inventions

Review

Comparative Assessment and Deployment of Zeolites, MOFs, and Activated Carbons for CO_2 Capture and Geological Sequestration Applications

Mohamadou Hamadama Mouctar [1], Mohamed G Hassan [1,*], Nuno Bimbo [1], Syed Zaheer Abbas [1] and Ihab Shigidi [2]

[1] School of Chemistry and Chemical Engineering, Faculty of Engineering and Physical Sciences, University of Southampton, Southampton SO17 1BJ, UK; m.z.hamadama-mouctar@soton.ac.uk (M.H.M.); n.bimbo@soton.ac.uk (N.B.); s.z.abbas@soton.ac.uk (S.Z.A.)

[2] Chemical Engineering Department, King Khalid University, P.O. Box 394, Abha 61411, Saudi Arabia; etaha@kku.edu.sa

* Correspondence: mghs1v19@soton.ac.uk

Abstract

The rising level of atmospheric carbon dioxide (CO_2) is a major driver of climate change, highlighting the need to develop carbon capture and storage (CCS) technologies quickly. This paper offers a comparative review of three main groups of porous adsorbent materials—zeolites, metal–organic frameworks (MOFs), and activated carbons—for their roles in CO_2 capture and long-term storage. By examining their structural features, adsorption capacities, moisture stability, and economic viability, the strengths and weaknesses of each material are assessed. Additionally, five different methods for delivering these materials into depleted oil and gas reservoirs are discussed: direct suspension injection, polymer-assisted transport, foam-assisted delivery, encapsulation with controlled release, and preformed particle gels. The potential of hybrid systems, such as MOF–carbon composites and polymer-functionalized materials, is also examined for improved selectivity and durability in underground environments. This research aims to connect materials science with subsurface engineering, helping guide the selection and use of adsorbent materials in real-world CCS applications. The findings support the optimization of CCS deployment and contribute to broader climate change efforts and the goal of achieving net-zero emissions. Key findings include CO_2 adsorption capacities of 3.5–8.0 mmol/g and surface areas up to 7000 m^2/g, with MOFs demonstrating the highest uptake and activated carbons offering cost-effective performance.

Keywords: zeolites; metal–organic frameworks; activated carbons; carbon capture; geological sequestration; delivery mechanisms; hybrid materials

Academic Editors: Said Al-Hallaj and Alessandro Dell'Era

Received: 24 June 2025
Revised: 29 July 2025
Accepted: 22 August 2025
Published: 28 August 2025

Citation: Mouctar, M.H.; Hassan, M.G.; Bimbo, N.; Abbas, S.Z.; Shigidi, I. Comparative Assessment and Deployment of Zeolites, MOFs, and Activated Carbons for CO_2 Capture and Geological Sequestration Applications. *Inventions* **2025**, *10*, 78. https://doi.org/10.3390/inventions10050078

1. Introduction

Carbon dioxide (CO_2) emissions have reached unprecedented levels in recorded human history, posing a formidable challenge to global climate stability. According to the Intergovernmental Panel on Climate Change (IPCC, 2023) [1], atmospheric CO_2 concentrations now exceed those observed at any time in the past two million years, driven primarily by industrial processes, fossil fuel combustion, and land-use change. This alarming trajectory has catalyzed a global consensus on the urgent need to mitigate greenhouse gas emissions through innovative technological interventions.

Among the most promising mitigation strategies is carbon capture and storage (CCS)—a suite of technologies aimed at isolating CO_2 emissions at their source, transporting the captured gas to appropriate geological sites, and injecting it deep underground for long-term containment. CCS has become particularly critical in hard-to-abate sectors such as cement production, steel manufacturing, and petrochemical refining, where emissions are process-related and cannot be fully eliminated through electrification alone [2,3].

A fundamental aspect of effective CCS implementation lies in the choice of sorbent material for capturing CO_2 and the method of delivering it into subsurface storage environments. Historically, CCS systems have relied on amine-based liquid solvents, which chemically bind with CO_2 under ambient or pressurized conditions. While these solvents offer relatively high capture efficiency, they come with several drawbacks, including high energy demand for regeneration, limited thermal stability, degradation over multiple cycles, and corrosive behavior that complicates plant operation and maintenance [4].

In contrast, solid porous adsorbents—including zeolites, metal–organic frameworks (MOFs), and activated carbons—have gained significant attention due to their superior physicochemical characteristics. Compared to conventional amine-based solvents, these materials offer significantly lower regeneration energy requirements, enhanced moisture resistance, and a substantially reduced environmental footprint across their lifecycle. These advantages position them as compelling alternatives for next-generation CCS applications, particularly in scenarios that demand resilience, cost-effectiveness, and scalability.

Solid adsorbents exhibit a diverse range of performance profiles. Zeolites are widely regarded for their structural robustness, affordability, and high selectivity under dry conditions. MOFs stand out for their tunable chemistry and exceptionally high surface areas, often exceeding 6000 m^2/g, which facilitate superior gas uptake capacities. Activated carbons, especially those derived from biomass, present a sustainable and economically viable solution with excellent tolerance to moisture and contaminants. Recent studies (e.g., Refs. [5,6] affirm the scalability and operational resilience of these materials under realistic field conditions.

However, the method of delivering these adsorbents into the target geological formation is as important as the material choice itself. Options include direct aqueous suspension injection, polymer-assisted transport, foam-based delivery, and advanced encapsulation or gel-based systems—all of which influence the material's placement, stability, and long-term sequestration efficacy [7].

This paper provides a comparative assessment of the most promising classes of porous adsorbents—zeolites, MOFs, and activated carbons—by analyzing their structural attributes, CO_2 adsorption properties, moisture and thermal stability, and regeneration behavior. It also critically examines delivery mechanisms and explores hybrid systems that combine the advantages of multiple materials to overcome individual limitations. The aim is to develop a practical framework for adsorbent selection and deployment, enabling the design of efficient and sustainable CCS strategies tailored to site-specific geological and operational conditions.

Ultimately, this review supports the broader effort to decarbonize industrial processes and achieve net-zero emissions by mid-century. Aligning material science innovations with subsurface engineering practices offers actionable insights for researchers, practitioners, and policymakers engaged in advancing climate mitigation technologies.

2. Background on Porous Materials for CO_2 Capture

Porous materials are crucial for carbon capture and storage (CCS) due to their ability to adsorb CO_2 from gas mixtures selectively. These materials use two main mechanisms for gas capture: physisorption and chemisorption. Physisorption involves weak van der

Waals forces and is usually characterized by rapid, reversible adsorption that requires low energy. This process is common in materials like activated carbons and many zeolites [6]. Conversely, chemisorption involves stronger chemical bonds between CO_2 molecules and functional groups on the surface, such as amines, leading to higher selectivity but often requiring more energy for desorption [8].

An ideal CO_2 adsorbent must balance several essential properties: high CO_2 uptake capacity, selectivity over gases like N_2 and CH_4, low regeneration energy, long-term stability under various environmental conditions, and scalable synthesis methods. Furthermore, surface area and pore size distribution are crucial factors affecting adsorption capacity. For example, micropores (<2 nm) generally provide high selectivity, while mesopores (2–50 nm) allow for faster diffusion and access to internal active sites [9]. Materials such as zeolites, metal–organic frameworks (MOFs), and activated carbons each offer distinct strategies to achieve these performance goals. Zeolites, which are crystalline aluminosilicates, feature well-defined pore structures and cation exchange capabilities. MOFs allow for extensive tuning through the selection of organic linkers and metal nodes, enabling precise functionalization [10]. Activated carbons, although less structurally uniform, are cost-effective and highly durable under harsh conditions [5].

As this review continues, the distinct strengths and limitations of each material type will be explored in detail. This foundational knowledge is vital for understanding how these materials can be effectively delivered into geological formations for permanent CO_2 sequestration.

2.1. Methodology and Evaluation Criteria

To quantitatively compare the performance of zeolites, metal–organic frameworks (MOFs), and activated carbons as CO_2 adsorbents, a radar chart (as seen in Figure 1 and Table 1) was created. The chart evaluates five key properties that influence the effectiveness of adsorbents in CCS applications: surface area, moisture resistance, ease of regeneration, cost (inverted, with higher values indicating lower relative cost), and CO_2 adsorption capacity. Zeolites demonstrate strong ease of regeneration and cost-effectiveness, but their performance is limited by low moisture resistance [8]. MOFs have the highest surface area and CO_2 uptake potential; however, their high cost and moderate regeneration requirements may restrict scalability [11]. Activated carbons offer a balanced profile with excellent moisture resistance, low cost, and good regeneration capabilities, though they generally have lower CO_2 selectivity compared to MOFs or zeolites [12]. This comparison highlights the trade-offs involved in selecting materials and supports the idea of hybrid systems that combine different adsorbents to maximize overall effectiveness across various geological conditions.

Table 1. Performance Comparison of Zeolites, MOF + C5:I16s, and Activated Carbons for CO_2 Capture and Storage Applications.

Property	Unit	Zeolites	MOFs	Activated Carbons	Normalization Notes	References
Surface Area	m^2/g	300–800	1000–7000	500–2500	Normalized from 300 (1) to 7000 (5)	[3,5,13]
Moisture Resistance	Qualitative	Low to Moderate	Variable (depends on MOF type)	High	Assigned ordinal scale (1–5) based on range	[3,12,14]
Regeneration Ease	Qualitative	High (via TSA/PSA)	Moderate to High (depends on MOF)	High	Based on regeneration temperature/load	[3,11,12]

Table 1. *Cont.*

Property	**Unit**	**Zeolites**	**MOFs**	**Activated Carbons**	**Normalization Notes**	**References**
Cost (Inverse)	USD/kg	~2–10	~100–500	~1–5	Inverted scale: higher cost = lower score	[2,12,14]
CO_2 Adsorption Cap.	mmol/g	3.5–5.0	5.0–8.0	3.0–5.0	Normalized from 3 (1) to 8 (5)	[2,5,11]
Normalized Scores (Used in Radar Chart Figure 1)						
Material	Surface Area	Moisture Resistance	Regeneration Ease	Cost (Inverse)	CO_2 Adsorption	
Zeolites	2	2	5	5	4	
MOFs	5	3	4	2	5	
Activated Carbon	3	5	4	5	3	

