

TECHNOLOGY SELECTION FOR CO₂ PURIFICATION WITH CATALYST AND ADSORBENT

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ABSTRACT

Carbon capture, utilization, and storage (CCUS) projects are increasingly recognized as a pivotal component in mitigating climate change and promoting sustainable industrial practices. This white paper explores the critical decision-making process involved in selecting the appropriate technology for carbon dioxide (CO₂) purification. Topics include oxygen (O₂) removal and the comparative advantages of silica gel over molecular sieves in dehydration.

The removal of O₂ from CO₂ can be achieved through a deoxygenation (DeOxo) process using a catalyst. A few technologies are available for oxygen removal, but one of the most common ones is utilizing either a platinum or palladium-based catalyst. The standard process involves adding hydrogen (H₂) to eliminate O₂, in turn producing water (H₂O).

There are two main technologies for CO₂ dehydration: triethylene glycol (TEG) or temperature swing adsorption (TSA). This paper will focus on TSA and compare two adsorbent material options, silica gel and molecular sieve. Silica gel exhibits superior acid resistance, lower carbon intensity, and an extended operational lifespan, lasting up to five years compared to the two-year lifespan typical of molecular sieves. Silica gel requires a lower regeneration temperature of 160-180 °C (320-356 °F), in contrast to the 230-290 °C (446-554 °F) needed for molecular sieves, which can lead to energy savings during operation. An example of a successful retrofit from an acid-resistant molecular sieve dryer to Sorbead showed significant improvement in changeout frequencies. This example not only informs technology selection for current projects but also contributes to a broader understanding of material performance in CO₂ purification technologies.

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Introduction

Carbon capture, utilization, and storage (CCUS) is critical for reducing carbon dioxide (CO₂) emissions and slowing down global warming. CCUS projects involve separating CO₂ from other gases at major industrial point sources such as natural gas processing plants, refineries, power plants, steel mills, and cement facilities, as well as directly from the atmosphere.

Purification of CO₂ is equally as important as the CO₂ capture. Raw CO₂ streams from amine units often contain residual water, oxygen, hydrocarbons, and other impurities that must be removed before utilization or transport. Achieving product specifications involves a multi-step process, including compression, contaminant removal, and dehydration.

This paper outlines the role of each purification step, highlights the importance of catalyst and adsorbent selection, and presents a successful commercial example that illustrates how silica gel adsorbents enhance performance and longevity in CO₂ dehydration compared to molecular sieve.

Process Overview

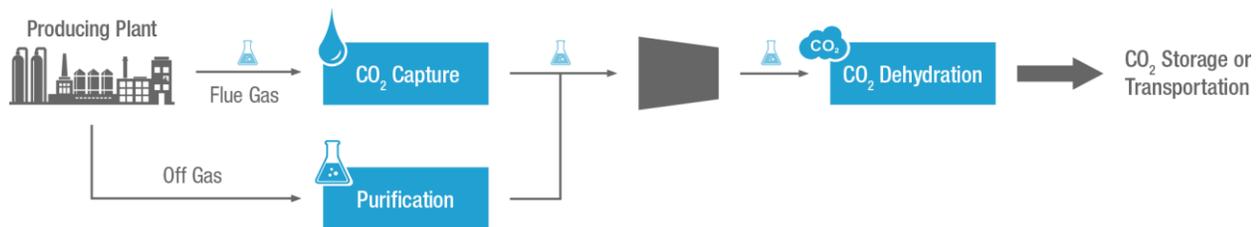


Figure 1 - Simplified process flow diagram for CCUS

CO₂ can come from different point sources, and each point source contains different types of contaminants.¹ After CO₂ is separated from the treated gas, the CO₂ is partially compressed and then undergoes purification. After CO₂ is separated from the treated gas, the CO₂ is partially compressed to reduce the amount of water that must be removed in the drying step and undergoes further purification to meet stringent pipeline specifications. A catalytic oxidation section can be used to remove hydrocarbon, oxygenates, and other carbon-based molecules that may impact the final product quality or liquefaction process. If only oxygen is present or hydrocarbon removal is not required, then a fuel such as hydrogen (H₂) or methane (CH₄) is used to react the trace amount of O₂ left in the CO₂ stream. Water is typically the last component to get removed due to the H₂O that might be generated upstream through the other process steps. The dry CO₂ is further compressed for utilization in industrial processes or converted into a supercritical fluid for transportation and storage. Further complicating the picture for CO₂ purification is the treated gas specifications that vary from project to project and region to region.

