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Chemistry of CO_2 Capture and Storage: From Molecular Interactions to Advanced Functional Materials

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ORIGINAL STUDY

Chemistry of CO_2 Capture and Storage: From Molecular Interactions to Advanced Functional Materials

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ABSTRACT

In light of the industrial development taking place, the burning of fossil fuels for transportation and electricity generation, and the accompanying carbon dioxide emissions, there is an urgent and continuing need to innovate methods of capture and storage, as well as competitive materials to address increasing carbon emissions. This review describes the importance of this procedure and the technologies that help solve this problem, some of which have been adopted by many countries and industrial institutions and differ in their efficiency, cost, and applicability.

Keywords: Carbon dioxide capturing, Purification, Porous materials, CCS

1. Introduction

Due to the rapid advancement of industrial and agricultural practices, the use of fossil fuels, and disparities in human quality of life, substantial quantities of pollutants are released into ecosystems as byproducts of these activities, posing a significant risk to human health [1–4]. Throughout the time of the Industrial Revolution, the atmospheric concentration of CO_2 increased by 35% (from approximately 270 parts per million to over 380 parts per million), leading to global warming, climate change, and ecosystem disruptions [5]. The temperature rise will lead to sea-level rise and Arctic ice melt, which will greatly harm the quality of life on Earth [6].

Capturing or converting carbon dioxide to mitigate climate change is crucial to protecting the environment.

It is the only way that allows the continued use of fossil fuels in industries and various purposes in the current century without exacerbating the global warming crisis. Finding

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suitable media for storing carbon dioxide through various physical and chemical trapping mechanisms has been the subject of ongoing research by the scientific community in recent decades, with the aim of developing more efficient and less expensive technologies while accounting for safety and ease of use.

The particular risks associated with carbon dioxide storage occur during both the operational and post-operation phases, with the primary concern being the potential for acute or chronic CO_2 leakage from the storage site. Therefore, it is essential to accurately assess and manage local health, safety, and environmental risks. Currently, there are very few practical processes, so many other methods are being studied, taking into account the time factor, as the concentration of carbon dioxide continues to increase every day. It is likely to reach 420 ppm by January 2023 (rate of increase: $\sim$0.5 ppm per year) [7].

The energy required to break the carbon dioxide double bond, known as bond dissociation energy, is significantly high at 532 kJ mol^{-1} [8].

2. Relationship between CO_2, GHGs, and global warming

Many chemical compounds in the atmosphere function as greenhouse gases (GHGs), which permit sunlight (shortwave radiation) to pass unimpeded through the Earth's atmosphere, thereby warming the land and oceans. The heated Earth subsequently releases this energy as infrared light (long-wave radiation), which is not visible to the human eye. Some of this infrared radiation escapes into space; however, greenhouse gases obstruct the passage of infrared rays through the atmosphere. They absorb a portion of this radiation and re-emit it back to the Earth's surface. This process, known as global warming, occurs naturally and is essential for maintaining the Earth's surface temperature. Without the effects of global warming, the average surface temperature would be approximately 60 degrees Fahrenheit cooler, rendering our current lifestyle unfeasible [9].

A variety of atmospheric chemicals may absorb heat, such CO_2, CH_4, N_2O, and chemical and industrial gases, including hydrofluorocarbons, perfluorocarbons, and sulphur hexafluoride. Atmospheric concentrations of several key greenhouse gases have risen substantially since the onset of large-scale industrial activities. Industrialization occurred about 200 years ago.

Carbon dioxide is the principal greenhouse gas (GHG) accountable for warming temperatures [10–16]. CO_2 emissions are rising predominantly due to increased fuel consumption in the industrial sector. This escalation has triggered climatic changes, including floods and droughts, due to disruptions in the natural balance. Recently, research efforts have focused on developing methods to capture greenhouse gases, including carbon dioxide [17, 18]. These systems enable efficient storage and transport of gases to protect the environment. Developing new materials and systems for the efficient storage and transport of gases is an important area of research.

Internationally, carbon capture and storage are important tools for decarbonizing the energy system. The capture, utilization, and storage of carbon dioxide must be a core component of strategies to eliminate net global greenhouse gas emissions, as efforts are underway to reach net zero by mid-century and to achieve global climate change objectives [19], as shown in Fig. 1.

