leverages temperature changes to adsorb and desorb gases from solid adsorbents.

**i. Adsorption. -** During the adsorption phase, a gas mixture containing $CO_2$ is passed through an adsorbent bed. Materials like zeolites, activated carbons, and MOFs are used due to their high surface area and selective adsorption properties. The $CO_2$ molecules adhere to the surface of the adsorbent at lower temperatures, while other gases pass through the bed. This selective adsorption is influenced by the adsorbent's affinity for $CO_2$ and its operating temperature [23], [24].

**ii. Heating. -** Once the absorbent bed is saturated with $CO_2$, the heating phase begins. The bed is heated, typically using steam or other heat sources, to increase the temperature. This heat causes the $CO_2$ molecules to desorb from the adsorbent surface. The efficiency of this step depends on the thermal properties of the adsorbent and the design of the heating system. Effective heat integration can significantly lower the energy penalty associated with this step [23], [24].

**iii. Desorption**. - As the temperature rises, the $CO_2$ is released from the adsorbent. This desorption process generates a concentrated $CO_2$ stream, which can be captured and stored. The purity and recovery rate of $CO_2$ depend on the adsorbent material and the operational parameters of the TSA cycle. MOFs, for example, have shown promising results due to their tunable properties and high selectivity for $CO_2$ [23], [24].

**iv. Cooling. -** After desorption, the adsorbent bed is cooled down to its initial temperature, readying it for the next cycle. Cooling can be achieved through heat exchange with ambient air or other cooling media. Efficient cooling ensures that the adsorbent retains its adsorption capacity for subsequent cycles [23], [24].

| Step | Description |
|---|---|
| 1. Adsorption | $CO_2$ laden gas is passed through the adsorbent bed, where $CO_2$ is selectively adsorbed at a lower temperature. The bed typically contains materials like zeolites, activated carbons, or metal-organic frameworks (MOFs) |
| 2. Heating | The adsorbent bed is heated to desorb the captured $CO_2$. This step increases the temperature of the bed to release the $CO_2$, making the adsorbent ready for the next cycle |
| 3. Desorption | $CO_2$ is released from the adsorbent material due to the increased temperature. This step produces a concentrated stream of $CO_2$, which can be captured for further use or storage |

*Table V. TSA Process Steps [25]*

**3.2 Evaluating Metal-Organic Frameworks (MOFs) for $CO_2$ Capture. -** Two MOFs, Zn4O(BTB)2 (MOF-177) and Mg2(dobdc) (Mg-MOF-74), were evaluated. Mg-MOF-74 demonstrated a higher working capacity and selectivity for $CO_2$ over $N_2$, which is critical for efficient $CO_2$ capture [26].

The study analyzed $CO_2$ adsorption isotherms at various temperatures, revealing that Mg2(dobdc) had superior performance, including a high working capacity of 17.6 wt% at 200°C. The presence of strong $CO_2$ adsorption sites in Mg-MOF-74 was crucial for its effectiveness in TSA processes [26].

**3.3 Electrochemical Conversion. -** The electrochemical conversion of $CO_2$ involves using electrical energy to drive chemical reactions that transform $CO_2$ into valuable products such as hydrocarbons, alcohols, and other chemicals. This process typically takes place in an electrochemical cell consisting of a cathode, an anode, and an electrolyte [22], [27].

**i. Cathode Reactions. -** At the cathode, $CO_2$ molecules are reduced to form products such as carbon monoxide (CO), formate, methanol, methane, ethylene, and other hydrocarbons. The specific product depends on the catalyst used and the operating conditions, such as potential and electrolyte composition.

The reduction of $CO_2$ involves multiple electron and proton transfer steps, making it a complex process. Effective catalysts are crucial to enhance selectivity and efficiency towards desired products [22], [27].

**ii. Anode Reactions. -** At the anode, water is typically oxidized to produce oxygen gas ($O_2$) and protons ($H^+$). This oxidation reaction provides the necessary protons and electrons for the reduction reactions at the cathode.

The overall efficiency of the process depends on the ability of the anode to facilitate the oxygen evolution reaction (OER) efficiently [22], [27].

**iii. Electrolyte. -** The electrolyte facilitates the movement of ions between the cathode and anode. It can be an aqueous solution, solid oxide, or ionic liquid, depending on the specific electrochemical system.

The choice of electrolyte affects the conductivity, stability, and overall efficiency of the electrochemical cell [22], [27].

**iv. Metallic Catalysts. -** Transition metals such as copper, silver, gold, and zinc are commonly used as catalysts for $CO_2$ reduction. Copper, in particular, is known for its ability to produce a wide range of hydrocarbons and alcohols.

Alloying and modifying these metals with other elements can enhance their catalytic properties and product selectivity [22], [27].

**v. Metal-Organic Frameworks (MOFs). -** MOFs are a class of porous materials that have shown promise as catalysts for $CO_2$ electroreduction. Their high surface area and tunable chemical environment make them suitable for optimizing catalytic activity and selectivity.

MOFs can be functionalized with various active sites to target specific reduction pathways [28].

**vi. Electrocatalyst Optimization. -** Research focuses on optimizing the structure, composition, and morphology of electrocatalysts to improve their performance. This includes developing nanostructured catalysts, bimetallic systems, and hybrid materials that combine the advantages of different components [28].

