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Life Cycle Assessment of CO_2 Post-Combustion Capture and Utilization for Wastewater Neutralization

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Abstract

The integration of carbon capture and utilization (CCU) technologies into industrial processes offers a sustainable approach to reducing CO_2 emissions while enhancing resource efficiency. This study explores the application of a Vacuum Swing Adsorption (VSA) process for capturing CO_2 from heat boiler flue gases and utilizing it for wastewater neutralization within the same industrial facility using real data from a pilot plant. By implementing an on-site CO_2 capture and reuse strategy, industries can minimize dependence on commercially bottled CO_2, thereby reducing costs and promoting a circular economy model that aligns with sustainability goals.

The CO_2 capture system employed in this study consists of a VSA unit equipped with zeolite 13X as the selective adsorbent for CO_2 capture. The system operates with a simple 2-bed and 3-step cycle with pressurization, adsorption and regeneration with vacuum. The CO_2 recovered through VSA is directly injected into alkaline industrial wastewater generated within the facility. When dissolved in water, CO_2 forms carbonic acid (H_2CO_3), which effectively reduces pH levels. In this study, CO_2 was used to neutralize wastewater with an initial pH of ≈ 12, bringing it down to a stable range between 7 and 8 in the neutralization tank. According to calculations, around 75% of the injected CO_2 was retained in the wastewater in the form of carbonates and bicarbonates, contributing to effective neutralization. The remaining 25% of the CO_2 was released to the atmosphere.

A Life Cycle Assessment (LCA) was carried out using the software Simapro 9.1 to assess the potential impacts of two different scenarios (Figure 1): one considering the use of commercially bottled CO_2 (Lineal CO_2) for wastewater neutralization and another considering the use of captured CO_2 (Circular CO_2) from the VSA process for the same purpose. The methodological framework for performing the LCA study is based on the ISO 14040:2006 standard, which comprises four steps: goal and scope definition, inventory analysis, impact assessment, and interpretation. The scope of the study is a cradle-to-gate. The system boundary includes all subprocesses such as bottle CO_2 production, adsorbent production, transportation, VSA plant infrastructure, electricity and process emissions. The functional unit

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will be 1 m^3 of neutralized wastewater. The life cycle inventory (LCI) of both scenarios includes the inputs and outputs of the materials and energy. All the background data such as bottled CO_2 production, adsorbents, electricity (electricity mix grid) and transportation are obtained from the Ecoinvent 3.3 database embedded in Simapro. To keep database consistency, it is assumed that the VSA carbon capture is located within the Spain and that the transportation of bottled CO_2 in the Lineal CO_2 scenario from production facilities are located at 200 km from the neutralization plant. The life cycle impact assessment of both scenarios is conducted using the CML-IA characterization (11 impact categories).