3. Carbon dioxide capture and storage (CCS)

The Goddard Institute for Studies (GISS) has recognized that global warming is coming because carbon dioxide concentrations have exceeded 400 ppm since 2013 [20–23]. Not

Fig. 1. A conceptual illustration of CO_2 emissions, greenhouse warming, and underground carbon capture and storage (CCS) as a pathway to mitigate climate change.

only that, atmospheric carbon dioxide levels are expected to reach 580 parts per million if fossil fuel use continues at the same pace over the next 50 years, leading to major global impacts on ecosystems. They will live in a hotter and more polluted world [24, 25].

Reducing carbon dioxide emissions into the atmosphere is a challenge; therefore, many efforts should be directed towards solving this problem. Several strategies can be adopted to overcome problems associated with increased greenhouse gas emissions. The first approach requires using an alternative green and renewable energy source to replace fossil fuels [26]. The use of solar energy, wind energy, nuclear power, and biomass represents an appealing and environmentally friendly approach to reducing CO_2 emissions [27]. This approach aims to prevent or eliminate gas emissions at the source. However, these renewable sources cannot provide enough energy to meet the growing industrial demand. In addition, these energy sources are more expensive than those obtained from fossil fuels [28].

The second strategy is a remedial approach that aims to reduce atmospheric gas emissions by using storage media [29].

For example, ammonia and ethanolamine have been used to remove carbon dioxide from natural gas [30]. Amines are volatile and poisonous, presenting environmental risks and limiting their application, and capture of CO_2 necessitates the separation and adsorption at elevated pressures onto porous substrates functioning as adsorbent particles [31–34]. Porous materials have several properties that can be used to capture carbon dioxide, and porous carbons (PCs) have received much attention for various catalytic reactions [35–37]. Their distinct porous structures (i.e., porosity < 2 nm, 2 nm $<$ porosity < 50 nm, and macropores > 50 nm) enable efficient adsorption of CCS gases and also facilitate catalytic reactions. [38–41] he most prevalent CO_2 adsorbents include zeolites, carbon-based materials, cross-linked polymers, inorganic materials, and metal-organic frameworks [42–45]. However, these materials have significant limitations. For instance, metal oxides exhibit limited adsorption capacity [46, 47], while activated carbon lacks selectivity and is unsuitable for flue gases [48–52]. Although organic polymers possess a high surface area [53–61], further research is necessary to enhance their performance.

Currently, there are very few operations worldwide that are practically based on such methods, such as injecting carbon dioxide into the ground. Still, this method has its own pros and cons, so research is underway to apply other methods, taking into account the time factor, as the concentration of carbon dioxide continues to increase. every day. It is likely to reach 420 ppm by January 2023 (rate of increase: ~0.5 ppm per year) [62].

Carbon capture, utilization, and storage (CCUS) technologies have been extensively researched to mitigate direct CO_2 emissions and to sequester atmospheric CO_2 [63, 64]. Various chemical processes for carbon capture and storage (CCS) have been developed, employing sorbents that selectively bind CO_2 molecules across a wide range of temperatures and pressures [65]. Additionally, significant efforts have been made to convert CO_2 into carbon through electrocatalysis, producing compounds such as formate, synthetic gases, alcohols, and fuels, or utilizing CO_2 as a raw material for metal-based carbon dioxide batteries for cleaning and energy storage [66, 67]. Despite these advancements, several challenges remain to be addressed to enable industrial-scale applications (Fig. 2).