**3.4 Mathematical Modelling of the TVSA system. -** The following assumptions were made to develop the mathematical model:

- Air is considered to have oxygen and nitrogen components in addition to the $CO_2$ (and 25% relative humidity), and the saturated steam is pure.
- Ideal gas law and ideal mixtures are assumed for the non-condensable components [29].
- Temperature and concentration variations are neglected in the radial direction in the adsorbent film and monolith wall leading to a lumped model in the radial coordinate for these model elements [30].
- Adsorbent film thickness is uniform in the axial direction [31].
- During the desorption step, condensed water does not penetrate inside the MOF pores due to the high flow rate of desorbed $CO_2$ from the MOF pores in the opposing direction. Thus, heat is conducted into the MOF and wall and is not transferred by diffusion of steam within the MOF phase following steam condensation [32], [33].
- Heat loss from the channel is negligible during all steps of the cycle

The pressure drop across the channel is given by the Hagen Poiseuille equation:

$$\Delta P = \frac{8L\mu v}{R_1^2} \tag{1}$$

where, $L$ = length of the channel
$v$ = velocity of gas inside the channel
$\mu$ = gaseous viscosity
$R_1$ = Channel Inner Radius

The other source of pressure drop is due to drag on the system, which is assumed to be negligible as compared to pressure drop by Hagen- Poiseuille Equation [eqn. (1)].

The $CO_2$ absorption rate is approximated by the linear driving force model as given by:

$$\frac{\partial \mathbf{Q_{CO2}}}{\partial \mathbf{t}} = \mathbf{k}(\mathbf{Q_{CO2}^{eq}} - \mathbf{Q_{CO2}}) \tag{2}$$

Where, $Q_{CO2}$ = absorbed $CO_2$ concentration
$Q_{CO2}^{eq}$ = equilibrium concentration of $CO_2$
$k$ = overall mass transfer coefficient

The mass transfer coefficient is calculated by the method proposed by A Sinha [12], which gives the final equation as:

$$\mathrm{k_m} = \frac{\mathrm{h_g M_{H_2O}}}{\mathrm{C_{p,g} M_g y_{lm} Le_{H_2O}^{2/3}}} \tag{3}$$

where, $h_g$ = convective heat transfer coefficient of moist air
$M_{H_2O}$ = Molar mass of water vapor
$c_{p,g}$ = Specific heat of moist air
$M_g$ = Molar mass of air
$y_{lm}$ = Log Mean Mole Fraction
$Le_{H_2O}$ = Lewis number of $H_2O$
$y_{lm}$ = Log mean mole fraction

$$y_{lm} = \frac{y_{ni} - y_{nb}}{\ln\left(\frac{y_{ni}}{y_{nb}}\right)} \tag{4}$$

Where, $y_{ni}$ = mole fraction of the non-condensable gases at the gas film interface
$y_{bi}$ = mole fraction in the bulk flow

The concentration at the interface is assumed to be in equilibrium with pure liquid water and thus estimated using the Antoine equation [eqn. (6)]:

$$-D_{H_2O}\frac{\partial y}{\partial x} \tag{5}$$

$$C_{H_2O}^{i} = \frac{\exp\left[a - \left(\frac{b}{T_g + c}\right)\right]}{RT_g} \tag{6}$$

where, $C_{H_2O}^{i}$ = saturation concentration of water vapor in the MOF channel interface
$a, b, c$ = Antoinne constants

The heat of absorption of $CO_2$ is determined using the Clausius–Clapeyron equation.

$$\ln\frac{P_2}{P_1} = \frac{\Delta H}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right) \tag{7}$$

The heat of absorption of $CO_2$ is calculated at 25°C, 50°C and 75°C

The system design specifications and mass and heat transfer properties are tabulated in Table VI and Table VII, respectively.

| Name | Symbol | Value | Unit |
|---|---|---|---|
| Air thermal conductivity | $k_g$ | 0.0257 | $W/m.K$ |
| Air heat capacity | $C_{p,g}$ | 1003 | $J/kg.K$ |
| Air density | $\rho_g$ | 1.1839 | $kg/m^3$ |
| Adsorbent Thermal Conductivity | $k_{ads}$ | 0.32 | $W/m.K$ |
| Adsorbent Heat Capacity | $C_{p,ads}$ | 892.5 | $J/kg.K$ |
| Adsorbent Density | $\rho_{ads}$ | 500 | $kg/m^3$ |
| Wall Thermal Conductivity | $k_{wall}$ | 1.6 | $W/m.K$ |
| Wall Heat Capacity | $C_{p,wall}$ | 840 | $J/kg.K$ |
| Wall density | $\rho_{wall}$ | 2050 | $kg/m^3$ |
| Antoine Constants | $a, b, c$ | 5.2,1733.9, -39.5 | - |

*Table VI. Properties of the TVSA $CO_2$ Capture System [12].*

| Parameter | Value |
|---|---|
| $D_g$ (m) | 0.000016 |
| h (W/m$^2$-K) | 75 |
| $T_{ambient}$ | 298 |
| $C_{CO2o}$ (mol/m$^3$) | 0.016 |
| $C_{inerto}$ (mol/m$^3$) | 40.88 |
| $\triangle$H (J/mol) | 55000 |
| $\triangle$H (J/mol) | 70000 |
| $A_1$ (m) | 0.00063 |
| $A_2$ (m) | 0.00052 |

*Table VII. Heat and Mass Transfer Properties [12]*

### 3.5 Estimating Energy Requirements

1) Electrical energy is required for the running of the fan. Higher air flow rates cause a larger pressure drop across the channel.
2) Energy required by the vacuum pump to decrease the pressure inside the channel.
3) Energy is required to provide sensible heat to the adsorbent.
4) Use of vacuum pumps to lower the partial pressure of water vapour.