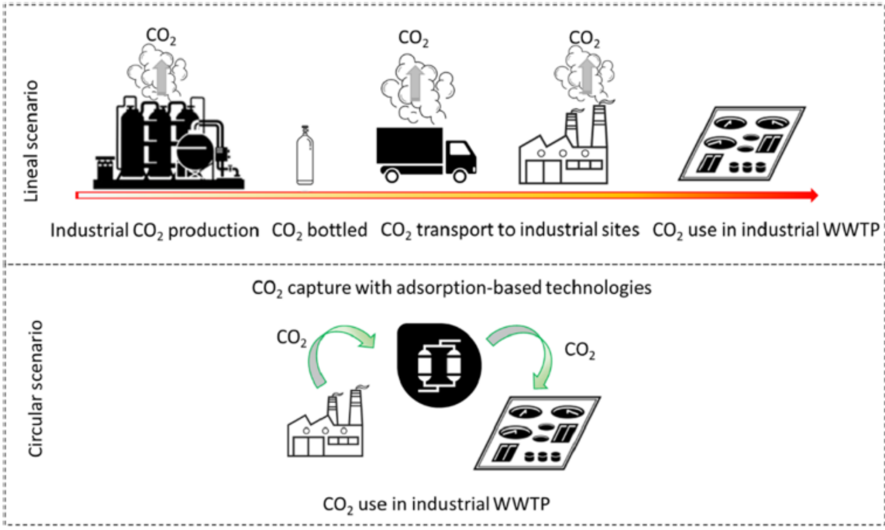
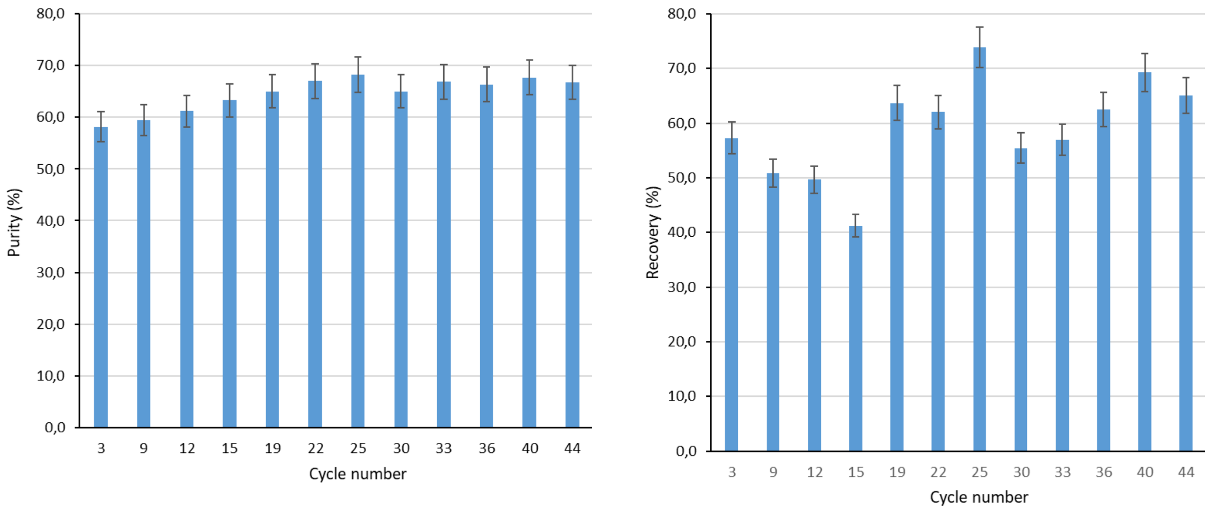


Figure 1. *Schematics of the lineal (conventional ex-situ production and transport of* CO_2*) and circular (using in-situ adsorption-based carbon capture technologies) approaches for the industrial use of* CO_2*.*

In Figure 2 are shown the main Key Performance (KPIs) Indicators obtained with the VSA process during 44 cycles. The average KPIs obtained during the last cycles have been used to perform the LCA. It can be observed that a productivity of 0.027 $kg_{CO2}/kg_{ads}\cdot h$ with a purity of 66.8% was obtained. The CO_2 recovery, which is calculated as the amount of CO_2 captured divided by the amount of CO_2 fed to the VSA unit, was 61.8%. The calculated energy consumption was 0.51 kWh/kg_{CO2}.