CO₂ Transport Specifications in CCUS Projects

CO₂ transport specifications are critical in CCUS projects because they define the composition and properties of CO₂ necessary for safe and efficient transport. These specifications ensure pipeline integrity, prevent corrosion, and mitigate operational risks during compression, shipping, and storage. While CO₂ quality requirements vary by project, common specifications focus on moisture, oxygen, sulfur, hydrocarbon and glycol content due to their significant impact on system reliability.

Transport Conditions and Water Specifications

CO₂ transport methods differ in operating conditions, which influence impurity limits. Pipelines typically carry supercritical CO₂ at 100–150 bara and ambient temperatures, with water specifications ranging from 100–400 ppmv. In contrast, shipping and trucking involve colder temperatures and lower pressures, requiring stricter water limits: <50 ppmv for medium-pressure shipping, <5 ppmv for low-pressure shipping, and <50 ppmv for rail or truck transport. These limits prevent hydrate formation and freezing during liquefaction².

There is no universally agreed upon pipeline specification for CO₂ transport. Regulations require equipment owners to assess safety and set entry requirements, resulting in CO₂ purity recommendations ranging from 93.5 to 96 mol%. This variability requires project-specific specifications and complicates the CO₂ treatment processes. Impurity inlet and outlet concentrations have a large impact on project costs and viability. In addition to impacting project economics, CO₂ specifications should be carefully examined to ensure safety and pipeline integrity.¹

Impurities

CCUS projects typically purify CO₂ for either EOR (gas phase) or saline storage (dense phase). Up until the One Big Beautiful Bill Act (OBBBA) of 2025, the U.S. 45Q previously offered \$60/ton for EOR and \$85/ton for saline storage. OBBBA raised the U.S. 45Q tax credit for CO₂ used in EOR from \$60/ton to \$85/ton. The same credit as for saline storage or permanent geological storage. Projects will require dense phase CO₂ if the product requires transportation via trucks, rail, or ships. This differentiation is important to understand because the corrosion concerns are more prevalent in dense phase.

Impurities can interact and amplify risks. CO₂ and water can form carbonic acid. Under high pressure, the acid becomes stronger as its dissociation increases. Carbonic acid can corrode carbon steel, and the presence of other acidic impurities such as H₂S, NO_x, and SO_x further accelerates corrosion.

Some project economics may favor glycol dehydration; however, glycol is hygroscopic. Glycol attracts water and increases corrosion potential. Oxygen can react with other components, causing unwanted side reactions. Consequently, many CCUS projects adopt conservative specifications: water <50 ppmv for freeze mitigation, glycol <50 ppbv for corrosion control, and oxygen <10 ppmv to minimize undesirable reactions.¹ The focus for this paper will be on technologies that

BASF offers, which does not include TEG. The paper will focus on dehydration using adsorbents and apply to CO₂ projects requiring drying CO₂ in preparation for dense phase.

Purification and Dehydration

Compression

Compression is required to meet delivery pressures and must be modeled before designing the catalyst and adsorbent units. The CO₂ stream at the outlet of the CO₂ separation step is at low pressure. The final CO₂ delivery pressure varies by project, but typically dehydration is done at an intermediate pressure between 20-60 bara, which allows water and water-soluble components such as amine and ammonia to get knocked out downstream of interstage cooling. The catalyst and adsorbent vendors require the stream conditions entering the catalyst and/or adsorbent unit. Therefore, it is important to quantify how much of each contaminant will get removed within the upstream compression stages to ensure optimized and accurate catalyst and adsorbent designs.

Deoxygenation (DeOxo)

If hydrocarbons and other oxidizable components are not present or not required to get removed, then a DeOxo is often used in CCUS for the purpose of O₂ removal. The amount of O₂ which might be present may typically range from 1-100 ppmv and presents a challenge for CO₂ pipelines where specs may range from 1-20 ppmv. Like CatOx, DeOxo uses either a platinum and/or palladium catalyst. The catalyst works by converting the O₂ to water using a reactant, most typically H₂, due to its low light-off temperature and high conversion efficiency.