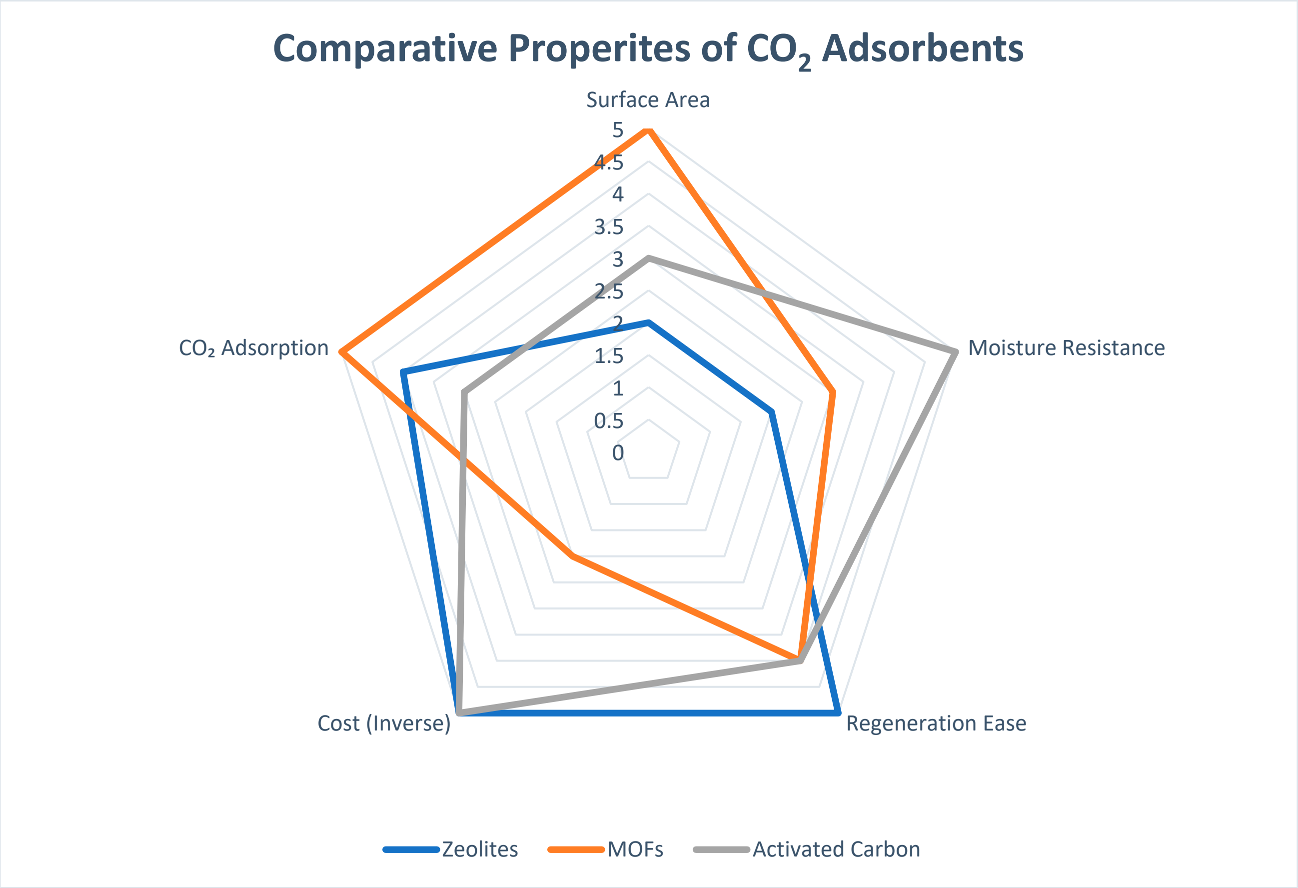


Figure 1. Radar chart comparing the performance features of zeolites, metal–organic frameworks (MOFs), and activated carbons for CO_2 capture and geological storage. The five evaluated criteria include surface area, moisture resistance, ease of regeneration, inverse cost (where higher values mean lower price), and CO_2 adsorption capacity. The data are normalized on a 1–5 scale based on typical literature-reported values. The chart highlights the strengths and weaknesses of each material type, emphasizing the potential advantages of hybrid adsorbent systems.

2.2. Definition of Properties

2.2.1. Surface Area (m^2/g)

Definition and Relevance: Surface area refers to the accessible internal surface of a material, typically measured in m^2/g. In CCS, higher surface areas provide more physisorption sites, increasing CO_2 absorption capacity. The BET method is commonly used to measure this.

Implications for CO_2 Capture: as seen in Table 1, MOFs often exceed 6000 m^2/g, offering excellent gas adsorption. Zeolites (300–800 m^2/g) and activated carbons (500–2500 m^2/g) have smaller surface areas, but their effectiveness depends more on pore accessibility and chemical functionality than on size alone. In geological sequestration, surface area directly influences adsorption efficiency under limited reservoir conditions.

2.2.2. CO_2 Adsorption Capacity (mmol/g)

Definition and Relevance: These measure the amount of CO_2 a material can hold per gram, expressed in millimoles. It is determined under standard pressure and temperature to allow for comparisons across materials.

Implications for CO_2 Capture: As seen in Table 1, high capacity reduces material volume and cost per ton of CO_2. MOFs lead with 5.5–8.0 mmol/g, followed by zeolites (3.5–5.0 mmol/g), and activated carbons (3.3–5.0 mmol/g). For subsurface injection, this parameter indicates the mass efficiency of the slurry or sorbent suspension.

2.2.3. Regeneration Ease

Definition and Relevance: Regeneration ease refers to the energy and process conditions needed to desorb CO_2, allowing for the material to be reused. Methods include TSA, PSA, and VSA.

Implications for CCS: Efficient regeneration lowers energy consumption and costs. Zeolites and activated carbons typically regenerate well with TSA/PSA. Though many MOFs have high uptake, they may degrade or require strict conditions, which can limit cyclic or field applications.

2.2.4. Cost (Inverse Scale, USD/kg)

Definition and Relevance: Material cost factors in synthesis complexity, precursor availability, and market scalability. Costs are inverted, so cheaper materials score higher.

Implications for CO_2 Capture: MOFs are costly (USD 100–500/kg), as seen in Table 1, due to complex synthesis and limited production. Zeolites (USD 2–10/kg) and activated carbons (~USD 1–5/kg) are more affordable and well-established. Cost per kilogram significantly influences system economics, especially for large-scale injections into reservoirs.

2.2.5. Moisture Resistance

Definition and Relevance: Moisture resistance evaluates a material's ability to maintain CO_2 adsorption in humid or aqueous environments, common in post-combustion capture and subsurface reservoirs.

Implications for CO_2 Capture: Zeolites' hydrophilicity can hinder CO_2 uptake because of water competition. MOFs' moisture tolerance varies depending on metal–ligand bonds and hydrophobicity. Activated carbons, being inherently hydrophobic, perform reliably in humid conditions. For long-term sequestration in aquifers or depleted reservoirs, moisture resistance is essential for stability and performance.

Performance data for each material type were compiled from a broad review of peer-reviewed sources. Because these properties span different units and magnitudes (e.g., surface area in m^2/g, cost in £/kg), a min–max normalization approach was used to enable comparative visualization. For each property, the minimum and maximum values across all three material classes were identified from the literature, and each value was rescaled to a normalized 1–5 scale, as per Equation (1). Each score on the radar chart is calculated using min–max normalization. For each performance metric, the minimum and maximum values across zeolites, MOFs, and activated carbons were scaled to a 1–5 range. References were used to ensure data consistency and relevance.

Equation (2) introduces a weighted scoring model for prioritizing adsorbents based on project-specific criteria (e.g., cost, capacity). Default weights can be adjusted to reflect technical or policy-driven priorities. This equation enables comparative ranking of adsorbents by emphasizing or downplaying certain attributes. The resulting score S_i supports application-specific deployment strategies by allowing decision-makers to identify trade-offs and synergies in adsorbent performance.

Equation (1): normalized score equation to scale the performance value of a polymer.

$$\text{Normalized score} = 1 + 4 \times \left(\frac{\text{Value} - \text{Min}}{\text{Max} - \text{Min}} \right) \tag{1}$$

Equation (2): Weighted Scoring Model for Adsorbent Evaluation.

$$S_i = \sum_{j=1}^{n} \left(w_j \times N_{ij} \right) \tag{2}$$

where

S_i = Total weighted score for material i (e.g., MOF, Zeolite, Activated Carbon);

N_{ij} = Normalized score (on 1–5 scale) of material i on criterion j;

w_j = Weight assigned to criterion j (e.g., cost, capacity, moisture resistance);

n = Total number of performance criteria;

$\sum w_j = 1$ (weights sum to 1).

MOFs with surface areas exceeding 6000 m^2/g received a top score of 5, while zeolites with typical areas around 700 m^2/g were scored lower on that axis. Conversely, cost data were inverted so that more affordable materials, such as activated carbon, scored higher (e.g., 5), while MOFs, which remain costly to synthesize, received a lower score. This normalization enables a balanced and interpretable graphical comparison, allowing decision-makers to identify trade-offs and synergies in adsorbent performance. Zeolites show strong ease of regeneration and cost-effectiveness, but limited moisture resistance. MOFs excel in surface area and CO_2 uptake but are hindered by higher costs and moderate stability. Activated carbons offer robust moisture resistance, low cost, and good regeneration, though they lag slightly in adsorption capacity and selectivity. This comparative analysis illustrates that no single material dominates all categories, supporting the rationale for hybrid systems or application-specific deployment strategies that combine complementary material properties.

3. Comparative Performance of Zeolites, MOFs, and Activated Carbons

Pore structure plays a key role in determining CO_2 adsorption and diffusion rates. Micropores (<2 nm) enhance selectivity while mesopores (2–50 nm) facilitate diffusion, with optimal performance often achieved through hierarchical structures.

3.1. Zeolites

Pore structure is a fundamental determinant of CO_2 adsorption efficiency and transport behavior in porous materials. Micropores (<2 nm) provide a high surface-to-volume ratio, promoting strong confinement effects and molecular selectivity—particularly for CO_2 over competing gases, such as N_2 and CH_4. However, the small pore size can hinder gas diffusion, especially under dynamic flow conditions. In contrast, mesopores (2–50 nm) improve diffusional accessibility and reduce mass transfer resistance. Thus, hierarchical zeolites—engineered to combine microporous and mesoporous domains—offer enhanced CO_2 capture by balancing selectivity and kinetics, particularly under industrial-scale flow rates.

Zeolites, a class of crystalline aluminosilicates, are among the most widely used solid adsorbents for CO_2 capture. Their structure comprises a three-dimensional framework of SiO_4 and AlO_4 tetrahedra, forming uniform microporous channels and cavities. The substitution of Si^{4+} with Al^{3+} imparts a net negative framework charge, which is balanced by exchangeable cations such as Na^+, K^+, or Ca^{2+}. This configuration enhances electrostatic interactions with polar molecules, making zeolites particularly effective in post-combustion CCS systems.

Recent advances in zeolite design have focused on improving mass transport and stability under practical operating conditions. Post-synthetic treatments—such as dealumination, desilication, and ion exchange—and template-assisted synthesis have been used to create hierarchical zeolites with interconnected mesopores embedded in the microporous framework. These modifications significantly increase diffusion rates and allow for higher working capacities under pressure swing (PSA), temperature swing (TSA), or vacuum swing (VSA) adsorption cycles.

Zeolites also score highly on sustainability metrics. They are synthesized from abundant and low-cost feedstocks, such as natural clays, volcanic tuffs, or industrial byproducts like fly ash [8]. Their recyclability, low toxicity, and ease of regeneration align well with circular economy and green chemistry principles.

Among the many zeolite types, Zeolite 13X (a FAU-type structure) stands out due to its relatively large micropore diameter (~0.74 nm), high surface area (~700 m^2/g), and CO_2 adsorption capacity of ~4.5–5.0 mmol/g under dry flue gas conditions [10]. Other variants, such as Zeolite 5A, ZSM-5, and SAPO-34, also demonstrate strong performance, depending on the target gas stream and operating conditions (Tables 2 and 3).

Table 2. Physicochemical properties and performance metrics of selected zeolites for CO_2 capture applications. This table summarizes the key characteristics of common zeolite materials, including surface area, CO_2 adsorption capacity, regeneration potential, moisture and thermal stability, regeneration energy, and the energy requirements for regeneration materials and industrial scalability. These metrics provide a comparative framework for evaluating the suitability of zeolites in carbon capture and subsurface injection scenarios.