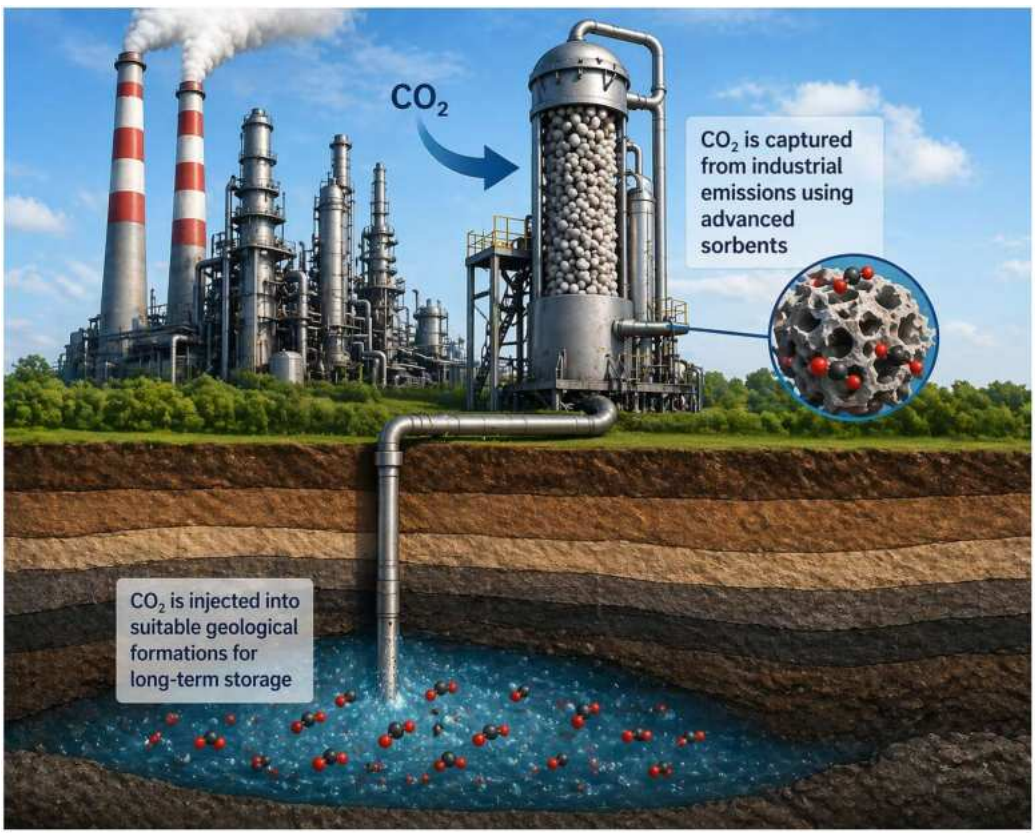

Fig. 2. A schematic representation of industrial CO_2 capture using advanced sorbents and its subsequent injection into deep geological formations for long-term storage (CCS).

- **Outlines the most relevant technologies for CO2 purification:**
- Absorption might be chemical or physical. In the first example, an absorbent molecule reacts with CO2. Second, the physical solvent dissolves CO_2 and weakly binds gas and

solvent molecules to retain it in solution. Regeneration often involves pressure swings [68].

- Adsorption: A porous substance with large surface area selects CO_2 molecules via intermolecular interactions. Temperature, partial pressures, surface forces, and pore-size distribution affect gas selective adsorption. Adsorbent beds are mostly renewed by pressure and temperature swings [69–71].
- Membranes: Semi-permeable barriers composed of organic or inorganic materials may separate substances by diverse methods, such as solution/diffusion, adsorption/diffusion, molecular sieving, ionic transport, and assisted transport [72], Fig. 3.

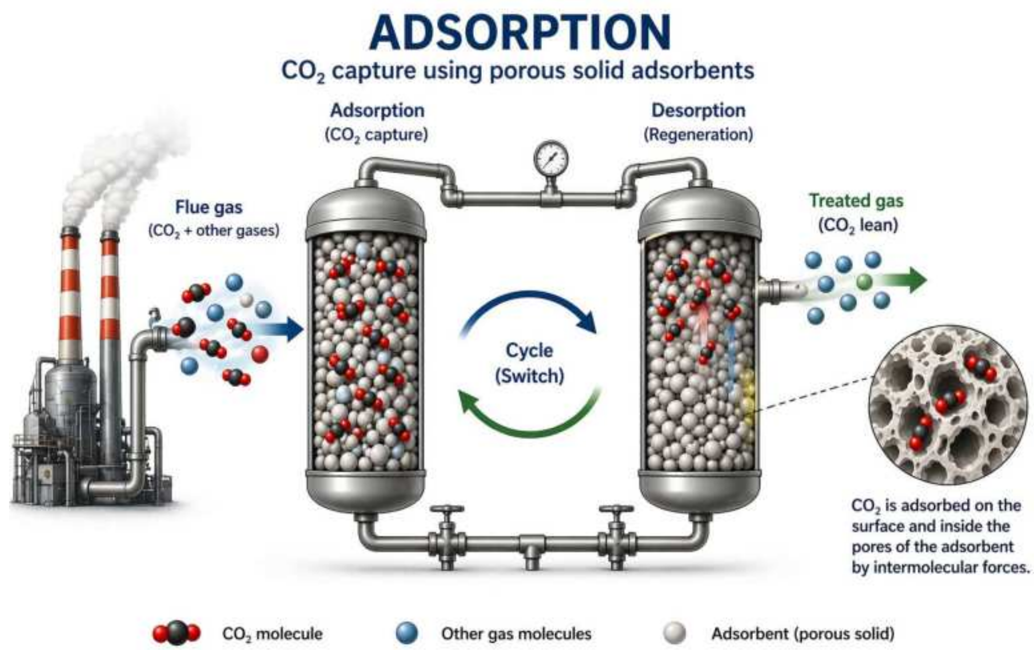

Fig. 3. Schematic illustration of CO_2 capture by adsorption using porous solid materials, showing adsorption–desorption cycles for efficient gas separation.