In some cases, H₂ is not available at the desired location, and it can be a costly addition if imports of H₂ are required. Besides H₂, other fuel sources such as methane, ethane, carbon monoxide, and other hydrocarbons that are already present in the CO₂ or available fuel gas at the site could be used. It is most common to install a DeOxo reactor upstream of a dehydration unit, which will typically come from the second stage compression at >20 bara and >140°C. Any additional heat required to reach the light-off temperature of the hydrocarbon would require additional energy or OpEx. This is why H₂ is the most common fuel source to use for CCUS projects as the light-off temperature is >30°C. The additional benefit of using H₂ is the ability to hydrogenate NO_x that could be present in many post-combustion applications which could be beneficial to projects that have a low tolerance to NO_x in the CO₂ product specification.

Dehydration

Following the DeOxo unit, the gas needs to be dehydrated to <50ppmv to meet pipeline transportation specifications. For the lower glycol and water specifications considered in this paper, Temperature Swing Adsorption (TSA) was considered. However, TEG is used to dehydrate CO₂ in many locations that feed pipelines, Nonetheless, for pipeline specifications that have a low maximum glycol specification, e.g., <50 ppb-mol, a sacrificial guard bed may be needed, which adds complexity and cost to the project.

The TSA process utilizes solid adsorbents in a fixed bed. Wet CO₂ is an acid gas; CO₂ and dense phase water form carbonic acid and can neutralize some adsorbents that have basic sites. The adsorbent for CO₂ dehydration must be acid resistant to prolong the bed life in CO₂ service since

although a dense phase is not expected, it is often present due to carryover or cooling. Sorbead is a specialty aluminosilicate gel that is produced using a unique oil drop process. Sorbead has a lower regeneration temperature (160-180°C) leading to lower OpEx and lower energy requirements compared to molecular sieves (regeneration temperature 230-280°C). The lower regeneration temperature, higher water capacity, and acid resistance of Sorbead makes it the recommended material for CO₂ dehydration. The material properties of Sorbead and molecular sieve are shown in the table below.

Table 2 - Material characteristics comparison of Sorbead and molecular sieves.

	Sorbead	Molecular Sieve
Morphology	Amorphous	Zeolite w/ clay binder
Crush Strength (N)	170	50
Attrition (wt.%)	0.05	0.2
Equilibrium H ₂ O capacity	45%	22%
Stability to liquids	Yes	No
Acid resistant	Yes	No

A TSA process works by adsorbing contaminants onto an adsorbent at low temperatures, then regenerating the bed at a higher temperature which drives off the adsorbed contaminants. The hot regeneration gas flows through a cooler and separator, where condensed water is removed to prevent building up in the system, before being recycled to the front of the unit. TSA units with Sorbead are designed to use wet (feed) gas for regeneration, eliminating the need for a regeneration gas compressor, bringing down the overall CapEx of the project and reducing the project execution time due to the long lead time of compressors. Sorbead TSAs can cycle >10,000 times in a lifetime, leading to many years of operation before a change out is required. A simplified TSA process flow diagram with silica gel is shown in Figure 2.