Parameter	**Zeolite 13X**	**Zeolite 4A (Na-A)**	**ZSM-5 (MFI-Type)**	**Zeolite Y**	**SAPO-34**
BET Surface Area (m^2/g)	~600–700	~400–500	~350–450	~600–800	~550–650
CO_2 Adsorption Capacity (mmol/g)	~4.5–5.0	~3.0–3.5	~2.5–3.5	~4.0–4.5	~3.5–4.0
Regenerability	Very High	Very High	Very High	Very High	High
Stability in Humid Conditions	Excellent	Excellent	Good	Excellent	Moderate
Thermal Stability	Up to ~700 °C	~500–600 °C	~800 °C	~700 °C	~600 °C
Chemical Stability	Excellent (alkaline-sensitive)	Excellent	Excellent	Moderate-to-Good	Moderate
Regeneration Energy (kJ/mol CO_2)	~20–30	~25–30	~30–40	~25–35	~25–35
Regeneration Method	TSA, PSA, VSA	TSA, PSA, VSA	TSA, PSA, VSA	TSA, PSA	TSA, PSA
Production Cost	Low	Very Low	Low to Moderate	Moderate	Moderate
Scalability	High	High	High	High	Moderate
Industrial Viability	Excellent	Excellent	Excellent	High	Good
References	[13]	[15]	[14]	[10]	[16]

Table 3. Performance characteristics of representative metal–organic frameworks (MOFs) for CO_2 adsorption and regeneration. The table displays surface areas, CO_2 uptake capacities, regeneration methods, stability profiles, and techno-economic considerations for selected MOFs. These parameters highlight the trade-offs and application-specific benefits of MOFs in CCS technologies, particularly under varying humidity and thermal conditions.

Parameter	**MOF-74**	**MOF-199 (HKUST-1)**	**MOF-177**	**UiO-66**
BET Surface Area (m^2/g)	1100–1500	1400–1800	4500–5100	1000–1500
CO_2 Adsorption Capacity (mmol/g)	Up to 8.0	~5.0–6.0	~6.0–7.5	~2.5–4.0
Regenerability	High	High	High (dry only)	Very High
Stability in Humid Conditions	Moderate to Poor	Poor	Poor	Excellent
Thermal Stability (°C)	~300–400	~240–300	~350	~500–550
Chemical Stability	Moderate	Limited	Limited	Very High
Regeneration Energy (kJ/mol CO_2)	~30–40	~25–35	~30–40	~20–30
Regeneration Method	TSA, PSA, VSA	TSA, PSA, VSA	TSA, PSA, VSA	TSA, PSA, VSA
Production Cost (USD /kg)	Moderate–High	Moderate	Moderate–High	Moderate
Scalability	Moderate	High	Limited	High
Industrial Viability	Promising (dry gases)	Promising (dry gases)	Limited	Excellent
References	[17]	[18]	[19]	[6]

However, a primary limitation of zeolites is their hydrophilicity, which results in competitive water adsorption under humid conditions. This significantly reduces CO_2 uptake in real-world flue gases. To mitigate this, researchers have explored hydrophobic zeolites like Silicalite-1 and amine-functionalized zeolites, which enhance both moisture resistance and CO_2 selectivity.

Zeolites are further valued for their thermal and chemical stability, enabling long-term regeneration cycles without significant degradation. This makes them suitable for demanding industrial environments, including natural gas purification, air separation, and flue gas scrubbing [8].

Uptake under humid conditions. To address this, researchers have explored hydrophobic zeolites, such as Silicalite-1, and functionalized them with amine groups to improve moisture resistance and CO_2 selectivity. Zeolites are also advantageous due to their thermal and chemical stability, allowing for repeated regeneration through thermal or pressure swing adsorption processes. This durability makes them suitable for long-term industrial applications, including natural gas purification, air separation, and environmental remediation [8].

Recent advancements include the development of hierarchical zeolites with mesoporous structures to enhance diffusion and adsorption kinetics, as well as composite materials that incorporate zeolite frameworks with other porous materials, such as MOFs or graphene, to leverage synergistic properties [12].

Overall, zeolites remain a cornerstone material in gas separation technologies due to their well-established performance, scalability, and cost-effectiveness, despite some challenges in humid environments.

This indicates a need to consider zeolites, which are crystalline aluminosilicates characterized by a three-dimensional framework of SiO_4 and AlO_4 tetrahedra. Their uniform microporous structures (typically 0.3–1.2 nm) and high thermal stability make them suitable for CO_2 capture and separation [8]. Zeolites, such as 13X and 5A, demonstrate high selectivity for CO_2 over other gases, like N_2, due to their surface polarity and ion-exchange capabilities. However, their adsorption performance can be negatively affected by moisture, although some zeolite structures exhibit substantial hydrothermal stability [12].

3.2. Metal–Organic Frameworks (MOFs)

Interestingly, a growing body of research is investigating the use of MOFs in dynamic gas environments, such as real-time CO_2 capture from automobile exhaust or fluctuating emissions from chemical plants. These studies aim to understand the structural integrity of MOFs under repeated adsorption–desorption cycles, particularly under conditions involving moisture and elevated temperatures.

It is also essential to highlight the versatility of MOFs in multifunctional applications. Some MOFs have been developed to adsorb gases simultaneously and catalyze chemical reactions, such as the conversion of captured CO_2 into valuable hydrocarbons or alcohols. This dual functionality positions MOFs at the boundary of integrated carbon capture and utilization (CCU) systems.

Metal–organic frameworks (MOFs) are a class of crystalline materials composed of metal ions or clusters coordinated to organic linkers, forming highly porous structures with exceptional surface areas and tunable pore sizes. Their modular construction enables precise control over chemical functionality and structural topology, making them ideal candidates for gas adsorption and separation applications [11].

One of the most notable characteristics of MOFs is their ultrahigh surface area, with materials such as MOF-210 and NU-110 achieving values exceeding 6000 m^2/g. This high surface area, combined with tuneable pore dimensions (typically 0.3–3+ nm), facilitates the adsorption of a variety of gases, including CO_2, CH_4, and H_2 [10,20]. From an applied standpoint, as seen in Table 3, MOFs such as HKUST-1 (Cu-BTC), ZIF-8, and UiO-66 have been widely studied due to their favorable adsorption characteristics and structural stability.

MOFs also demonstrate high selectivity for CO_2 over other gases due to their ability to incorporate functional groups such as amines, azoles, and hydroxyls that enhance CO_2 affinity. For instance, amine-functionalized MOFs, such as mmen-Mg_2(dobpdc), exhibit exceptional performance for post-combustion CO_2 capture under low partial pressures.

Despite their outstanding properties, a key limitation of many metal–organic frameworks (MOFs) is their sensitivity to moisture. Some MOFs, particularly those with unsaturated metal centers, degrade in humid environments, limiting their industrial applicability. This suggests, however, that recent advancements in the development of water-stable MOFs, such as UiO-66 (based on Zr clusters) [6], have significantly enhanced their practical application potential.

The regeneration of MOFs after gas adsorption is typically achieved through temperature or pressure swing processes. Some MOFs also show reversible adsorption behaviors, which is advantageous for cyclic operations. However, the cost of synthesis and scale-up challenges remain significant barriers to widespread adoption.

Ongoing research efforts are focusing on improving the hydrothermal stability of MOFs, developing cost-effective synthesis methods, and exploring hybrid materials that combine MOFs with other porous frameworks or polymers for enhanced performance [11].

In summary, MOFs represent one of the most promising material classes for gas storage and separation due to their high surface area, tunable chemistry, and structural versatility. With continued advancements in stability and scalability, MOFs have the potential to revolutionize carbon capture and clean energy technologies.

MOFs are crystalline materials formed by the coordination of metal ions or clusters with organic ligands. They are notable for their ultrahigh surface areas (up to 7000 m^2/g)

and tunable pore sizes [11]. These features allow for the precise tailoring of MOFs for selective gas adsorption, including CO_2, H_2, and CH_4. This suggests the need to consider MOFs such as MOF-5, ZIF-8, and HKUST-1, which have demonstrated exceptional gas uptake properties under optimized conditions. However, the stability of MOFs under humid or acidic conditions can be a limiting factor in industrial applications.

3.3. Activated Carbons

Activated carbons also offer exceptional promise in applications requiring rapid adsorption kinetics, such as respiratory protection, emergency filtration systems, and pressure swing adsorption (PSA) systems for gas purification. Their relatively inert surface chemistry makes them compatible with a wide range of gases and volatile compounds.

One must recognize that emerging trends in activated carbon research include the use of biomass-derived precursors, such as agricultural waste and lignocellulosic residues. These sustainable feedstocks not only reduce production costs but also contribute to circular economy strategies aimed at valorizing waste into high-value materials.

Activated carbons are among the most extensively used adsorbents in gas storage and separation technologies due to their cost-effectiveness, high surface area, and chemical stability. From an applied standpoint, they are typically derived from carbon-rich precursors such as coal, coconut shells, wood, or synthetic polymers through physical or chemical activation processes. These treatments create a highly porous structure composed mainly of micropores (<2 nm), mesopores (2–50 nm), and occasionally macropores (>50 nm) [5].

The surface area of activated carbons can range from 500 to over 2500 m^2/g, depending on the precursor material and activation conditions. It is worth noting that this extensive porosity provides a large number of active sites for gas adsorption, making them highly effective for capturing gases such as CO_2, CH_4, and volatile organic compounds (VOCs). It is worth noting that their hydrophobic surface character also contributes to their stability in humid environments, which is advantageous compared to some hydrophilic materials, such as zeolites.

For CO_2 capture, activated carbons can achieve uptake capacities of up to 3–5 mmol/g under moderate pressures and temperatures. In practical terms, however, unlike zeolites and MOFs, their selectivity for CO_2 over N_2 or CH_4 is typically lower due to the lack of strong specific interactions with CO_2 molecules. To enhance selectivity and uptake, surface functionalization techniques such as amination, oxidation, and impregnation with alkali metal salts have been investigated [2].

Activated carbons are also effective in methane storage applications, particularly under high-pressure conditions. Densified activated carbon materials have demonstrated high volumetric methane storage capacities, making them suitable for use in natural gas vehicles and storage tanks [5]. Additionally, their thermal and oxidative stability enables repeated regeneration with minimal degradation in performance.

A key advantage of activated carbons is their scalability and low production cost, which makes them ideal for industrial-scale applications. They are already widely used in commercial air and water purification systems, solvent recovery, and flue gas treatment. From an applied standpoint, however, their relatively disordered pore structure and limited tunability compared to MOFs may constrain their performance in applications requiring precise gas separation.

Recent research efforts have focused on developing hierarchical activated carbons with improved porosity gradients and hybrid materials that combine activated carbon with metal–organic frameworks (MOFs) or metal oxides to leverage the strengths of both classes [5].

Activated carbons are amorphous carbonaceous materials with a wide range of pore sizes, primarily micropores and mesopores. They are typically derived from organic precursors, such as coconut shells or coal, through physical or chemical activation processes. Although their surface area (500–2500 m^2/g) is generally lower than that of MOFs, activated carbons offer significant advantages in terms of cost, scalability, and thermal stability. They have been widely used in CO_2 capture and methane storage, particularly under high-pressure conditions [5].

Table 4 below summarizes the key physical and operational characteristics of zeolites, MOFs, and activated carbons.

Table 4. Key physical and operational characteristics of zeolites, MOFs, and activated carbons.