- Cryogenic separation process: Distillation of CO_2 can be performed at low temperatures and high pressures. Hybrid processes: Two or more separation subsystems can be combined to improve separation efficiency and reduce costs, as in combined adsorption/membrane systems [73, 74].
- The initial stage of hydrate separation entails exposing the CO_2-rich exhaust gas stream to water under high pressure, resulting in hydrate formation. The formation of hydrates captures CO_2. Following separation, the hydrates dissociate, releasing pure carbon dioxide. [75].
- Biofixation Autotrophic microorganisms fix CO_2 to synthesize biological organic materials and extracellular products, capturing CO_2 from the atmosphere or other sources (including flue gases) with the help of different cultivation systems. As a result, CO_2 is sequestered as organic biomass, which can be converted into various chemicals and biofuels through biorefining processes [76, 77].
- Mineralization refers to the reaction of CO2 with substances that contain alkaline earth oxides, such as magnesium oxide (MgO) and calcium oxide (CaO). Useful carbonate products can be derived from industrial byproducts and waste materials [78].

- Calcium looping processes (CLP) refer to a specific mineralization technique that extracts CO_2 from flue gas by converting calcium oxide (CaO) into calcium carbonate ($CaCO_3$) [79].
- Molten carbonate fuel cell (MCFC) technology employs a molten carbonate salt suspended within a porous ceramic matrix as an electrolyte, facilitating the internal reforming reaction, which converts alternative fuels into hydrogen [80].
- Electrochemically mediated amine regeneration (EMAR) technology represents an alternative method for regenerating amines used in carbon capture from flue gas sources, eliminating the need for thermal regeneration, thereby conserving energy and enhancing CO2 capture efficiency [81].

4. Conclusion

Carbon capture, utilization, and storage (CCUS) technologies represent a critical and rapidly advancing strategy for mitigating anthropogenic CO_2 emissions and addressing global climate change. This review highlights that conventional capture methods, namely absorption, adsorption, and membrane separation-remain the backbone of current industrial applications, each offering distinct advantages in terms of efficiency, selectivity, and operational flexibility. Among these, adsorption using porous materials has emerged as a particularly promising approach due to its high surface area, tunable pore structure, and energy-efficient regeneration processes. In parallel, significant progress has been achieved in CO_2 utilization pathways, especially through electrocatalytic conversion into value-added chemicals such as formate, syngas, and fuels, as well as their integration into emerging energy storage systems. These developments support the transition toward a circular carbon economy, where CO_2 is no longer viewed solely as a waste product but as a valuable resource. Despite these advancements, several challenges continue to hinder large-scale deployment, including high operational costs, energy requirements for regeneration, material stability, and process scalability. Therefore, future research should focus on the rational design of advanced materials (e.g., metal-organic frameworks, porous polymers, and hybrid nanocomposites), optimization of process integration, and development of cost-effective, sustainable systems. Overall, CCUS technologies are indispensable for achieving global decarbonization targets and net-zero emissions. Continued innovation, combined with supportive policy frameworks and industrial implementation, will be essential to unlock their full potential and ensure a sustainable environmental future.

Conflicts of interest

The authors declare that there are no conflicts of interest regerding the publication of the manuscript.

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ORIGINAL STUDY

Chemistry of CO_2 Capture and Storage: From Molecular Interactions to Advanced Functional Materials

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ABSTRACT

In light of the industrial development taking place, the burning of fossil fuels for transportation and electricity generation, and the accompanying carbon dioxide emissions, there is an urgent and continuing need to innovate methods of capture and storage, as well as competitive materials to address increasing carbon emissions. This review describes the importance of this procedure and the technologies that help solve this problem, some of which have been adopted by many countries and industrial institutions and differ in their efficiency, cost, and applicability.