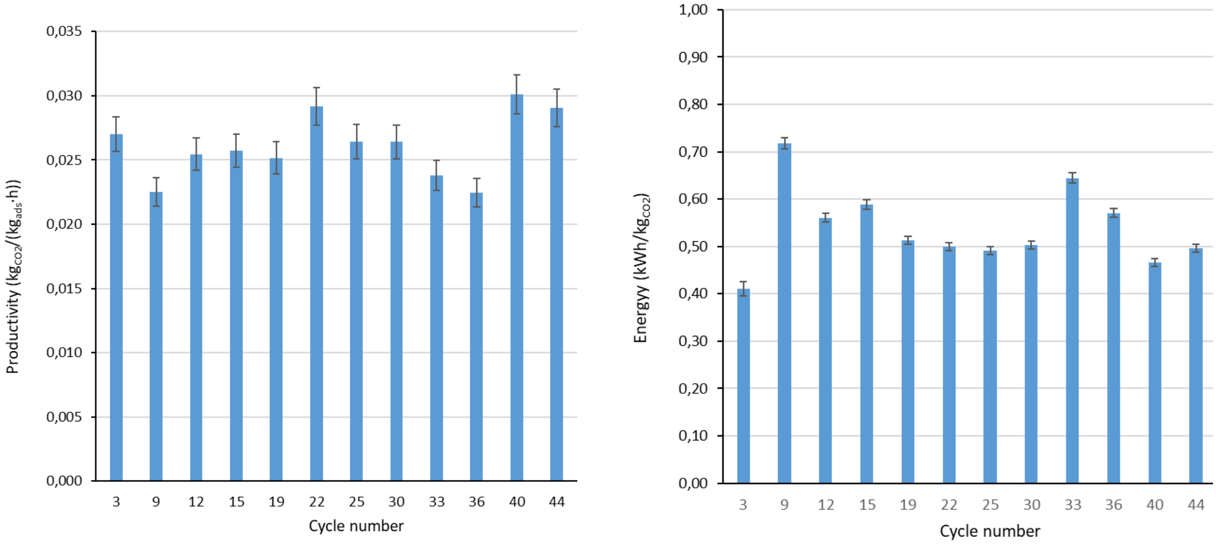


Figure 2. *Key performance indicators of the post-combustion VSA process. a) purity, b) recovery, c) productivity and d) energy consumption*

As an example of the impact assessment, Figure 3 presents the main results obtained for the climate change impact category with the two studied scenarios. The results are expressed in kg CO_2-equivalent needed to neutralize 1 m^3 of wastewater, illustrating the carbon footprint associated with each option. The Lineal CO_2 scenario has a significantly higher carbon footprint, around 1.50 kg CO_2-eq, compared to the Circular CO_2 scenario, which is approximately 0.64 kg CO_2-eq. In the Lineal CO_2 scenario, the dominant contributor is boiler emissions, followed by industrial CO_2 production, wastewater neutralization, and transportation, with the latter having a minor contribution. For the Circular CO_2 scenario, the total impact is much lower, mainly driven by direct emissions from the VSA, electricity consumption for VSA operation and emissions in the wastewater neutralization process while adsorbent usage and plant infrastructure contribute minimally.

The elimination of CO_2 transportation and commercial production reduces the carbon footprint and operational costs associated with purchasing bottled CO_2. Additionally, the on-site utilization of captured CO_2 aligns with sustainability goals by reducing industrial emissions from the boiler and enhancing process efficiency. These results highlight that the use of circular approaches with CO_2 offers a clear environmental advantage, reducing the carbon footprint by approximately 57%. The impact in the VSA system could be optimized by integrating renewable energy sources and improving process recovery and energy efficiency. In contrast, the high contribution of boiler emissions in the Lineal CO_2 scenario underscores the benefits of CCU as a decarbonization strategy.

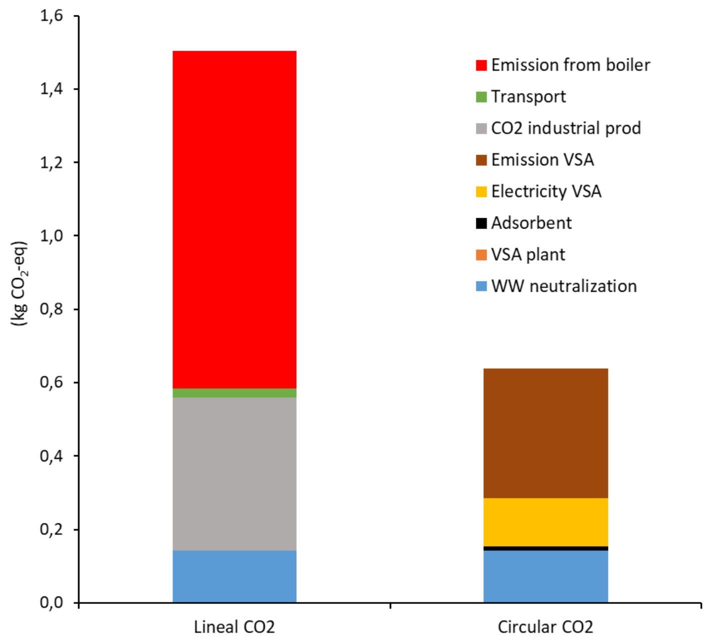


Figure 2. *Carbon footprint of neutralizing 1 m^3 of wastewater with Lineal CO_2 and Circular CO_2 scenarios.*

This study demonstrates that a VPSA-based CO_2 capture and reuse system is a viable and effective solution for industrial wastewater neutralization. By repurposing flue gas CO_2 from heat boilers for in-situ use, such as neutralization, industries can enhance sustainability, reduce operational costs, and contribute to circular economy practices. The findings suggest that adopting such integrated CCU strategies can play a key role in achieving greener industrial operations while maintaining process efficiency and compliance with environmental regulations.

Keywords: Vacuum Swing Adsorption (VSA); Carbon capture; Use and storage (CCUS); Zeolite;; Circular economy.