The efficiency of the pump is considered to be 85 % [12]. The equations for the energy requirement for the various components are given in Table VII.

| Components | Energy requirement (Joules per mole of CO₂) |
|---|---|
| Electrical energy for blowers | $E_1 = \frac{\triangle PQ.t}{N}$ |
| Adsorbent sensible heat | $E_2 = \frac{mads\ Cads}{LN} \int_{t=tstep\ 4}^{tstep\ 5} \int_{z=0}^{L} (\frac{dTads}{dt}\ dz) dt$ |
| Monolithic wall sensible heat | $E_3 = \frac{mads\ Cwall}{LN} \int_{t=tstep\ 4}^{tstep\ 5} \int_{z=0}^{L} (\frac{dTwall}{dt}\ dz) dt$ |
| CO$_2$ desorption heat | $E_4 = \triangle H$ |
| Electrical energy for vacuum Pump | $E_5 = -\frac{P_1 V_1^{\gamma}}{N_m} \frac{(V_2^{1-\gamma} - V_1^{\gamma})}{1-\gamma}$ |
| Energy in uncondensed steam | $E_6 = \frac{2\pi L'}{N_m} \int_{t=tstep4}^{tstep5} ( \int_{r=0}^{R1} v_{step4} r C_{H2O}(L) dr )\, dt$ |

*Table VIII. Energy Requirements [12]*

### 3.6 Economic Modelling of the System

- O&M cost of the device (includes energy, loading and unloading of a sorbent (**$N_{O\&M}$**))
- Scrap value of the sorbent at the end of its lifetime (**$N_S$**)
  $N_S$ = Sorbent Price **$V_s$** + Installation cost **$I_s$**
- The amount spent on the hardware is taken into consideration; hence, the running expense is the capital cost of the plant **$N_{BoP}$.**

For NPV of a DAC system:

$$NPV_0 = N_{rev} - (N_{O\&M} + N_{BoP} + N_S) \quad (8)$$

The net present value of the system has to be zero or greater than zero at some point during the operation.

To find $t_{life,}$ the first derivative of the NPV equation concerning time must be zero:

$$@t = t_{life} \ \frac{dNPV_0}{dt} = n_{rev} - (n_{O\&M} + N_{BoP}) = 0 \quad (9)$$

Revenue generated per unit of time can be calculated as,

$$n_{rev}(t) = \frac{PC_0}{t_{cycle}} e^{\frac{-t}{\tau D}} e^{\frac{-t}{\tau M}} \tag{10}$$

where **P** is the market price of carbon dioxide per unit mass, $\mathbf{C_0}$ is the initial capacity of sorbent (the amount of $CO_2$ captured per cycle), and $\mathbf{t_{cycle}}$ is the duration of one loading/unloading cycle. **D** is the time constant of the sorbent capacity degradation, and **M** is a time constant that accounts for the time value of money. The costs of MIL-101(Cr)-PEI-800 and mmen-Mg2 (dobpdc) are taken as $15/kg and $50/kg, respectively taken from local market survey.

In summary, achieving economic viability for a Direct Air Capture (DAC) device necessitates meeting the conditions outlined in Equations (8), (9) and (10). While equation (9) allows for the calculation of the device's lifetime, a positive value for $t_{life}$ does not automatically ensure a positive Net Present Value (NPV).

**4. Results and Discussions. -** The flow of CO2 through the material is shown in Figure 4, which shows how quickly $CO_2$ starts to pass through the material without being captured. For MIL-101(Cr)-PEI-800, $CO_2$ breaks through earlier, meaning this material gets saturated faster and starts letting $CO_2$ through sooner, while for mmen-Mg2(dobpdc), $CO_2$ breaks through later, indicating this material can capture more $CO_2$ before it gets saturated. At a time, step of approximately 4200s, the concentration stays constant since most of the $CO_2$ is adsorbed on the surface by the adsorbent.

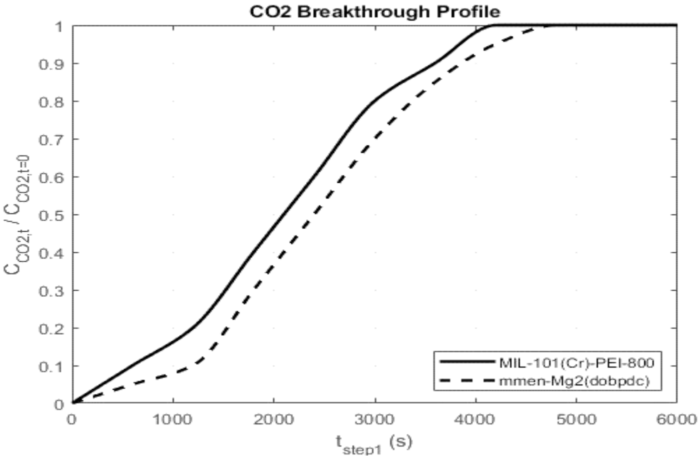

*Figure IV. $CO_2$ breakthrough curve.*

The holding time of $CO_2$ for each material is shown in Figure 5. From where one can conclude that since mmen-$Mg_2$(dobpdc) has a higher capacity of approximately 2.9 mmol/g, so it can hold more $CO_2$ while MIL-101(Cr)-PEI-800 has a lower capacity of approximately 1.2 mmol/g, so it holds less $CO_2$. In simple terms, mmen-Mg2(dobpdc) is better at capturing and holding more $CO_2$ for a longer time compared to MIL-101(Cr)-PEI-800.