Property/Feature	**Zeolites**	**MOFs**	**Activated Carbons**
Structure	Crystalline aluminosilicates	Crystalline MOFs	Amorphous carbon structures
Surface Area (m^2/g)	300–800	Up to 7000	500–2500
Thermal Stability	High (>700 °C)	Moderate to High	Very High (>900 °C)
Hydrothermal Stability	Good	Often Limited	Excellent
Moisture Sensitivity	High	Varies	Low
Regenerability	Easy	Moderate	Easy
Cost	Low to Moderate	High	Low
Pore Size Range (nm)	0.3–1.2	0.3–3+	0.5–50
Hydrogen Storage	Low to Moderate	High	Moderate
Methane Storage	Moderate	High	High
CO_2 Selectivity	High	Very High	Moderate
CO_2/N_2 Selectivity	High	Very High	Moderate
Regeneration Ease	High	Moderate	High
Scalability	High	Moderate	Very High
Reference	[12]	[12]	[12]

This comparison highlights that while MOFs lead in terms of adsorption capacity and tunability, their drawbacks, including cost and stability, limit their widespread deployment. Zeolites, though less flexible, are robust and cost-effective. Activated carbons offer a practical middle ground with excellent scalability and moisture tolerance. This leads to activated carbons remaining indispensable in gas adsorption applications due to their versatility, affordability, and robustness. With continued innovation in surface modification and composite development, their role in clean energy storage and carbon management is expected to expand further.

4. Delivery Mechanisms for Subsurface Sequestration

Notably, field deployments such as Zeolite 13X core injections [13] and MOF-polymer suspensions in synthetic reservoirs [20] demonstrate early-stage field validation of these methods.

Efficient subsurface deployment of porous materials, such as zeolites, metal–organic frameworks (MOFs), and activated carbons, is crucial for ensuring effective CO_2 storage in depleted oil and gas reservoirs. Current research and field trials consider five main delivery strategies: direct suspension injection, polymer-assisted transport, foam-assisted delivery, encapsulation with controlled release, and preformed particle gels (PPGs). Each mechanism offers unique advantages and limitations in terms of injectivity, stability, material retention, and compatibility with formation conditions, as seen in Figures 2–4.

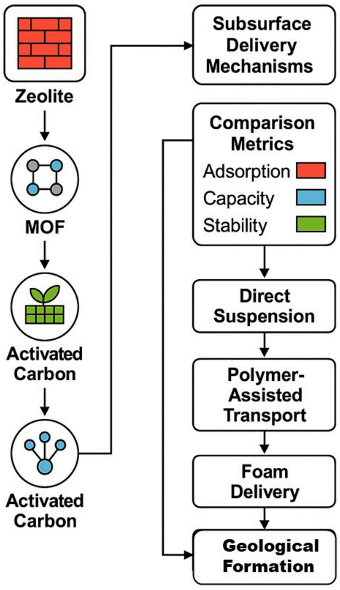


Figure 2. Integrated flowchart illustrating the evaluation and deployment pathway for CO_2 adsorbents in carbon capture and storage (CCS) systems. Zeolites, metal–organic frameworks (MOFs), and activated carbons are assessed based on key performance metrics—adsorption capacity, structural stability, and CO_2 selectivity. These materials are then delivered into geological formations via engineered strategies, including direct suspension, polymer-assisted transport, and foam delivery. The diagram emphasizes the interdependence of material properties and delivery mechanisms in achieving efficient, scalable CO_2 sequestration.

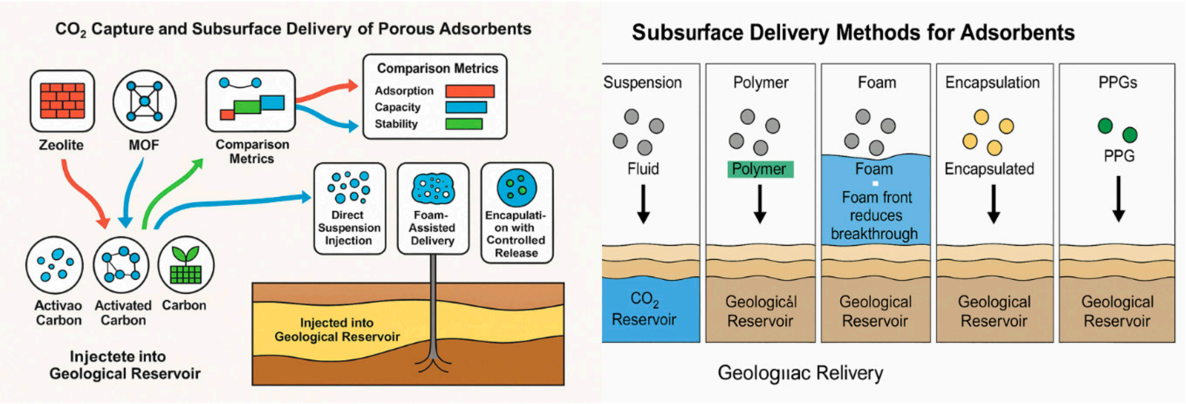


Figure 3. Integrated flowchart showing the CO_2 capture potential of zeolites, MOFs, and activated carbons (**left**) alongside subsurface delivery methods (**right**). Adsorbents are assessed based on performance metrics (adsorption, capacity, stability) and then transported into geological formations using techniques such as direct suspension and polymer particle gels. This visual summary aids in material selection and deployment strategies for carbon capture and storage (CCS) systems.

Direct suspension injection is the most straightforward technique, involving the dispersion of porous particles into an aqueous or brine-based fluid and injecting them into the reservoir. Zeolites and activated carbons are particularly well-suited for this approach due to their mechanical and thermal stability. Key challenges include particle agglomeration, settling, and clogging of pore throats. To mitigate these effects, surfactants and stabilizing agents are often added to enhance the homogeneity of the suspension. Studies by [13,21] have shown the successful injection of Zeolite 13X suspensions into sandstone cores, leading to minimal permeability damage and effective CO_2 capture. This method provides operational simplicity and is compatible with existing oilfield infrastructure, but it necessitates careful control of particle size distribution and fluid rheology.

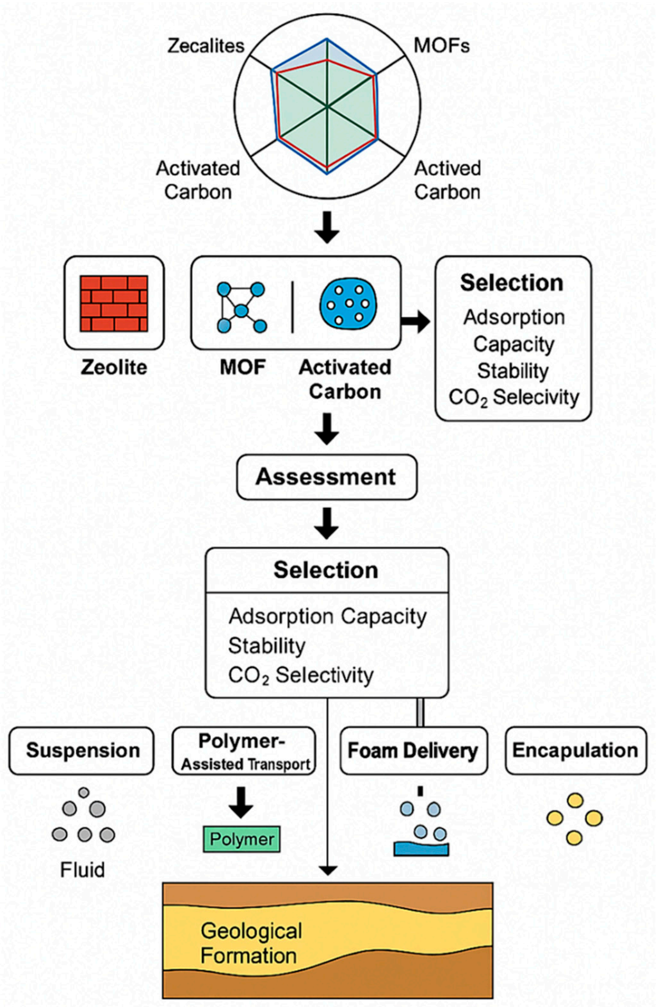


Figure 4. Integrated visual framework for material selection and delivery in CO_2 capture and geological sequestration systems. The top panel presents a radar chart comparing zeolites, MOFs, and activated carbons across key performance metrics—adsorption capacity, structural stability, and cost. Based on this assessment, the most suitable adsorbent is selected and matched to an appropriate subsurface delivery method such as suspension, polymer-assisted transport, foam delivery, or encapsulation. These pathways culminate in the injection of the adsorbent into a geological formation for long-term CO_2 sequestration. This flowchart highlights the end-to-end decision-making process in adsorbent-based CCS deployment.

Polymer-assisted delivery involves dispersing porous adsorbents in a polymer solution, typically using high-viscosity polymers such as partially hydrolyzed polyacrylamide (HPAM) or xanthan gum. These solutions minimize particle settling and enhance sweep efficiency. MOFs, which are susceptible to hydrolytic degradation, particularly benefit from this protective matrix. The polymer also modifies fluid mobility, allowing for deeper penetration into low-permeability zones. A study by [20,22] showed that HPAM-MOF composites maintained their CO_2 adsorption efficiency in synthetic core environments, supporting the viability of this method. However, the retention of polymers on reservoir rock and their potential for formation damage must be managed through optimization of concentration and compatibility testing to ensure effective use.

Foam-based systems leverage the benefits of gas–liquid interfaces to improve mobility control and reduce gravity override. CO_2 or nitrogen-based foams stabilized with surfactants or nanoparticles can efficiently transport zeolite or MOF particles into heterogeneous formations. This method is vital in high-permeability or fractured zones. Experimental work by [23] indicated that nanoparticle-stabilized foams carrying MOFs showed uniform placement and improved contact with CO_2-rich regions, enhancing sequestration efficiency. Foam stability, influenced by reservoir salinity and temperature, is a crucial factor for success.

Encapsulation techniques involve enclosing the adsorbent material within a protective barrier that dissolves or ruptures under specific reservoir conditions (e.g., temperature, pH, or salinity). Hydrogels, such as poly(*N*-isopropylacrylamide) (PNIPAM) and silica shells, are utilized to protect sensitive metal–organic frameworks (MOFs) during injection and to ensure targeted release. The work by [24] demonstrated that ZIF-8 encapsulated in PNIPAM hydrogels retained 80% of its CO_2 adsorption capacity after repeated thermal cycling, highlighting the durability of this method. However, the complexity and cost of synthesis, along with the potential effects of degradation byproducts on formation chemistry, pose challenges for encapsulation.

Preformed Particle Gels (PPGs) are cross-linked polymer matrices designed to swell upon contact with water, enabling the in situ deployment of embedded adsorbent particles. These gels can block high-permeability channels and gradually release active materials. When impregnated with zeolites or MOFs, they function as both flow modifiers and sorbent carriers. PPGs enhanced CO_2 sweep efficiency by reducing bypassing and channelling in fractured reservoirs [25]. However, the irreversible nature of gel swelling and potential for formation plugging in productive zones requires a tailored design based on site-specific permeability profiles.

Table 5 presents a comparative summary of delivery methods across factors, such as reservoir compatibility, injectivity, and maturity level, to assist in selecting the most appropriate strategy.

Table 5. Comparative Evaluation of Delivery Methods for Subsurface CO_2 Adsorbents.