Keywords: Carbon dioxide capturing, Purification, Porous materials, CCS

1. Introduction

Due to the rapid advancement of industrial and agricultural practices, the use of fossil fuels, and disparities in human quality of life, substantial quantities of pollutants are released into ecosystems as byproducts of these activities, posing a significant risk to human health [1–4]. Throughout the time of the Industrial Revolution, the atmospheric concentration of CO_2 increased by 35% (from approximately 270 parts per million to over 380 parts per million), leading to global warming, climate change, and ecosystem disruptions [5]. The temperature rise will lead to sea-level rise and Arctic ice melt, which will greatly harm the quality of life on Earth [6].

Capturing or converting carbon dioxide to mitigate climate change is crucial to protecting the environment.

It is the only way that allows the continued use of fossil fuels in industries and various purposes in the current century without exacerbating the global warming crisis. Finding

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suitable media for storing carbon dioxide through various physical and chemical trapping mechanisms has been the subject of ongoing research by the scientific community in recent decades, with the aim of developing more efficient and less expensive technologies while accounting for safety and ease of use.

The particular risks associated with carbon dioxide storage occur during both the operational and post-operation phases, with the primary concern being the potential for acute or chronic CO_2 leakage from the storage site. Therefore, it is essential to accurately assess and manage local health, safety, and environmental risks. Currently, there are very few practical processes, so many other methods are being studied, taking into account the time factor, as the concentration of carbon dioxide continues to increase every day. It is likely to reach 420 ppm by January 2023 (rate of increase: $\sim$0.5 ppm per year) [7].

The energy required to break the carbon dioxide double bond, known as bond dissociation energy, is significantly high at 532 kJ mol^{-1} [8].

2. Relationship between CO_2, GHGs, and global warming

Many chemical compounds in the atmosphere function as greenhouse gases (GHGs), which permit sunlight (shortwave radiation) to pass unimpeded through the Earth's atmosphere, thereby warming the land and oceans. The heated Earth subsequently releases this energy as infrared light (long-wave radiation), which is not visible to the human eye. Some of this infrared radiation escapes into space; however, greenhouse gases obstruct the passage of infrared rays through the atmosphere. They absorb a portion of this radiation and re-emit it back to the Earth's surface. This process, known as global warming, occurs naturally and is essential for maintaining the Earth's surface temperature. Without the effects of global warming, the average surface temperature would be approximately 60 degrees Fahrenheit cooler, rendering our current lifestyle unfeasible [9].

A variety of atmospheric chemicals may absorb heat, such CO_2, CH_4, N_2O, and chemical and industrial gases, including hydrofluorocarbons, perfluorocarbons, and sulphur hexafluoride. Atmospheric concentrations of several key greenhouse gases have risen substantially since the onset of large-scale industrial activities. Industrialization occurred about 200 years ago.

Carbon dioxide is the principal greenhouse gas (GHG) accountable for warming temperatures [10–16]. CO_2 emissions are rising predominantly due to increased fuel consumption in the industrial sector. This escalation has triggered climatic changes, including floods and droughts, due to disruptions in the natural balance. Recently, research efforts have focused on developing methods to capture greenhouse gases, including carbon dioxide [17, 18]. These systems enable efficient storage and transport of gases to protect the environment. Developing new materials and systems for the efficient storage and transport of gases is an important area of research.

Internationally, carbon capture and storage are important tools for decarbonizing the energy system. The capture, utilization, and storage of carbon dioxide must be a core component of strategies to eliminate net global greenhouse gas emissions, as efforts are underway to reach net zero by mid-century and to achieve global climate change objectives [19], as shown in Fig. 1.

3. Carbon dioxide capture and storage (CCS)

The Goddard Institute for Studies (GISS) has recognized that global warming is coming because carbon dioxide concentrations have exceeded 400 ppm since 2013 [20–23]. Not

Fig. 1. A conceptual illustration of CO_2 emissions, greenhouse warming, and underground carbon capture and storage (CCS) as a pathway to mitigate climate change.

only that, atmospheric carbon dioxide levels are expected to reach 580 parts per million if fossil fuel use continues at the same pace over the next 50 years, leading to major global impacts on ecosystems. They will live in a hotter and more polluted world [24, 25].

Reducing carbon dioxide emissions into the atmosphere is a challenge; therefore, many efforts should be directed towards solving this problem. Several strategies can be adopted to overcome problems associated with increased greenhouse gas emissions. The first approach requires using an alternative green and renewable energy source to replace fossil fuels [26]. The use of solar energy, wind energy, nuclear power, and biomass represents an appealing and environmentally friendly approach to reducing CO_2 emissions [27]. This approach aims to prevent or eliminate gas emissions at the source. However, these renewable sources cannot provide enough energy to meet the growing industrial demand. In addition, these energy sources are more expensive than those obtained from fossil fuels [28].