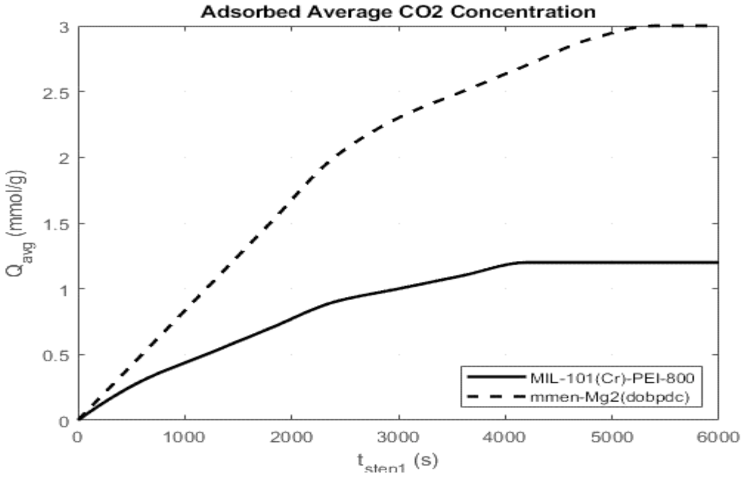

*Figure V. Adsorbed average $CO_2$ concentration.*

Energy requirements of the both MOFs mmen-Mg2 (dobpdc) and MIL-101 (Cr)-PEI-800 are given in Figure VI and Figure VII, respectively. Since the thermal efficiency was taken to be 85% [12], the minimum primary combustion energy requirements for the MIL-101(Cr)-PEI-800 and mmen-Mg2 (dobpdc) adsorbents are around 0.150 MJ/mole and 0.125 MJ/mole.