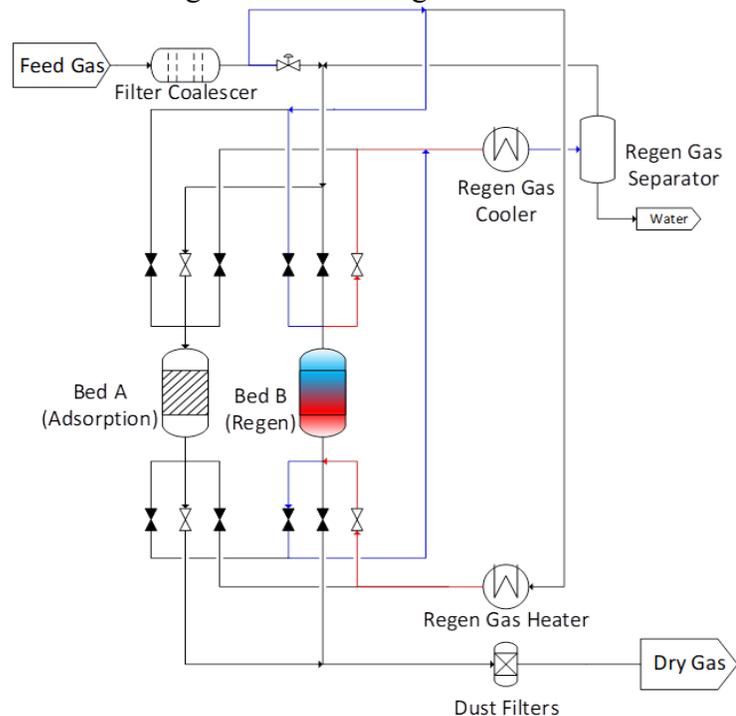


Figure 2 - Simplified process flow diagram of a TSA unit with wet gas regeneration scheme

CO₂ Dehydration Commercial Example

Background

The adsorbent selection is a critical decision for maximizing the performance of a CO₂ dehydration unit. This section will cover one example of how changing the type of adsorbent from acid-resistant molecular sieve to Sorbead can greatly improve the adsorbent changeout interval. The example will cover a retrofit at Whitecap Resources Inc.

Weyburn facility in Saskatchewan, which is one of the world's largest and most recognized CCUS plants. Since 2000, it has safely stored 41 million tons of third-party CO₂, primarily in the Midale formation.

Retrofit from acid resistant molecular sieve to aluminosilicate gel

Whitecap Resources Inc. installed a Temperature Swing Adsorption (TSA) unit for the dehydration of CO₂ in 2013. The feed consists primarily of carbon dioxide at 92 mol%, with a small fraction of heavier hydrocarbons (C₆+) at 0.164 mol% and saturated water. The system operates with a four-tower configuration, including two adsorption towers, one heating tower, and one cooling tower. The TSA unit was originally designed with acid-resistant molecular sieves for acid gas dehydration. The acid-resistant molecular sieve design experienced rapid degradation and had a 3-6 month lifetime before change out was required. Different types of acid-resistant molecular sieves from various suppliers were used without success to extend the bed life.

In 2016, BASF was engaged to troubleshoot the issue. Sorbead was recommended for the following reasons:

- Sorbead will help protect the molecular sieves in the mass transfer zone from heavy hydrocarbons and coking.
- Sorbead WS is not a binder containing product and it is water stable; therefore, unaffected by retrograde reflux condensation as typically seen in some of the MS dehydrators.
- Sorbead WS is a more structurally stable and liquid resilient product when compared to molecular sieves.
- Sorbead is proven to be impervious to acid attacks by wet acid gas stream.

The discussion led to a 2018 change to a layered configuration of Sorbead and acid-resistant molecular sieve (1:1). This bed configuration led to a significant increase in lifetime and was not replaced again until 2021. The addition of Sorbead in the top half of the adsorbent beds increased the lifetime from 6 months to >3 years, a six-fold increase in adsorbent lifespan. After further review, BASF recommended utilizing Sorbead throughout the bed and the removal of all molecular sieves. This configuration, with 100% Sorbead in the bed, was operated for over 4 years before the next change out was required. Molecular sieves are employed when tight water specifications (<1 ppmv) are required. However, in the case of Weyburn and most CCS projects, that strict water specification is not required. Sorbead is recommended instead as a more robust material that does not suffer from the well-known degradation modes of molecular sieves.