The second strategy is a remedial approach that aims to reduce atmospheric gas emissions by using storage media [29].

For example, ammonia and ethanolamine have been used to remove carbon dioxide from natural gas [30]. Amines are volatile and poisonous, presenting environmental risks and limiting their application, and capture of CO_2 necessitates the separation and adsorption at elevated pressures onto porous substrates functioning as adsorbent particles [31–34]. Porous materials have several properties that can be used to capture carbon dioxide, and porous carbons (PCs) have received much attention for various catalytic reactions [35–37]. Their distinct porous structures (i.e., porosity <2 nm, 2 nm $<$ porosity <50 nm, and macropores >50 nm) enable efficient adsorption of CCS gases and also facilitate catalytic reactions. [38–41] he most prevalent CO_2 adsorbents include zeolites, carbon-based materials, cross-linked polymers, inorganic materials, and metal-organic frameworks [42–45]. However, these materials have significant limitations. For instance, metal oxides exhibit limited adsorption capacity [46, 47], while activated carbon lacks selectivity and is unsuitable for flue gases [48–52]. Although organic polymers possess a high surface area [53–61], further research is necessary to enhance their performance.

Currently, there are very few operations worldwide that are practically based on such methods, such as injecting carbon dioxide into the ground. Still, this method has its own pros and cons, so research is underway to apply other methods, taking into account the time factor, as the concentration of carbon dioxide continues to increase. every day. It is likely to reach 420 ppm by January 2023 (rate of increase: ~0.5 ppm per year) [62].

Carbon capture, utilization, and storage (CCUS) technologies have been extensively researched to mitigate direct CO_2 emissions and to sequester atmospheric CO_2 [63, 64]. Various chemical processes for carbon capture and storage (CCS) have been developed, employing sorbents that selectively bind CO_2 molecules across a wide range of temperatures and pressures [65]. Additionally, significant efforts have been made to convert CO_2 into carbon through electrocatalysis, producing compounds such as formate, synthetic gases, alcohols, and fuels, or utilizing CO_2 as a raw material for metal-based carbon dioxide batteries for cleaning and energy storage [66, 67]. Despite these advancements, several challenges remain to be addressed to enable industrial-scale applications (Fig. 2).