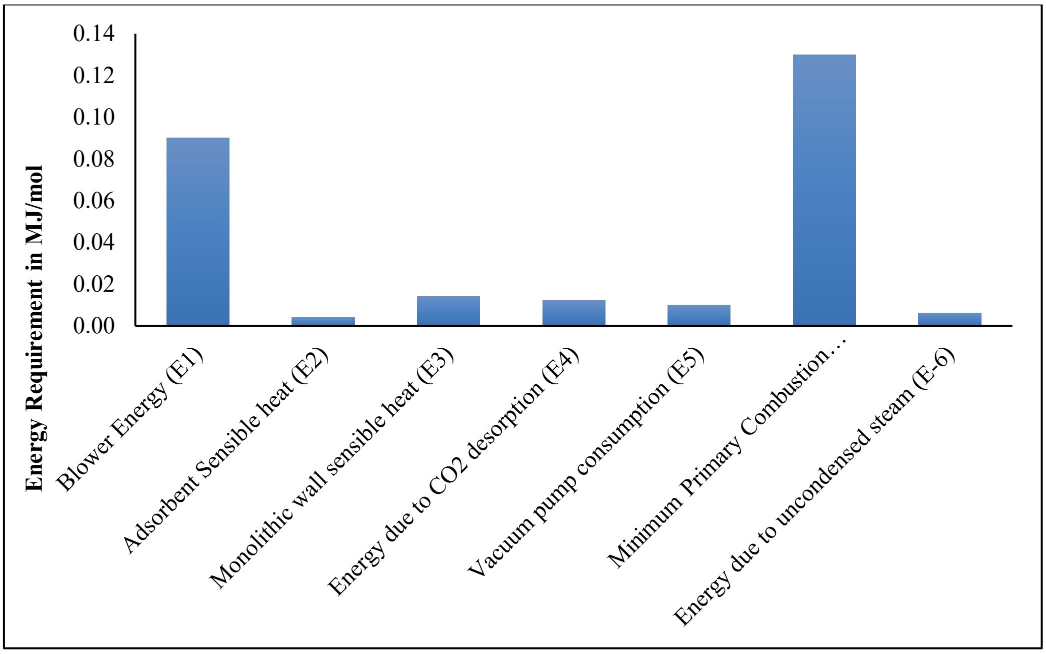

*Figure VI. Energy requirements for mmen-Mg2 adsorbent.*

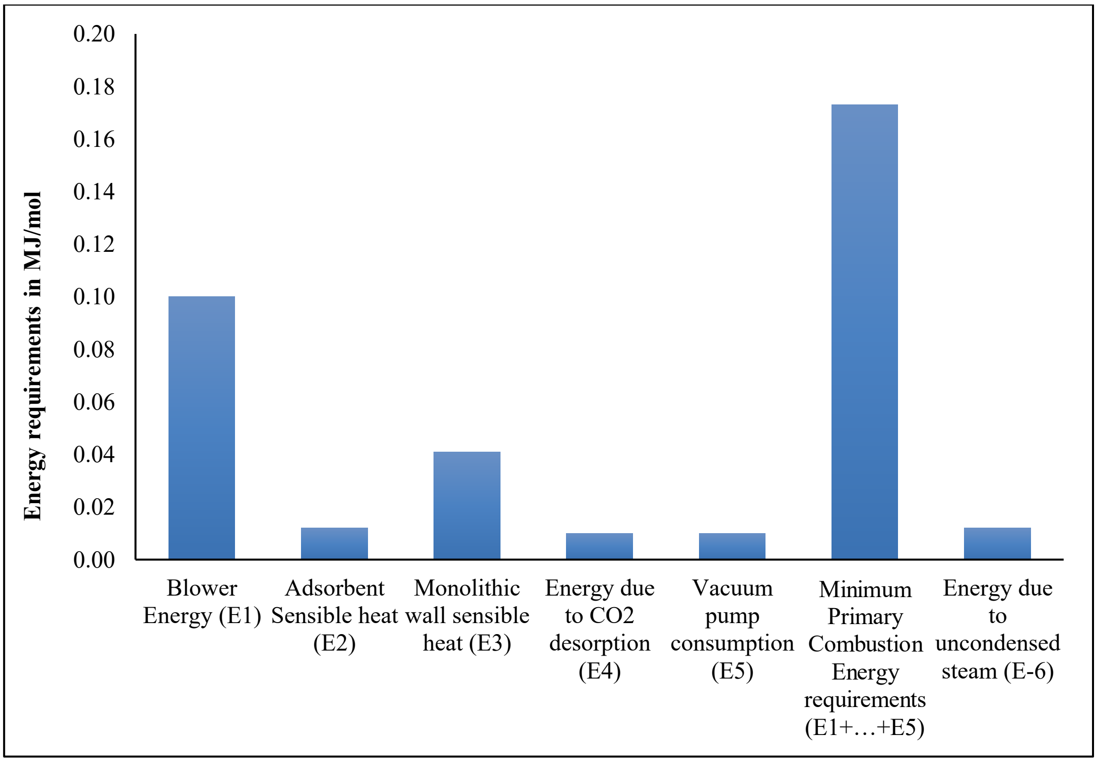

*Figure VII. Energy requirements for MIL-101 (Cr)-PEI-800 adsorbent.*

The cost comparison of both MOFs is shown in Figure 6. The curve shows the cost components for MIL-101(Cr)-PEI-800 and mmen-Mg-2(dobpdc), indicating that mmen-Mg-2(dopdc) generally incurs lower costs in key areas such as steam and blower operation. Specifically, MIL-101(Cr)-PEI-800 shows higher costs for blower Opex and steam, suggesting it is less economical in operational expenditure. While both materials have similar costs for monoliths and vacuum pump Capex, mmen-Mg-2(dobpdc) offers cost savings in most categories, highlighting it as the more cost-effective option for these processes.

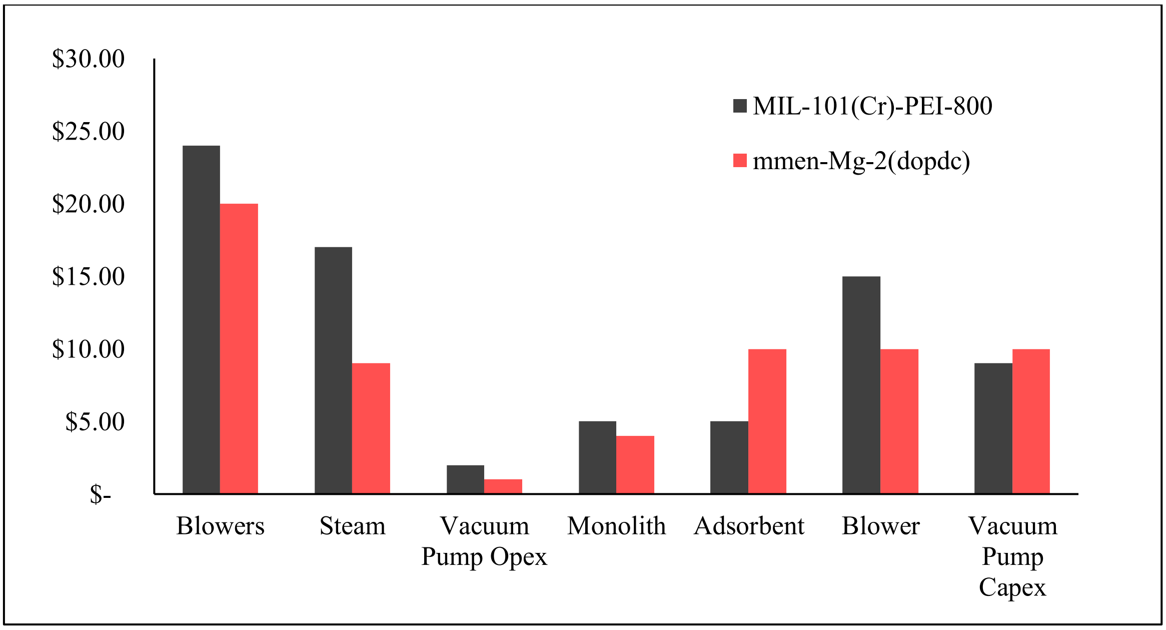

*Figure VIII. Cost comparison between both adsorbents.*

The Figure 7 looks at how the cost of the Direct Air Capture (DAC) process changes with different steam velocities for two materials MIL-101(Cr)-PEI-800 and mmen-Mg2(dobpdc). The curve shows that cost is the strong function of steam velocity. For MIL-101(Cr)-PEI-800, the cheapest operation is found at a steam velocity of 0.04 m/s while for mmen-Mg2(dobpdc), the lowest cost is at a steam velocity of about 0.06 m/s.

The study performed an analysis to find the best adsorption and desorption times by varying certain parameters and keeping the air velocity constant at 3 m/s. For this analysis, the steam velocity was kept at the optimal points identified (0.04 m/s for MIL-101(Cr)-PEI-800 and 0.06 m/s for mmen-$Mg_2$(dobpdc)). This helps to optimize the DAC process for cost and efficiency.