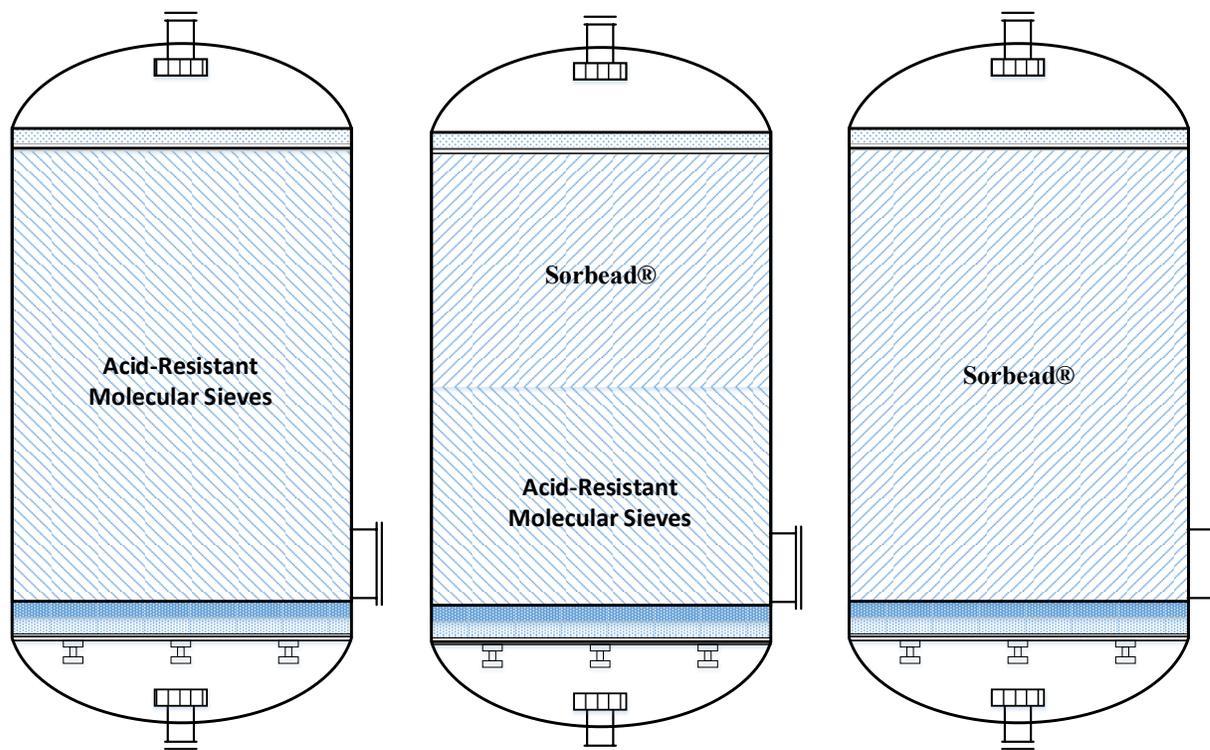


Figure 3 - Different loading configuration

During the 2018 molecular sieve changeout, spent samples revealed significant coking levels of 7–14% attributed to heavy hydrocarbons. Additionally, 40% of the fines were detected in the mid-section of the bed, likely due to regeneration reflux issues. Solid caking of the molecular sieve was also observed during unloading, indicating severe degradation of adsorbent performance.

Sorbead has variable pore sizes and can adsorb some of the hydrocarbons present while being more effective at higher relative humidity. The ability to co-adsorb some of the hydrocarbon allows for a cleaner product gas that is used for regeneration. The ability to regenerate using cleaner gas reduces the rate of accumulation of coke. Sorbead has almost double the water equilibrium capacity as most molecular sieves. This allows Sorbead to have a longer bed life.

BASF TSA bed designs utilize a water-stable Sorbead in the upper portion of the bed to protect the bottom section of the bed from liquid carry over. Molecular sieves are not water stable and are made with binders that can migrate in high water environments that can form solid cakes that lengthen the maintenance schedule for unloading. Sorbead is amorphous and does not have binders; thus, mitigating the risk of caking altogether.

The combination of benefits of using Sorbead in CO₂ dehydration service not only extends the life of bed life but also improves the operational expense of regeneration temperature.

Conclusion

The purification and dehydration of CO₂ for CCUS applications are required to meet pipeline specifications and ensure operational reliability. Technology and material selection for these processes are critical to ensure economic feasibility, operability, and safety of transported CO₂. While compression primarily serves to increase pressure, it also plays a critical role in removing water and water-soluble contaminants, reducing downstream complexity for catalyst and adsorbent design. CatOx and DeOxo units address residual hydrocarbons and oxygen, respectively, using platinum- or palladium-based catalysts to achieve high CO₂ purity. Finally, dehydration is essential to meet stringent moisture limits, where Temperature Swing Adsorption (TSA) with Sorbead offers significant advantages over traditional molecular sieves. Sorbead's acid resistance, lower regeneration temperature, and ability to handle liquids and hydrocarbon contamination extend bed life and reduce operational costs, as demonstrated in Whitecap Resources Inc's commercial reference. Together, these integrated processes ensure efficient CO₂ conditioning for safe and economical pipeline transport, while optimizing long-term performance and minimizing maintenance challenges.

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