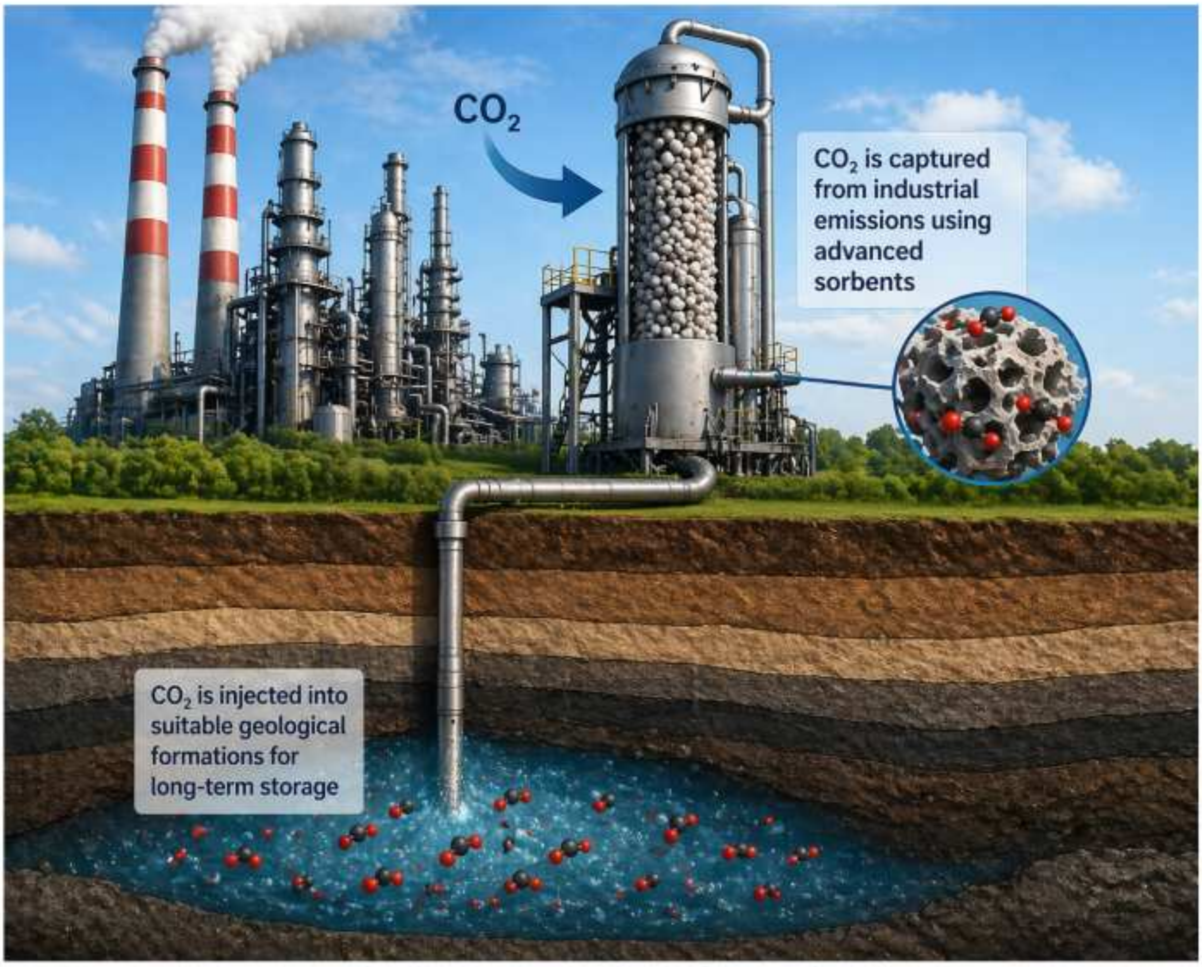

Fig. 2. A schematic representation of industrial CO_2 capture using advanced sorbents and its subsequent injection into deep geological formations for long-term storage (CCS).

- **Outlines the most relevant technologies for CO2 purification:**
- Absorption might be chemical or physical. In the first example, an absorbent molecule reacts with CO2. Second, the physical solvent dissolves CO_2 and weakly binds gas and

solvent molecules to retain it in solution. Regeneration often involves pressure swings [68].

- Adsorption: A porous substance with large surface area selects CO_2 molecules via intermolecular interactions. Temperature, partial pressures, surface forces, and pore-size distribution affect gas selective adsorption. Adsorbent beds are mostly renewed by pressure and temperature swings [69–71].
- Membranes: Semi-permeable barriers composed of organic or inorganic materials may separate substances by diverse methods, such as solution/diffusion, adsorption/diffusion, molecular sieving, ionic transport, and assisted transport [72], Fig. 3.