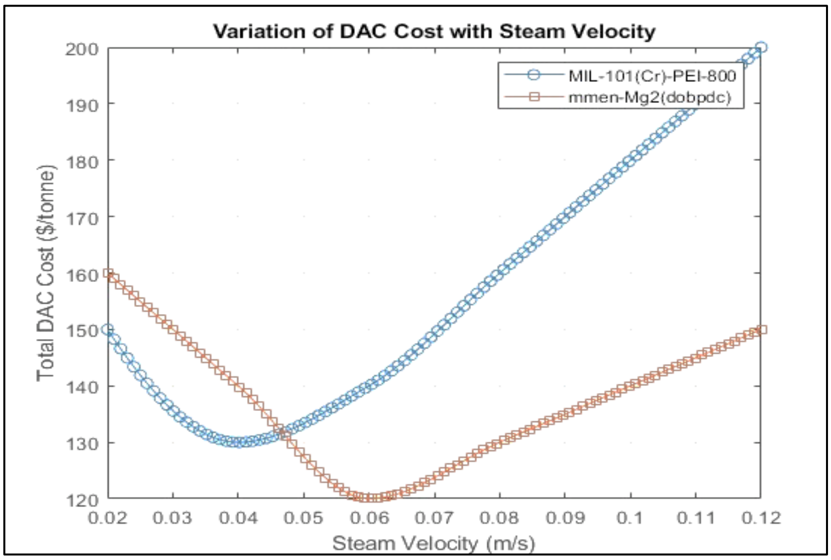

*Figure IX. Total DAC Cost v/s Steam velocity.*

MOF-based adsorbents, such as mmen-$Mg_2$(dobpdc), can potentially reduce energy demands and operational costs in DACC systems. However, transitioning these materials from lab-scale success to industrial deployment requires addressing unresolved challenges. These include energy-intensive synthesis (e.g., solvent reliance, high-temperature activation), mechanical brittleness during pelletization (critical for industrial reactor integration), and stability under cyclic TVSA conditions, where thermal degradation or moisture sensitivity could compromise long-term performance. It also requires advancements in scalable synthesis methods like continuous flow reactors [34]. A thorough understanding of how MOFs integrate into different CO2 capture technologies and regeneration processes [35], and the effective use of computational tools for material design and performance prediction under realistic operating conditions [36]. Addressing these multifaceted challenges is crucial for transitioning the promise of MOFs into practical, large-scale solutions for carbon capture.

**5. Conclusion. -** This study investigates the performance of a TVSA (Temperature Vacuum Swing Adsorption) process for Direct Air Capture (DAC) of $CO_2$ using two advanced materials, MIL-101(Cr)-PEI-800 and mmen-Mg2(dobpdc). The latter material demonstrated superior $CO_2$ adsorption capacity (2.9 mmol/g compared to 1.2 mmol/g for MIL-101(Cr)-PEI-800). Key optimizations included air and steam flow rates, with 3 m/s airflow and steam velocities of 0.04 m/s for MIL-101(Cr)-PEI-800 and 0.06 m/s for mmen-Mg2(dobpdc). Energy requirements were minimized to below the $CO_2$ combustion energy, and costs were estimated at $77-142 per tonne for MIL-101(Cr)-PEI-800 and $64-194 per tonne for mmen-Mg2(dobpdc). Future improvements could include using solar energy and enhancing material stability, aiming to further optimize energy efficiency and reduce costs in scalable DAC solutions. The thickness of the adsorbent film is crucial in determining energy costs, as a thicker film captures more $CO_2$, thereby reducing the energy required for the desorption step. Maintaining a normal air flow rate is essential, since higher air flow rates would lead to $CO_2$ bypassing the adsorbent without being captured. It was observed that increasing air velocity beyond 3 m/s does not enhance adsorption. Additionally, utilizing a solar thermal cycle to produce steam can further decrease the system's overall energy cost.

On the other hand, the economic modelling of the Direct Air Capture (DAC) system includes the operation and maintenance (O&M) costs, which cover energy and the loading/unloading of the sorbent ($\mathbf{N_{O\&M}}$), and the scrap value of the sorbent at the end of its lifetime ($\mathbf{N_S}$). The scrap value ($\mathbf{N_S}$) is calculated as the sum of the sorbent price ($\mathbf{V_s}$) and the installation cost ($\mathbf{I_s}$). The hardware cost is also considered, making the capital cost of the plant ($\mathbf{N_{BoP}}$) part of the running expenses. The net present value (NPV) of the DAC system is determined by eq (8). For the system to be economically viable, the NPV must be zero or greater at some point during operation. To find the lifetime ($\mathbf{t_{life}}$) of the system, the first derivative of the NPV equation with respect to time is set to zero in eq (9). Key takeaways include that the NPV starts negatively due to the initial sorbent cost, increases with revenue from captured $CO_2$, and $\mathbf{t_{life}}$ is the point where the NPV reaches its maximum. The revenue generated per unit of time is calculated using eq (10).

The economic analysis indicates that MOFs can significantly reduce storage costs compared to traditional methods. The study evaluated the lifecycle costs of MOF-based storage systems and found that they offer competitive advantages in terms of both capital and operational expenses. This makes MOFs a cost-effective option for carbon capture.

**Acknowledgment. -** The Authors acknowledge the support provided by Sindh Higher Education Commission through the project SRSP/NPS SC. & Tech-09/314/2023-24.