Delivery Method	**Compatible Material(s)**	**Reservoir Compatibility**	**Advantages**	**Challenges**	**Technology Readiness Level (TRL)**
Direct Suspension Injection	Zeolites, Activated Carbons	High-permeability sandstone, depleted reservoirs	Simple implementation, compatible with existing infrastructure	Particle settling, clogging risks	7–9
Polymer-Assisted Transport	MOFs, Zeolites	Low-permeability formations, heterogeneous zones	Improves sweep efficiency, protects sensitive materials	Polymer retention, formation damage	5–7
Foam-Assisted Delivery	Zeolites, MOFs	Fractured formations, high-permeability layers	Mobility control, deep penetration	Foam stability under salinity/temperature	5–6
Encapsulation with Controlled Release	MOFs	Saline aquifers, variable pH zones	Targeted release, material protection	High complexity, cost	4–5
Preformed Particle Gels (PPGs)	MOFs, Zeolites	Fractured or bypassed zones	Dual function: flow diversion and adsorption	Swelling risks, limited reusability	4–6

Each delivery strategy offers distinct advantages tailored to specific geological contexts and the characteristics of the materials used. Direct injection, for instance, is ideal for sturdy materials such as zeolites and activated carbons, ensuring effective deployment without compromising material integrity. On the other hand, polymer and encapsulation techniques are more suitable for delicate metal–organic frameworks (MOFs), providing protection and controlled release in sensitive environments.

Foam and Propellant Placement Gels (PPGs) excel in scenarios involving complex reservoir geometries and fractured zones, offering enhanced control over material distribution and penetration. These strategies enhance the efficiency and effectiveness of deployment depending on the geological challenges and material properties encountered.

Recent findings [26,27] indicate that hybrid materials, such as MOF–carbon composites, offer 20–25% improvement in moisture resistance while maintaining high CO_2 uptake (6.5–7.5 mmol/g).

5. Hybrid Systems and Advanced Materials for CO_2 Sequestration

The limitations of single-component sorbents under complex field conditions—such as fluctuating temperature, high salinity, and moisture saturation—have catalyzed the development of hybrid and multifunctional materials. These systems synergistically combine the advantages of metal–organic frameworks (MOFs), zeolites, activated carbons, polymers, and emerging smart technologies to produce sorbents with enhanced adsorption kinetics, regeneration efficiency, mechanical robustness, and environmental resilience. Section 5 presents a comprehensive overview of recent advances in hybrid material strategies, intelligent design frameworks, and next-generation carbon capture technologies.

5.1. MOF–Zeolite and MOF–Carbon Composites

MOF-based composites represent a promising class of materials for scalable, high-performance CO_2 capture systems. MOF–zeolite hybrids integrate the high thermal and hydrothermal stability of zeolites with the structural tunability and large surface area of MOFs. These composites have shown 15–25% greater humidity resistance and retained CO_2 uptake capacities of 6.0–7.0 mmol/g under simulated flue gas conditions [27].

In parallel, MOF–carbon composites exploit the hydrophobic nature, high conductivity, and mechanical flexibility of activated carbon to stabilize MOF particles in humid and corrosive environments. These hybrids achieve 6.5–7.5 mmol/g CO_2 capacity—comparable to pristine MOFs—while maintaining structural integrity after repeated regeneration cycles. Additionally, carbon frameworks enhance compatibility with electro-swing and pressure-swing adsorption techniques by reducing hysteresis and energy consumption.

Collectively, these composites address key barriers to field deployment, including material degradation under moisture and salinity and cost-effective regeneration during continuous operation.

5.2. Polymer-Integrated Smart Adsorbents

The integration of stimuli-responsive polymers has given rise to a new generation of "smart" CO_2 adsorbents capable of adapting dynamically to environmental changes. These systems respond to inputs such as temperature, pH, ionic strength, or salinity, altering their structural conformation to expose or conceal adsorption sites.

For instance, poly(*N*-isopropylacrylamide)-based hydrogels exhibit reversible swelling and contraction, enabling programmable CO_2 capture–release cycles. Laboratory tests demonstrated 10–15% higher CO_2 uptake under high-salinity conditions compared to static materials, while also displaying enhanced cycling durability and salt tolerance. These features make smart adsorbents particularly suited for fractured reservoirs and chemically aggressive aquifers, where precision deployment and environmental robustness are paramount.

5.3. AI-Guided Materials Design and Screening

Artificial intelligence (AI) and machine learning (ML) have become integral tools in accelerating the discovery and optimization of CCS sorbents. Data-driven platforms like MOF-ML [28] use high-throughput screening data to identify promising candidates based on multi-objective performance metrics, including CO_2 uptake, regeneration energy, and material stability under various conditions.

By mining databases containing millions of hypothetical frameworks, AI algorithms can rapidly narrow down viable structures, reducing both experimental workload and development timelines. For example, generative models like ZeoliteGAN and property predictors such as AdsorbNet have accurately forecasted high-performance materials tailored to specific pressure–temperature–humidity envelopes, outperforming traditional trial-and-error approaches.

AI-guided design is also being combined with robotic synthesis and in silico testing to create closed-loop platforms, significantly speeding up the path from prediction to validation.

5.4. Environmental and Economic Considerations

While performance is paramount, the environmental footprint and cost structure of hybrid materials must be evaluated for long-term sustainability. MOFs, though highly tunable, often involve energy-intensive and solvent-heavy synthesis routes. However, recent advances in green synthesis, including aqueous processing and bio-derived linkers, are reducing these concerns.

In contrast, activated carbons and natural zeolites, particularly those derived from agricultural or industrial waste streams, offer a low-cost and sustainable base for hybrid sorbent development. Economic models show that even modest improvements of 10–15% in moisture resistance or sorption capacity can significantly reduce operational costs across the lifecycle of industrial CCS systems.

Overall, a holistic techno-economic assessment is critical for translating advanced materials from laboratory scale to field deployment at commercial scale.

5.5. Smart Adsorbents for Saline and Harsh Subsurface Environments

Saline aquifers, a primary geological target for CO_2 sequestration, pose a unique set of challenges—including ionic competition, mineral scaling, and brine-induced degradation. Traditional adsorbents are prone to performance loss under such conditions, necessitating the development of salt-tolerant and chemically resilient smart systems.

New classes of adsorbents now feature protective surface modifications, such as fluoropolymer coatings, hydrophobic functionalization, or amphiphilic barriers, that significantly reduce water and salt interference. For example, Zeolite 13X coated with a cross-linked fluorinated polymer retained 90% of its original CO_2 capacity in 3.5% NaCl brine, compared to a 50% drop in untreated controls [10]. Similarly, graphene-supported MOFs achieved stable adsorption (6.8 mmol/g) under high-salinity conditions, with negligible pore blockage.

Smart materials also include phase-responsive composites that adapt their pore structures when triggered by salinity or ionic changes. Some hydrogel-based carriers and ionic-liquid infused sorbents have demonstrated cycling stability for over 10 salinity exposure cycles, marking a substantial advance in performance under reservoir-mimicking conditions.

5.6. AI-Assisted Discovery and Deployment of Hybrid Materials

Beyond material design, AI is now being employed to predict field-specific performance, integrating models that account for geological variables, gas composition, and fluid dynamics in CCS sites. These tools aid in matching sorbents to subsurface environments with high precision, facilitating customized deployment strategies.

Moreover, AI-driven inverse design algorithms can identify hybrid material combinations with targeted properties (e.g., hydrophobicity, surface polarity, or binding energy) to meet niche requirements. Coupled with economic modeling, these systems also evaluate trade-offs between performance, cost, and environmental impact, enabling decision-makers to optimize material selection for different CCS scenarios, such as direct air capture, post-combustion flue gas, or saline aquifer injection.

This integration of materials informatics, machine learning, and field simulation is redefining how sorbents are discovered, scaled, and implemented across the CCS value chain.

6. Discussion: Deployment Challenges and Climate Policy Alignment

The successful deployment of porous adsorbents for CO_2 capture and storage hinges not only on their physicochemical performance but also on a broader array of logistical, regulatory, and policy considerations. Section 6 examines the practical obstacles and systemic enablers that will influence the transition from laboratory-scale validation to large-scale implementation.

6.1. Infrastructure and Field Compatibility

One of the most pressing challenges is integrating novel adsorbents into existing carbon capture and storage (CCS) infrastructure. Although zeolites and activated carbons are already commercially available for industrial gas separations, the upscaling of MOFs or hybrid materials remains a bottleneck due to limited bulk production capabilities, lengthy synthesis times, and high costs [3]. Ensuring compatibility with pipelines, injection systems, and reservoir conditions is essential for transitioning from batch testing to field trials. Furthermore, matching the adsorbent's performance profile to reservoir-specific temperature, pressure, and salinity conditions is crucial. Customization and pre-deployment characterization of material behavior under site-specific conditions—such as high brine content or fluctuating pressure gradients—can enhance sequestration efficiency and mitigate operational risks.

6.2. Monitoring and Verification Technologies

Regulatory frameworks require robust tools for verifying the containment and stability of injected CO_2. While geophysical monitoring techniques, such as seismic imaging and pressure mapping, are well-established, they often lack the resolution to track the placement or behavior of adsorbents in situ. This necessitates the development of new monitoring strategies that can track CO_2 adsorption in real time, including the use of tracer particles, reactive gels with optical markers, and geochemical fingerprinting methods.

Without reliable tracking, the risk of leakage or inefficient usage of adsorbents increases, undermining both environmental safety and economic feasibility. Continued investment in sensor miniaturization, wireless data logging, and real-time analytics is needed to close this gap.

6.3. Lifecycle and Economic Viability

From a cost-benefit perspective, the full lifecycle of adsorbent materials must be assessed, including synthesis, transportation, field deployment, regeneration (if applicable), and eventual disposal or repurposing [12]. MOFs, while promising in performance, are still expensive to produce at scale and may involve energy-intensive regeneration depending on the capture conditions [3].

Conversely, activated carbons and natural zeolites sourced from low-cost or recycled materials offer a favorable environmental and economic profile. Hybrid materials that combine these with high-performance elements—such as metal–organic frameworks (MOFs) or metal oxides—could bridge the cost-performance gap. Techno-economic models suggest that increasing the longevity of adsorbents by 25–50% could reduce total carbon capture and storage (CCS) costs by over 15% in specific configurations.

6.4. Policy Incentives and International Commitments

Achieving the deployment of CCS technologies at a scale relevant to climate targets will require not only technological maturity but also strong policy support. The inclusion of CCS in nationally determined contributions (NDCs), international funding programs, and carbon trading markets is crucial for commercial viability.

Incentives such as tax credits (e.g., the U.S. 45Q credit), public–private partnership models, and CCS demonstration grants in the EU and Asia–Pacific have already begun to stimulate innovation and early deployment. Embedding CCS materials development in climate finance mechanisms can ensure broader adoption while addressing equity and sustainability concerns.

6.5. Toward Integrated CCS Ecosystems

The future of CCS may lie in integrated ecosystems where porous materials not only adsorb CO_2 but also facilitate downstream processes, such as catalytic conversion to fuels or feedstocks. The development of multifunctional systems that integrate capture, conversion, and reuse within the same physical matrix aligns with circular economy principles and could significantly enhance the value proposition of CCS technologies [29].

In this context, porous materials, particularly metal–organic frameworks (MOFs) with catalytic functionalities, could play a transformative role. However, achieving this vision requires cross-disciplinary collaboration, from material scientists and geologists to economists and policymakers.

6.6. Extrapolating Laboratory Data to Field Conditions

While laboratory testing provides critical insights into adsorbent performance, translating these results to real-world conditions remains a major scientific and operational hurdle. Factors such as particle agglomeration, pore clogging, hydrothermal cycling, and mineral scaling can significantly reduce efficiency in subsurface or flue gas environments. Moreover, field-relevant parameters—such as fluctuating pressures, elevated temperatures, and brine salinity—can alter adsorption dynamics and compromise long-term material stability.