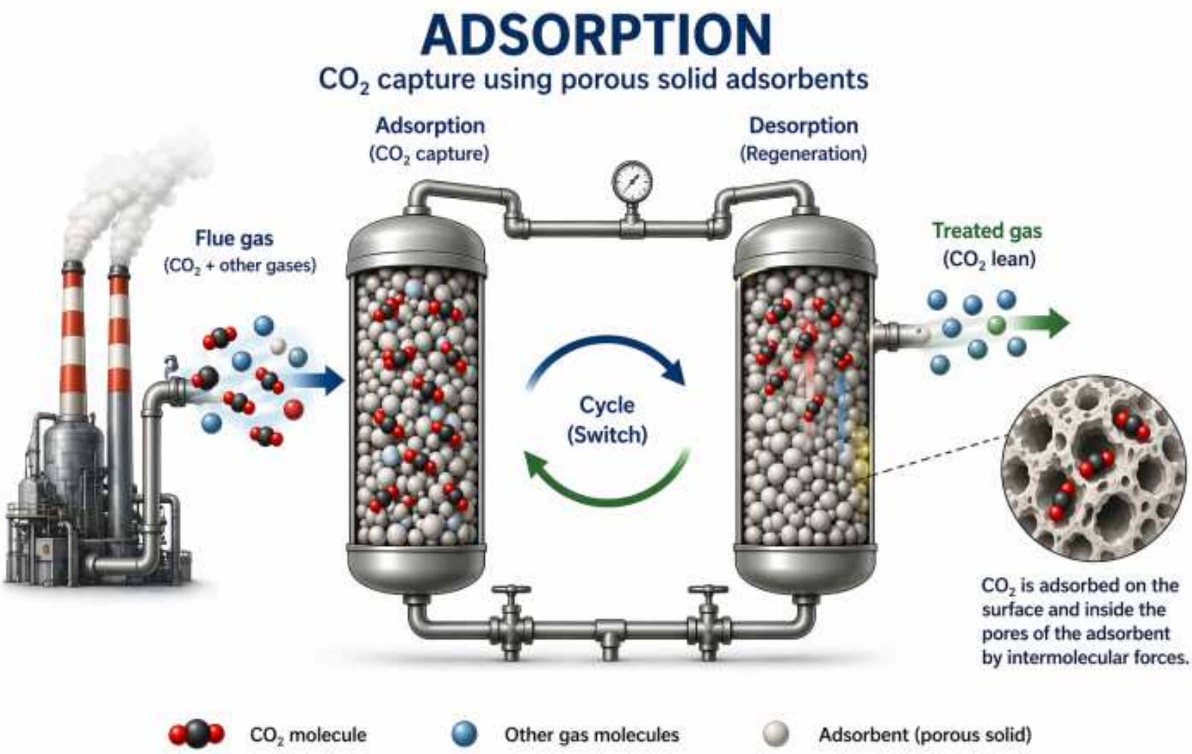

Fig. 3. Schematic illustration of CO_2 capture by adsorption using porous solid materials, showing adsorption–desorption cycles for efficient gas separation.

- Cryogenic separation process: Distillation of CO_2 can be performed at low temperatures and high pressures. Hybrid processes: Two or more separation subsystems can be combined to improve separation efficiency and reduce costs, as in combined adsorption/membrane systems [73, 74].
- The initial stage of hydrate separation entails exposing the CO_2-rich exhaust gas stream to water under high pressure, resulting in hydrate formation. The formation of hydrates captures CO_2. Following separation, the hydrates dissociate, releasing pure carbon dioxide. [75].
- Biofixation Autotrophic microorganisms fix CO_2 to synthesize biological organic materials and extracellular products, capturing CO_2 from the atmosphere or other sources (including flue gases) with the help of different cultivation systems. As a result, CO_2 is sequestered as organic biomass, which can be converted into various chemicals and biofuels through biorefining processes [76, 77].
- Mineralization refers to the reaction of CO2 with substances that contain alkaline earth oxides, such as magnesium oxide (MgO) and calcium oxide (CaO). Useful carbonate products can be derived from industrial byproducts and waste materials [78].

- Calcium looping processes (CLP) refer to a specific mineralization technique that extracts CO_2 from flue gas by converting calcium oxide (CaO) into calcium carbonate ($CaCO_3$) [79].
- Molten carbonate fuel cell (MCFC) technology employs a molten carbonate salt suspended within a porous ceramic matrix as an electrolyte, facilitating the internal reforming reaction, which converts alternative fuels into hydrogen [80].
- Electrochemically mediated amine regeneration (EMAR) technology represents an alternative method for regenerating amines used in carbon capture from flue gas sources, eliminating the need for thermal regeneration, thereby conserving energy and enhancing CO2 capture efficiency [81].

4. Conclusion

Carbon capture, utilization, and storage (CCUS) technologies represent a critical and rapidly advancing strategy for mitigating anthropogenic CO_2 emissions and addressing global climate change. This review highlights that conventional capture methods, namely absorption, adsorption, and membrane separation-remain the backbone of current industrial applications, each offering distinct advantages in terms of efficiency, selectivity, and operational flexibility. Among these, adsorption using porous materials has emerged as a particularly promising approach due to its high surface area, tunable pore structure, and energy-efficient regeneration processes. In parallel, significant progress has been achieved in CO_2 utilization pathways, especially through electrocatalytic conversion into value-added chemicals such as formate, syngas, and fuels, as well as their integration into emerging energy storage systems. These developments support the transition toward a circular carbon economy, where CO_2 is no longer viewed solely as a waste product but as a valuable resource. Despite these advancements, several challenges continue to hinder large-scale deployment, including high operational costs, energy requirements for regeneration, material stability, and process scalability. Therefore, future research should focus on the rational design of advanced materials (e.g., metal-organic frameworks, porous polymers, and hybrid nanocomposites), optimization of process integration, and development of cost-effective, sustainable systems. Overall, CCUS technologies are indispensable for achieving global decarbonization targets and net-zero emissions. Continued innovation, combined with supportive policy frameworks and industrial implementation, will be essential to unlock their full potential and ensure a sustainable environmental future.

Conflicts of interest

The authors declare that there are no conflicts of interest regerding the publication of the manuscript.

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