## References

[1] R. A. Kerr, “It’s Official: Humans Are Behind Most of Global Warming,” Science, vol. 291, no. 5504, pp. 566–566, Jan. 2001, doi: 10.1126/science.291.5504.566A.

[2] A. Kaithwas, M. Prasad, A. Kulshreshtha, and S. Verma, “Industrial wastes derived solid adsorbents for CO2 capture: A mini review,” Chem. Eng. Res. Des., vol. 90, no. 10, pp. 1632–1641, Oct. 2012, doi: 10.1016/j.cherd.2012.02.011.

[3] S. A. Montzka, E. J. Dlugokencky, and J. H. Butler, “Non-CO2 greenhouse gases and climate change,” Nature, vol. 476, no. 7358, pp. 43–50, Aug. 2011, doi: 10.1038/nature10322.

[4] R. Checa-Garcia, K. P. Shine, and M. I. Hegglin, “The contribution of greenhouse gases to the recent slowdown in global-mean temperature trends,” Environ. Res. Lett., vol. 11, no. 9, p. 094018, Sep. 2016, doi: 10.1088/1748-9326/11/9/094018.

[5] J. G. Canadell et al., “Contributions to accelerating atmospheric CO 2 growth from economic activity, carbon intensity, and efficiency of natural sinks,” Proc. Natl. Acad. Sci., vol. 104, no. 47, pp. 18866–18870, Nov. 2007, doi: 10.1073/pnas.0702737104.

[6] Y. Wu, J. Xu, K. Mumford, G. W. Stevens, W. Fei, and Y. Wang, “Recent advances in carbon dioxide capture and utilization with amines and ionic liquids,” Green Chem. Eng., vol. 1, no. 1, pp. 16–32, Sep. 2020, doi: 10.1016/j.gce.2020.09.005.

[7] J. Zhang, S. Wang, X. Cheng, C. Chen, L. Zhang, and Z. Wang, “Design strategies and advantages of metal-organic frameworks@ lignocellulose-based composite aerogel for CO2 capture: A review,” Sep. Purif. Technol., vol. 356, p. 129878, Apr. 2025, doi: 10.1016/j.seppur.2024.129878.

[8] A. Sodiq et al., “A review on progress made in direct air capture of CO2,” Environ. Technol. Innov., vol. 29, p. 102991, Feb. 2023, doi: 10.1016/j.eti.2022.102991.

[9] M. Liu et al., “Recent advances and principles of metal–organic framework for the detection of chloramphenicol: Perspectives and challenges,” Microchem. J., vol. 207, p. 111878, Dec. 2024, doi: 10.1016/j.microc.2024.111878.

[10] Y. An et al., “The stability of MOFs in aqueous solutions—research progress and prospects,” Green Chem. Eng., vol. 5, no. 2, pp. 187–204, Jun. 2024, doi: 10.1016/j.gce.2023.07.004.

[11] I. K. Shah, P. Pre, and B. J. Alappat, “Steam Regeneration of Adsorbents: An Experimental and Technical Review,” Chem. Sci. Trans., vol. 2, no. 4, Oct. 2013, doi: 10.7598/cst2013.545.

[12] A. Sinha, L. A. Darunte, C. W. Jones, M. J. Realff, and Y. Kawajiri, “Systems Design and Economic Analysis of Direct Air Capture of CO2 through Temperature Vacuum Swing Adsorption using MIL-101(Cr)-PEI-800 and mmen-Mg2(dobpdc) MOF Adsorbents”.

[13] J. K. Stolaroff, D. W. Keith, and G. V. Lowry, “Carbon dioxide capture from atmospheric air using sodium hydroxide spray: Supporting Information”.

[14] “Sodium Hydroxide-Based CO2 Direct Air Capture for Soda Ash Production─Fundamentals for Process Engineering | Industrial & Engineering Chemistry Research.” Accessed: Sep. 25, 2024. [Online]. Available: https://pubs.acs.org/doi/10.1021/acs.iecr.3c00357

[15] K. Heidel, D. Keith, A. Singh, and G. Holmes, “Process design and costing of an air-contactor for air-capture,” Energy Procedia, vol. 4, pp. 2861–2868, Jan. 2011, doi: 10.1016/j.egypro.2011.02.192.

[16] P. Tabarzadi and A. Ghaemi, “Modeling and optimization of CO2 capture in spray columns via artificial neural networks and response surface methodology,” Case Stud. Chem. Environ. Eng., vol. 10, p. 100783, Dec. 2024, doi: 10.1016/j.cscee.2024.100783.

[17] M. Mahmoudkhani and D. W. Keith, “Low-energy sodium hydroxide recovery for CO2 capture from atmospheric air—Thermodynamic analysis,” Int. J. Greenh. Gas Control, vol. 3, no. 4, pp. 376–384, Jul. 2009, doi: 10.1016/j.ijggc.2009.02.003.

[18] W. R. Lee et al., “Exceptional CO 2 working capacity in a heterodiamine-grafted metal–organic framework,” Chem. Sci., vol. 6, no. 7, pp. 3697–3705, 2015, doi: 10.1039/C5SC01191D.

[19] L. A. Darunte, K. S. Walton, D. S. Sholl, and C. W. Jones, “CO2 capture via adsorption in amine-functionalized sorbents,” Curr. Opin. Chem. Eng., vol. 12, pp. 82–90, May 2016, doi: 10.1016/j.coche.2016.03.002.