Recent work by [21] has demonstrated that CO_2 uptake for MOFs and composite materials can decrease by up to 30% under high-salinity brine conditions compared to dry lab conditions, primarily due to site blocking and pore flooding. Additionally, the regeneration energy may increase by 10–20% due to thermal degradation or altered kinetics in scaled systems.

This underscores the need for pilot-scale validation, site-specific conditioning of materials, and the development of adaptive sorbent formulations tailored to real-world CCS deployment. Bridging this gap is critical for ensuring that material innovations contribute meaningfully to national and global decarbonization goals.

7. Sustainability and Environmental Performance of Adsorbent-Based CO_2 Sequestration

The sustainability of carbon capture and storage (CCS) technologies is increasingly evaluated not only by technical feasibility and economic cost, but also by their environmental footprint and life cycle performance. The use of solid adsorbents such as zeolites, metal–organic frameworks (MOFs), and activated carbons offers a pathway toward more environmentally conscious CCS strategies, particularly when these materials are sourced or synthesized with sustainable practices in mind (Figure 5).

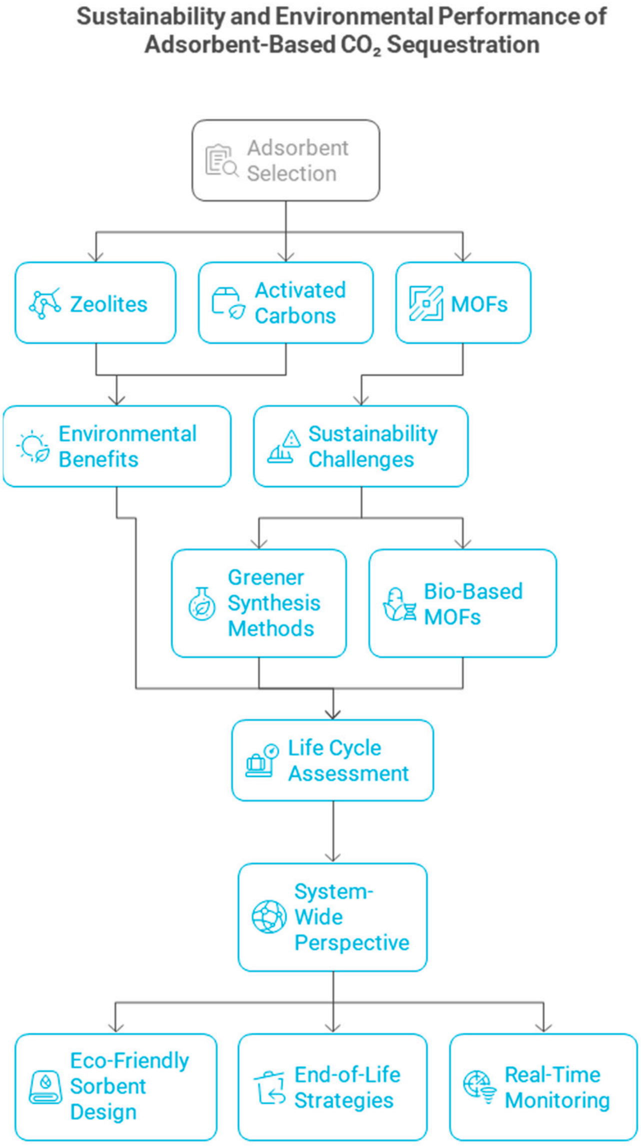


Figure 5. Sustainability and Environmental Performance of Adsorbent-Based CO_2 Sequestration.

Zeolites, typically synthesized from abundant aluminosilicate minerals or even industrial waste (e.g., fly ash), are considered among the most environmentally benign adsorbents due to their thermal stability, long service life, and recyclability with minimal degradation [30]. However, their sensitivity to moisture and relatively lower uptake capacity can limit their standalone effectiveness under field conditions.

Activated carbons, particularly those derived from biomass (e.g., coconut shells, sawdust, or agricultural residues), are widely recognized for their low environmental impact and high circularity potential [31]. Their production involves relatively low energy input, and carbonization processes can be integrated into waste valorization streams, further improving sustainability metrics. Additionally, activated carbons demonstrate strong tolerance to impurities and moisture, reducing the need for extensive pre-treatment of flue gases or subsurface fluids.

MOFs, while offering outstanding tunability and adsorption performance, present significant sustainability challenges. Many MOFs are synthesized using rare or toxic metals (e.g., Cr, Zn) and organic linkers through solvent-intensive processes [32]. Recent research has focused on greener synthesis methods—such as water-based or mechanochemical synthesis—to reduce environmental burdens, as well as the development of bio-based

MOFs [33]. Lifecycle assessments (LCAs) of MOFs are still limited, and further studies are needed to determine their cradle-to-grave impacts, especially for large-scale deployment.

From a system-wide perspective, life cycle assessment (LCA) tools have to be applied to adsorbent-based CCS systems to estimate environmental trade-offs. These include greenhouse gas (GHG) emissions from material synthesis, energy consumption during regeneration cycles, and the environmental impact of delivery mechanisms such as polymer additives and surfactants [34]. Polymer-stabilized or foam-based delivery systems must be evaluated for biodegradability, persistence, and potential interactions with subsurface ecosystems. Researchers have called for more holistic sustainability frameworks that integrate techno-economic performance with carbon intensity, material criticality, and ecological toxicity.

To ensure environmental integrity and societal acceptance, the future development of CCS systems should prioritize eco-friendly sorbent design, minimize solvent and energy use in production, and support end-of-life strategies such as adsorbent regeneration, reuse, or safe subsurface immobilization. Moreover, incorporating real-time monitoring and adaptive management can further mitigate ecological risks during and after deployment.

Life Cycle Assessment (LCA) of Adsorbent Materials

A robust evaluation of adsorbent-based CCS systems must include quantitative life cycle assessment (LCA) to determine their net environmental impact across stages of material production, operation, and end-of-life. Recent LCA studies underscore that although many porous adsorbents demonstrate high CO_2 uptake and selectivity, their embodied energy, carbon footprint, and environmental toxicity can vary significantly depending on synthesis methods and feedstock sources.

MOFs, for instance, despite their superior adsorption properties, often require high energy input (up to 200–400 MJ/kg) during solvothermal synthesis, especially when using rare metals such as chromium or zinc and organic solvents like DMF or ethanol. The estimated cradle-to-gate carbon footprint for MOF production ranges from 10–30 kg CO_2-eq per kg MOF, depending on the type of linker and metal center used [34]. These values can be reduced by switching to water-based or mechanochemical synthesis routes, which cut solvent usage by up to 90% and lower GHG emissions by 40–60% [32]. Still, end-of-life strategies for MOFs remain underdeveloped, with concerns about metal leaching and safe degradation.

By contrast, activated carbons derived from biomass (e.g., coconut shells or wood waste) have a much lower LCA burden. Studies indicate that their production energy ranges from 30 to 70 MJ/kg, with a carbon footprint of 2–5 kg CO_2-eq per kg AC, depending on activation methods (e.g., steam vs. chemical activation). Furthermore, their integration into circular bio-economy streams enhances their sustainability profile by valorizing agricultural residues and enabling carbon-negative scenarios in some configurations [31].

Zeolites occupy a middle ground. Natural zeolites or those synthesized from fly ash typically require 80–150 MJ/kg of input energy and generate 4–7 kg CO_2-eq per kg zeolite. Their thermal and chemical stability supports long-term reuse across multiple regeneration cycles, extending service life and improving overall environmental performance [30]. However, performance trade-offs—particularly under humid or saline conditions—may necessitate the use of hybridized systems, potentially increasing material and energy demands. An LCA comparison of these adsorbents is summarized in Table 6.

LCA tools have revealed that regeneration energy and material degradation during operational cycles account for over 30–40% of the total environmental impact in adsorbent-based CCS systems. This highlights the importance of optimizing regeneration protocols (e.g., low-temperature TSA, moisture-tolerant swing processes) to minimize cumulative GHG emissions and improve lifecycle performance.

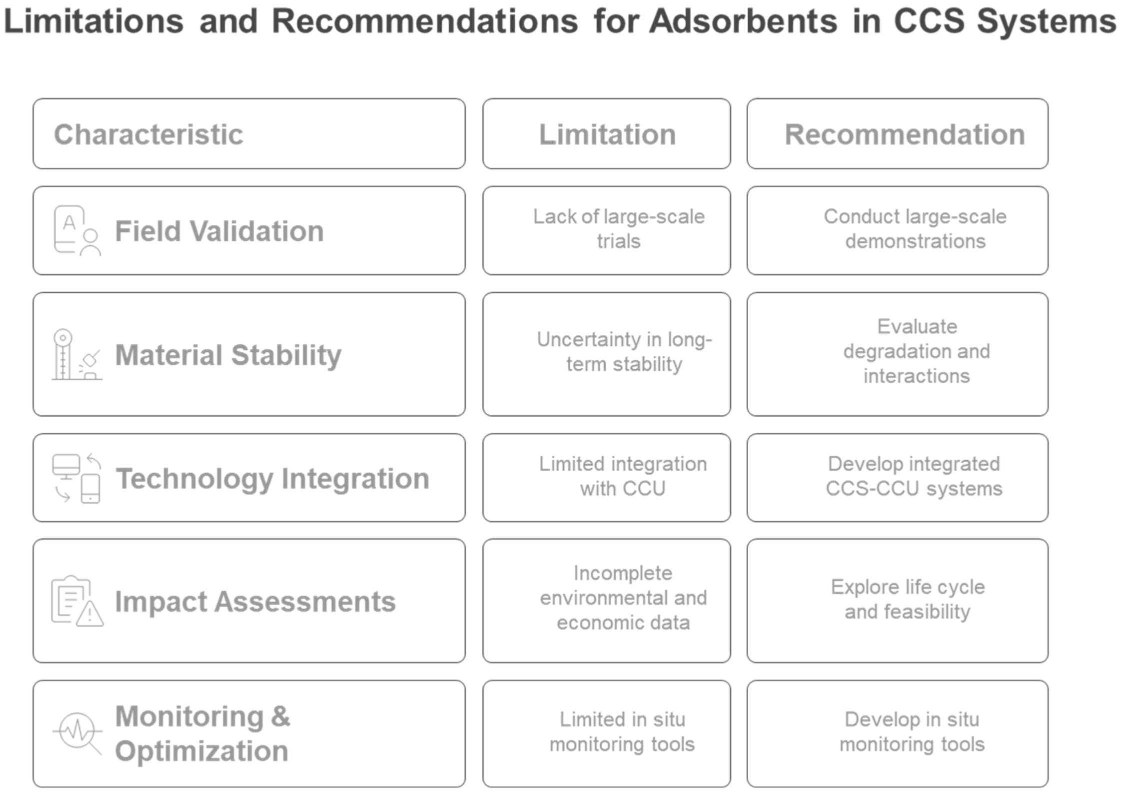
Table 6. Comparative Life Cycle Assessment (LCA) Parameters for Major CO_2 Adsorbent Classes.

Parameter	**MOFs (Conventional)**	**MOFs (Green Synthesis)**	**Activated Carbon**	**Zeolites (Synthetic/Natural)**
Energy Input (MJ/kg)	200–400 MJ/kg [34]	80–150 MJ/kg [32]	30–70 MJ/kg [31]	80–150 MJ/kg [30]
GHG Emissions (kg CO_2-eq/kg)	10–30 kg CO_2-eq/kg [34]	4–12 kg CO_2-eq/kg [32]	2–5 kg CO_2-eq/kg [31,35]	4–7 kg CO_2-eq/kg [30,35]
Solvent Use	High (e.g., DMF, ethanol) [34]	Low (e.g., water, mechanochemical) [32]	Low [31]	Low to Moderate [30,36]
Circularity Potential	Low–Moderate [34]	Moderate [32]	High [31,36]	Moderate–High [30]
End-of-Life Management	Limited recyclability [34]	Emerging (e.g., bio-MOFs, recyclable linkers) [32]	Mature (reusable, degradable) [31,36]	High reusability and mineral stability [30,36]

In future work, it is essential to embed LCA integration into the early stages of sorbent material development, allowing researchers to co-optimize performance and sustainability. Decision-support frameworks incorporating techno-economic assessment (TEA) alongside LCA can guide material selection for specific deployment scenarios (e.g., saline aquifers, industrial flue gas streams), aligning innovation with the principles of green chemistry and climate justice.

8. Limitations and Recommendations for Future Research

Despite the promising developments reviewed, several critical limitations must be addressed to facilitate the broader deployment of porous adsorbents in CCS systems (see Figure 6).



Limitations and Recommendations for Adsorbents in CCS Systems

Characteristic	Limitation	Recommendation
Field Validation	Lack of large-scale trials	Conduct large-scale demonstrations
Material Stability	Uncertainty in long-term stability	Evaluate degradation and interactions
Technology Integration	Limited integration with CCU	Develop integrated CCS-CCU systems
Impact Assessments	Incomplete environmental and economic data	Explore life cycle and feasibility
Monitoring & Optimization	Limited in situ monitoring tools	Develop in situ monitoring tools

Figure 6. Limitations and Recommendations for Adsorbents in CCS Systems.

8.1. Data Gaps and Standardization Deficiencies

A significant obstacle to advancing porous material applications for carbon capture lies not in performance but in the inconsistency of available data and the absence of universally accepted testing protocols. While the literature is replete with claims of high adsorption capacities or exceptional regenerability, these often arise from disparate testing conditions, limiting their comparability and usefulness in practical settings.

For example, two studies [37,38] might report CO_2 uptake for similar MOFs, but use different pressures, temperatures, or gas mixtures, making the results essentially non-comparable. Inconsistent definitions of key properties worsen this issue. Terms like "stability" or "regeneration energy" are used without clear thresholds or standardized methods, causing confusion rather than clarity.

Also, a few materials are tested beyond initial characterization. Long-term behavior under repeated cycling, exposure to flue gas contaminants, or performance in humidified streams is either underreported or ignored. This lack of durability data undermines confidence in field readiness and complicates lifecycle modelling.

Compared to more mature clean technologies, such as photovoltaics or lithium–ion batteries, which benefit from community-driven benchmarking frameworks, porous CCS materials remain methodologically fragmented. The creation of an open-access, peer-reviewed performance database could enable more accurate screening of candidate materials and provide critical input for techno-economic evaluations.

Moreover, integrating machine learning tools with curated datasets could reveal performance trends across structural families, expediting material discovery. But until a consensus emerges around data reporting standards and validation protocols, the field risks stagnation. Only through collective effort and transparency can porous materials fulfil their potential as cornerstones of next-generation CCS strategies.

8.2. Scaling and Integration Challenges of Porous Materials

Although porous materials such as MOFs, zeolites, and activated carbons exhibit great promise for carbon capture, their widespread application remains constrained by significant barriers to industrial scaling. MOFs in particular—despite their impressive structural tunability and high adsorption capacities—require intricate and often inefficient synthetic routes that are not yet conducive to cost-effective bulk production. This poses practical limits on their availability for deployment in CCS settings.

In contrast, zeolites and activated carbons benefit from more established commercial production lines. However, the superior performance of MOFs, especially under dry gas conditions, raises the question of how to balance availability with efficacy. One overlooked issue is that lab-scale synthesis methods rarely translate into scalable, continuous production, and attempts to upscale often compromise structural fidelity or porosity.

Moreover, materials intended for geological injection must conform to a range of physical specifications, including suitable particle morphology and mechanical strength, to ensure compatibility with subsurface conditions. This includes resistance to pressure-induced deformation, pore blockage, or chemical alteration under in situ conditions. The lack of robust field data confirming such stability under variable reservoir environments further exacerbates deployment uncertainty.

Integrating novel materials into legacy CCS infrastructure introduces additional complexity. The materials must work seamlessly with existing gas separation systems, pipeline configurations, and injection equipment without necessitating major retrofits. Until a harmonized approach emerges—one that aligns material design with practical engineering constraints—the gap between laboratory innovation and industrial deployment is likely to persist.

8.3. Field Deployment Uncertainty and Environmental Sensitivity

The real-world deployment of porous adsorbents faces a host of challenges that are not adequately captured by laboratory experiments. While controlled environments offer insight into fundamental performance, they fail to represent the dynamic conditions found in subsurface reservoirs, where fluctuations in salinity, moisture, and temperature can significantly alter sorbent behavior. Such environmental complexity introduces a degree of unpredictability that complicates both operational planning and risk mitigation.

Zeolites, for example, exhibit high CO_2 uptake in dry conditions; however, their performance rapidly deteriorates in the presence of water vapor due to competitive adsorption. Similarly, although some MOFs have been designed to resist hydrolysis, many variants remain vulnerable to degradation under humid or acidic environmental conditions often encountered during CO_2 injection into saline aquifers or depleted reservoirs.

Beyond the issue of chemical robustness, current CCS operations lack tools for real-time monitoring of adsorbent saturation or structural integrity post-injection. Technologies such as seismic imaging or pressure logging provide indirect data but are insufficient for tracking the fate of materials at the molecular or pore level. This results in an information gap that impairs system optimization and hinders adaptive responses to changes within the reservoir.

To address these gaps, a multi-pronged approach is essential. More representative pre-deployment testing that mimics real reservoir conditions must become standard practice. Additionally, the development of advanced sensing technologies—such as embedded tracers or reactive nanomaterials—could significantly improve our ability to observe and manage the behavior of injected sorbents. Without these innovations, the practical use of porous materials will remain uncertain, regardless of their theoretical potential.

9. Conclusions, Challenges, and Opportunities

9.1. Conclusions

This review has evaluated the comparative performance of three leading classes of porous adsorbents: zeolites, metal–organic frameworks (MOFs), and activated carbons for CO_2 capture and geological sequestration. Zeolites offer robust thermal stability, high selectivity, and low cost, yet exhibit performance limitations under humid conditions. MOFs demonstrate superior tunability and CO_2 uptake capacity, though challenges in hydrothermal stability and scale-up economics constrain their industrial deployment. Activated carbons, widely available and moisture-tolerant, provide a practical middle ground, particularly when derived from sustainable biomass feedstocks.

In addition to material selection, this study examined five primary subsurface delivery mechanisms: direct suspension injection, polymer-assisted transport, foam-assisted delivery, encapsulation with controlled release, and preformed particle gels (PPGs). These methods each offer unique operational benefits and limitations, depending on reservoir properties, particle stability, and required placement precision.

Emerging innovations in hybrid systems, such as MOF–carbon composites and smart polymer-integrated sorbents, are reshaping the landscape of adsorbent design by improving environmental resilience and adaptive deployment capabilities. Furthermore, the integration of AI-guided materials discovery is accelerating the optimization of CO_2 capture materials tailored to specific geological and operational conditions.

The transition to commercial-scale carbon capture and storage (CCS) requires not only technical advancements but also supportive policy mechanisms, robust monitoring infrastructure, and comprehensive lifecycle assessments. When implemented holistically, these systems have the potential to transform depleted geological reservoirs into high-efficiency carbon sinks, positioning porous adsorbents at the heart of sustainable carbon management.

9.2. Challenges and Opportunities in Advancing Adsorbent-Based Carbon Storage

Despite the progress in developing advanced materials and delivery strategies for carbon capture and storage (CCS), several critical challenges remain before these technologies can be deployed at scale. Addressing these will require coordinated efforts across disciplines and sectors (Figure 6).

1. Lack of Large-Scale Field Validation: While many adsorbent materials and delivery techniques have shown great promise in laboratory settings or small-scale pilot studies, there is still a significant gap in demonstrating their performance in real-world, large-scale environments. Subsurface geological formations are highly complex and variable, and without full-scale field trials, it is difficult to fully understand how these systems will behave. Key questions remain around how well materials can be injected, how long they will stay in place, and how effectively they can capture and retain CO_2 in different geological conditions. Long-term field validation is crucial to prove these technologies are not only effective but also reliable and safe over time;
2. Uncertainty in Long-Term Material Stability: Another major concern is the durability of the materials used—especially porous adsorbents like MOFs (metal–organic frameworks), zeolites, and activated carbons. These materials may be exposed to harsh subsurface conditions, including high pressures, fluctuating temperatures, and varying salinity levels. Over time, this can lead to chemical degradation, changes in mechanical strength, or loss of adsorption capacity. Currently, we lack a clear understanding of how these materials behave over the long term, particularly over periods of several years or decades. Research is needed to explore their degradation pathways, resilience under cyclical loading, and potential interactions with native reservoir fluids;
3. Integration with Carbon Capture and Utilization (CCU): Beyond simply storing CO_2, there is a growing interest in turning captured carbon into useful products—what is known as Carbon Capture and Utilization (CCU). For this vision to be realized, adsorbents must not only capture CO_2 efficiently but also allow for its recovery and regeneration so that it can be fed into catalytic processes or industrial value chains. Designing materials that can be regenerated repeatedly and are compatible with downstream applications is a critical next step toward circular and economically viable carbon management;
4. Environmental and Economic Assessments: To ensure that these technologies are both sustainable and practical, we need a better understanding of their environmental and economic impacts. This includes analyzing the full life cycle of adsorbent materials—from raw material extraction and manufacturing to deployment and disposal—as well as considering their supply chain emissions and overall cost-effectiveness. This is especially important for newer materials like MOFs and hybrids, which may involve rare or energy-intensive components. Robust life cycle assessment (LCA) and techno-economic analysis (TEA) can help guide responsible development and inform policy and investment decisions;
5. Smart Monitoring and Data-Driven Optimization: One of the most exciting frontiers lies in using smart sensing and data analytics to improve the performance and safety of CCS systems. For example, adsorbents could be functionalized with tracers or responsive sensors that enable real-time tracking of CO_2 movement and material behavior underground. These innovations would not only enhance the reliability of the storage process but also allow for adaptive control strategies, reducing risk and

improving efficiency. Integrating such tools into deployment strategies could be a game-changer for field operations.

Author Contributions: Conceptualization, I.S. and M.G.H.; methodology, M.H.M., N.B. and S.Z.A.; resources, M.G.H., M.H.M. and I.S.; data curation, M.H.M., M.G.H., S.Z.A., N.B. and I.S.; writing—original draft preparation, M.H.M., M.G.H., S.Z.A., N.B. and I.S.; writing—review and editing, M.H.M., M.G.H., S.Z.A., N.B. and I.S.; visualization, M.G.H. and M.H.M.; supervision, N.B., S.Z.A. and M.G.H.; project administration, M.H.M.; funding acquisition, I.S. All authors have read and agreed to the published version of the manuscript.

Funding: The authors extend their appreciation to the Deanship of Research and Graduate Studies at King Khalid University, KSA, for funding aspects of this work through small group research under grant number RGP1/70/46.

Data Availability Statement: Available from the corresponding author upon communication.

Conflicts of Interest: The authors have no conflicts of interest.