[20] D. Wu et al., “Thermodynamic complexity of carbon capture in alkylamine-functionalized metal–organic frameworks,” J. Mater. Chem. A, vol. 3, no. 8, pp. 4248–4254, Feb. 2015, doi: 10.1039/C4TA06496H.

[21] Z. Yuan, M. R. Eden, and R. Gani, “Toward the Development and Deployment of Large-Scale Carbon Dioxide Capture and Conversion Processes,” Ind. Eng. Chem. Res., vol. 55, no. 12, pp. 3383–3419, Mar. 2016, doi: 10.1021/acs.iecr.5b03277.

[22] “Maximum and Comparative Efficiency Calculations for Integrated Capture and Electrochemical Conversion of CO2 | ACS Energy Letters.” Accessed: Sep. 24, 2024. [Online]. Available: https://pubs.acs.org/doi/10.1021/acsenergylett.3c02489

[23] L. Joss, M. Hefti, Z. Bjelobrk, and M. Mazzotti, “On the Potential of Phase-change Adsorbents for CO2 Capture by Temperature Swing Adsorption,” Energy Procedia, vol. 114, pp. 2271–2278, Jul. 2017, doi: 10.1016/j.egypro.2017.03.1375.

[24] A. Ntiamoah, J. Ling, P. Xiao, P. A. Webley, and Y. Zhai, “CO2 Capture by Temperature Swing Adsorption: Use of Hot CO2-Rich Gas for Regeneration,” Ind. Eng. Chem. Res., vol. 55, no. 3, pp. 703–713, Jan. 2016, doi: 10.1021/acs.iecr.5b01384.

[25] E. S. Sanz-Pérez, C. R. Murdock, S. A. Didas, and C. W. Jones, “Direct Capture of CO 2 from Ambient Air,” Chem. Rev., vol. 116, no. 19, pp. 11840–11876, Oct. 2016, doi: 10.1021/acs.chemrev.6b00173.

[26] J. A. Mason, K. Sumida, Z. R. Herm, R. Krishna, and Jeffrey. R. Long, “Evaluating metal–organic frameworks for post-combustion carbon dioxide capture via temperature swing adsorption,” Energy Environ. Sci., vol. 4, no. 8, p. 3030, 2011, doi: 10.1039/c1ee01720a.

[27] “Electrochemical Approaches for CO2 Conversion to Chemicals: A Journey toward Practical Applications | Accounts of Chemical Research.” Accessed: Sep. 25, 2024. [Online]. Available: https://pubs.acs.org/doi/10.1021/acs.accounts.1c00674

[28] “Techno-economic Analysis of Metal–Organic Frameworks for Hydrogen and Natural Gas Storage | Energy & Fuels.” Accessed: Sep. 24, 2024. [Online]. Available: https://pubs.acs.org/doi/10.1021/acs.energyfuels.6b02510

[29] T. Ahmed, “Chapter 3 - Natural Gas Properties,” in Equations of State and PVT Analysis (Second Edition), T. Ahmed, Ed., Boston: Gulf Professional Publishing, 2016, pp. 189–238. doi: 10.1016/B978-0-12-801570-4.00003-9.

[30] M. S. Shafeeyan, W. M. A. Wan Daud, and A. Shamiri, “A review of mathematical modeling of fixed-bed columns for carbon dioxide adsorption,” Chem. Eng. Res. Des., vol. 92, no. 5, pp. 961–988, May 2014, doi: 10.1016/j.cherd.2013.08.018.

[31] J. L. Plawsky, M. Ojha, A. Chatterjee, and P. Wayner, “Review of the effects of surface topography, surface chemistry, and fluid physics on evaporation at the contact line,” Chem. Eng. Commun., vol. 196, pp. 658–696, May 2009, doi: 10.1080/00986440802569679.

[32] “Water and Metal–Organic Frameworks: From Interaction toward Utilization | Chemical Reviews.” Accessed: Sep. 25, 2024. [Online]. Available: https://pubs.acs.org/doi/10.1021/acs.chemrev.9b00746

[33] “CO2 capture materials: a review of current trends and future challenges - ScienceDirect.” Accessed: Sep. 25, 2024. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S2589234723001690

[34] J. L. Woodliffe et al., “Continuous flow synthesis of MOF UTSA-16(Zn), mixed-metal and magnetic composites for CO2 capture – toward scalable manufacture,” J. Environ. Chem. Eng., vol. 12, no. 6, p. 114167, Dec. 2024, doi: 10.1016/j.jece.2024.114167.

[35] M. Kong et al., “A review on development of post-combustion CO2 capture technologies: Performance of carbon-based, zeolites and MOFs adsorbents,” Fuel, vol. 371, p. 132103, Sep. 2024, doi: 10.1016/j.fuel.2024.132103.

[36] Z. Deng and L. Sarkisov, “Multi-Scale Computational Design of Metal–Organic Frameworks for Carbon Capture Using Machine Learning and Multi-Objective Optimization,” Chem. Mater., vol. 36, no. 19, pp. 9806–9821, Oct. 2024, doi: 10.1021/acs.chemmater.4c01969.

**Author contribution:**
1. Conception and design of the study
2. Data acquisition
3. Data analysis
4. Discussion of the results
5. Writing of the manuscript
6. Approval of the last version of the manuscript

MMUZS has contributed to: 1, 2, 3, 4, 5 and 6.
AT has contributed to: 1, 2, 3, 4, 5 and 6.

**Acceptance Note:** This article was approved by the journal editors Dr. Rafael Sotelo and Mag. Ing. Fernando A. Hernández Gobertti.