References

1. Intergovernmental Panel On Climate Change (IPCC). *Climate Change 2021—The Physical Science Basis: Working Group I Contribution to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change*, 1st ed.; Cambridge University Press: Cambridge, UK, 2023; ISBN 978-1-009-15789-6. [CrossRef]
2. Pardakhti, M.; Jafari, T.; Tobin, Z.; Dutta, B.; Moharreri, E.; Shemshaki, N.S.; Suib, S.; Srivastava, R. Trends in Solid Adsorbent Materials Development for CO_2 Capture. *ACS Appl. Mater. Interfaces* **2019**, *11*, 34533–34559. [CrossRef]
3. Sumida, K.; Rogow, D.L.; Mason, J.A.; McDonald, T.M.; Bloch, E.D.; Herm, Z.R.; Long, J.R. Carbon Dioxide Capture in Metal—Organic Frameworks. *Chem. Rev.* **2012**, *112*, 724–781. [CrossRef] [PubMed]
4. Singh, J.; Chaowamalee, S.; Pitayachinchot, H.; Kaewngam, C.; Chotirattanachote, A.; Thiensuwan, N.; Poompradub, S.; Yokoi, T.; Ngamcharussrivichai, C. Bifunctionality of Amine-Modified Metal-Organic Frameworks for CO_2 Capture and Selective Utilization in Cycloaddition. *Carbon Capture Sci. Technol.* **2024**, *13*, 100262. [CrossRef]
5. Jedli, H.; Almonnef, M.; Rabhi, R.; Mbarek, M.; Abdessalem, J.; Slimi, K. Activated Carbon as an Adsorbent for CO_2 Capture: Adsorption, Kinetics, and RSM Modeling. *ACS Omega* **2024**, *9*, 2080–2087. [CrossRef]
6. Adegoke, K.A.; Akpomie, K.G.; Okeke, E.S.; Olisah, C.; Malloum, A.; Maxakato, N.W.; Ighalo, J.O.; Conradie, J.; Ohoro, C.R.; Amaku, J.F.; et al. UiO-66-Based Metal-Organic Frameworks for CO_2 Catalytic Conversion, Adsorption and Separation. *Sep. Purif. Technol.* **2024**, *331*, 125456. [CrossRef]
7. Wang, B.; Feng, Y.; Blears, J.; Thompson, K.; Hughes, R. Streamline-Based Simulation of Nanoparticle Transport in Field-Scale Heterogeneous Subsurface Systems. *Adv. Water Resour.* **2021**, *148*, 103842. [CrossRef]
8. Breck, D.W. *Zeolite Molecular Sieves: Structure, Chemistry, and Use*; John Wiley & Sons: New York, NY, USA, 1974. [CrossRef]
9. Coasne, B.; Farrusseng, D. Gas Oversolubility in Nanoconfined Liquids: Review and Perspectives for Adsorbent Design. *Microporous Mesoporous Mater.* **2019**, *288*, 109561. [CrossRef]
10. Bahmanzadegan, F.; Ghaemi, A. Modification and Functionalization of Zeolites to Improve the Efficiency of CO_2 Adsorption: A Review. *Case Stud. Chem. Environ. Eng.* **2024**, *9*, 100564. [CrossRef]
11. Zhang, Z.; Ding, H.; Pan, W.; Ma, J.; Zhang, K.; Zhao, Y.; Song, J.; Wei, C.; Lin, F. Research Progress of Metal–Organic Frameworks (MOFs) for CO_2 Conversion in CCUS. *J. Energy Inst.* **2023**, *108*, 101226. [CrossRef]
12. Kong, M.; Song, L.; Liao, H.; Zhang, S.; Wang, Y.; Deng, X.; Feng, W. A Review on Development of Post-Combustion CO_2 Capture Technologies: Performance of Carbon-Based, Zeolites and MOFs Adsorbents. *Fuel* **2024**, *371*, 132103. [CrossRef]
13. Chen, C.; Park, D.-W.; Ahn, W.-S. CO_2 Capture Using Zeolite 13X Prepared from Bentonite. *Appl. Surf. Sci.* **2014**, *292*, 63–67. [CrossRef]
14. Jedli, H.; Almoneef, M.M.; Mbarek, M.; Jbara, A.; Slimi, K. Adsorption of CO_2 onto Zeolite ZSM-5: Kinetic, Equilibrium and Thermodynamic Studies. *Fuel* **2022**, *321*, 124097. [CrossRef]
15. Panda, D.; Kumar, E.A.; Singh, S.K. Introducing Mesoporosity in Zeolite 4A Bodies for Rapid CO_2 Capture. *J. CO_2 Util.* **2020**, *40*, 101223. [CrossRef]
16. Usman, M.; Ghanem, A.S.; Niaz Ali Shah, S.; Garba, M.D.; Yusuf Khan, M.; Khan, S.; Humayun, M.; Laeeq Khan, A. A Review on SAPO-34 Zeolite Materials for CO_2 Capture and Conversion. *Chem. Rec.* **2022**, *22*, e202200039. [CrossRef]
17. Díaz-García, M.; Mayoral, Á.; Díaz, I.; Sánchez-Sánchez, M. Nanoscaled M-MOF-74 Materials Prepared at Room Temperature. *Cryst. Growth Des.* **2014**, *14*, 2479–2487. [CrossRef]

18. Lin, K.-S.; Adhikari, A.K.; Ku, C.-N.; Chiang, C.-L.; Kuo, H. Synthesis and Characterization of Porous HKUST-1 Metal Organic Frameworks for Hydrogen Storage. *Int. J. Hydrog. Energy* **2012**, *37*, 13865–13871. [CrossRef]
19. Saha, D.; Deng, S. Hydrogen Adsorption on Metal-Organic Framework MOF-177. *Tsinghua Sci. Technol.* **2010**, *15*, 363–376. [CrossRef]
20. Demir, H.; Aksu, G.O.; Gulbalkan, H.C.; Keskin, S. MOF Membranes for CO_2 Capture: Past, Present and Future. *Carbon Capture Sci. Technol.* **2022**, *2*, 100026. [CrossRef]
21. Tavagh Mohammadi, B.; Jahanbani Ghahfarokhi, A.; Grimstad, A.-A. A Review of Modeling Approaches for CO_2 Injection into Depleted Gas Reservoirs: Coupling Transient Wellbore and Reservoir Dynamics. *Int. J. Greenh. Gas Control* **2025**, *145*, 104406. [CrossRef]
22. Zhao, G.; Li, Z.; Cheng, B.; Zhuang, X.; Lin, T. Hierarchical Porous Metal Organic Framework Aerogel for Highly Efficient CO_2 Adsorption. *Sep. Purif. Technol.* **2023**, *315*, 123754. [CrossRef]
23. Bello, A.; Dorhjie, D.B.; Ivanova, A.; Cheremisin, A. A Numerical Feasibility Study of CO_2 Foam for Carbon Utilization and Storage in a Depleted, High Salinity, Carbonate Oil Reservoir. *Sci. Rep.* **2024**, *14*, 20585. [CrossRef] [PubMed]
24. Neubertová, V.; Švorčík, V.; Kolská, Z. Amino-Modified ZIF-8 for Enhanced CO_2 Capture: Synthesis, Characterization and Performance Evaluation. *Microporous Mesoporous Mater.* **2024**, *366*, 112956. [CrossRef]
25. Salunkhe, B.; Schuman, T.; Al Brahim, A.; Bai, B. Ultra-High Temperature Resistant Preformed Particle Gels for Enhanced Oil Recovery. *Chem. Eng. J.* **2021**, *426*, 130712. [CrossRef]
26. Choi, H.L.; Jeong, Y.; Lee, H.; Bae, T.-H. High-Performance Mixed-Matrix Membranes Using a Zeolite@MOF Core–Shell Structure Synthesized via Ion-Exchange-Induced Crystallization and Post-Synthetic Conversion. *JACS Au* **2024**, *4*, 253–262. [CrossRef]
27. Ullah, S.; Rehman, A.U.; Najam, T.; Hossain, I.; Anjum, S.; Ali, R.; Shahid, M.U.; Shah, S.S.A.; Nazir, M.A. Advances in Metal-Organic Framework@activated Carbon (MOF@AC) Composite Materials: Synthesis, Characteristics and Applications. *J. Ind. Eng. Chem.* **2024**, *137*, 87–105. [CrossRef]
28. Park, H.; Yan, X.; Zhu, R.; Huerta, E.A.; Chaudhuri, S.; Cooper, D.; Foster, I.; Tajkhorshid, E. A Generative Artificial Intelligence Framework Based on a Molecular Diffusion Model for the Design of Metal-Organic Frameworks for Carbon Capture. *Commun. Chem.* **2024**, *7*, 21. [CrossRef]
29. Dalla Longa, F.; Detz, R.; Van Der Zwaan, B. Integrated Assessment Projections for the Impact of Innovation on CCS Deployment in Europe. *Int. J. Greenh. Gas Control* **2020**, *103*, 103133. [CrossRef]
30. Silveira, T.; Awano, C.M.; Donatti, D.A.; Vicente, F.S.; Vollet, D.R. About the thermal stability and pore elimination in the ordered hexagonal mesoporous silica SBA-15. *Microporous Mesoporous Mater.* **2014**, *190*, 227–233. [CrossRef]
31. Ioannidou, O.; Zabaniotou, A. Agricultural residues as precursors for activated carbon production—A review. *Renew. Sustain. Energy Rev.* **2007**, *11*, 1966–2005. [CrossRef]
32. Karan, H.; Roles, J.; Ross, I.L.; Ebrahimi, M.; Rackemann, D.; Rainey, T.; Hankamer, B. Solar biorefinery concept for sustainable co-production of microalgae-based protein and renewable fuel. *J. Clean. Prod.* **2022**, *368*, 132981. [CrossRef]
33. Zhang, Q.; Yan, S.; Yan, X.; Lv, Y. Recent advances in metal-organic frameworks: Synthesis, application and toxicity. *Sci. Total Environ.* **2023**, *902*, 165944. [CrossRef] [PubMed]
34. Pan, S.Y.; Chen, Y.H.; Fan, L.S.; Kim, H.; Gao, X.; Ling, T.C.; Chiang, P.C.; Pei, S.; Gu, G. CO_2 mineralization and utilization by alkaline solid wastes for potential carbon reduction. *Nat Sustain* **2020**, *3*, 399–405. [CrossRef]
35. Zhang, K.; Nalaparaju, A.; Jiang, J. CO_2 Capture in Rht Metal–Organic Frameworks: Multiscale Modeling from Molecular Simulation to Breakthrough Prediction. *J. Mater. Chem. A* **2015**, *3*, 16327–16336. [CrossRef]
36. Indira, V.; Abhitha, K. A Review on Polymer Based Adsorbents for CO_2 Capture. In *IOP Conference Series: Materials Science and Engineering*; IOP Publishing: Bristol, UK, 2021; Volume 1114, p. 012081. [CrossRef]
37. Gajda, A.; Pajdak, A.; Skoczylas, N.; Kudasik, M.; Kozieł, K.; Kurowski, G.; Hyjek, K.; Dymek, K.; Sitarz, M.; Jodłowski, P. Effective Heat Transfer Associated with CO_2 and CH_4 Adsorption on HKUST-1 Metal-Organic Framework Deposited in Situ on Heat Exchanger. *Energy* **2024**, *307*, 132525. [CrossRef]
38. Kim, J.S.; Lee, S.; Kim, T.; Oh, K.H.; Choi, Y.; Byun, H.; Lee, C.-H.; Ravi, S.; Bae, Y.-S. Enhanced Hydrogen Storage via Microporous Defects and Cu(I) Sites in HKUST-1. *Int. J. Hydrog. Energy* **2024**, *90*, 941–949. [CrossRef]