



Evaluating Lewatit® VP OC 1065 Performance as a Solid Sorbent for Direct Air Carbon Capture

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In this study, we have evaluated the CO₂ sorption characteristics of Lewatit® VP OC 1065 and assessed its potential application as a solid sorbent for direct air capture (DAC) of CO₂. This material is an amine-functionalized polymeric resin, and materials of this type have a unique benefit: CO₂ sorption potential is enhanced in the presence of humidity. Nevertheless, its complex swelling behavior and oxidative degradation pathways often impact its properties during sorption and cycling. Complementary gravimetric and breakthrough analysis techniques, using instruments such as the DVS Carbon and BTA Frontier, allow users to simulate common co-sorption scenarios to mimic DAC conditions and assess this material's performance and suitability as a CCUS material under realistic conditions.

Introduction

Carbon dioxide removal (CDR) is a critical pillar in the global strategy to limit temperature rise to 1.5°C above pre-industrial levels [1]. Among emerging technologies, Direct Air Capture (DAC) using solid adsorbents promises a scalable solution [2]. This study evaluates Lewatit® VP OC 1065, an amine-functionalized polymeric resin, specifically assessing its performance under realistic atmospheric conditions.

Unlike many sorbents that suffer from competitive sorption, Lewatit® exhibits a synergistic effect where CO₂ uptake is enhanced by the presence of humidity. Using the Surface Measurement Systems DVS Carbon Advanced and BTA Frontier, we utilize the complementary techniques of high-resolution gravimetric and breakthrough analysis to characterize and evaluate Lewatit's® sorption performance and suitability as a realistic solid sorbent for DAC carbon capture. This study aims to map the co-sorption performance of H₂O and CO₂ to measure this enhancement effect and assess the sorbent's lifetime over multiple sorption-desorption cycles.

Methods

Single and multicomponent isotherms were recorded using the DVS Carbon Advanced, a gravimetric sorption analyzer. The instrument combines a high-resolution UltraBalance with precise control of gas composition and temperature. Control of CO₂ concentration from low ppm levels up to 100 vol% at atmospheric pressure, together with humidity control from dry to near-saturated conditions across a wide temperature range is available.

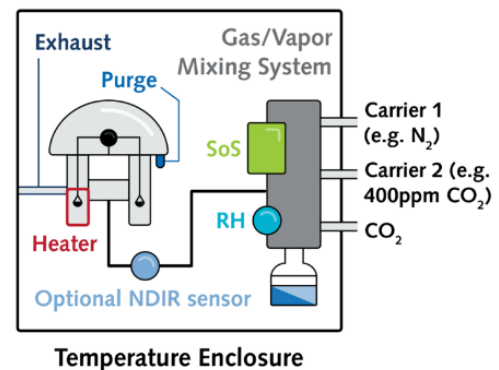


Figure 1: A schematic of the DVS Carbon.



Concentrations can be programmed in either stepwise or ramped profiles, enabling complex co-sorption, cycling, and regeneration protocols. Temperature control from 5°C to 450°C is achieved through a combination of a thermostatted sample enclosure and a high-temperature local heater.

Packed bed breakthrough experiments were performed using the BTA Frontier, a state-of-the-art breakthrough measurement system capable of handling multicomponent gas and vapor uptake and desorption measurements. The instrument exposes the adsorbent, placed within a fixed-bed column, to multicomponent gas streams comprising of up to five gases and up to two vapors under precisely controlled temperature and flow conditions. The concentration and flow rate of the column effluent are continuously monitored via a series of integrated sensors, as shown in Figure 2.

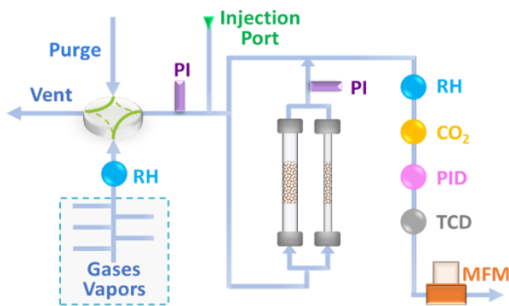


Figure 2: Schematic representation of the BTA Frontier system.

Lewatit® VP OC 1065 was purchased from Sigma-Aldrich and was used as received as the model amine-functionalized resin for DAC studies. The material consists of macroporous styrene-divinylbenzene co-polymer matrix shaped into beads (<0.5 mm diameter) functionalized with primary amine groups, specifically benzylamine groups. These primary amine groups are highly reactive and bind strongly to CO₂ and water in the gas phase, giving Lewatit® high sorption capacity for both species. For both DVS and BTA measurements, the resin was pre-dried in situ at 110 °C under inert gas (nitrogen) to remove residual moisture and contaminants.

For DVS experiments, sample masses of approximately 10-25 mg were used to provide a

balance of relatively fast equilibration rates while maintaining an adequate signal-to-noise ratio. The DVS camera accessory was used for in situ photos. For the BTA experiments, 120 mg of sample was packed into the sample tube. For dead volume and sensor response corrections to breakthrough capacities, blank adsorption and desorption experiments were carried under identical conditions except the adsorbent being replaced by an inert glass bead materials of same volume as the adsorbent.

Results

Single Component Isotherms

Equilibrium CO₂ sorption isotherms were measured at 25 °C and 40°C. The CO₂ concentration was increased stepwise until a mass equilibrium was achieved at each step according to a predefined mass stability criterion (<0.002%/min over 10 minutes). The resulting isotherms, including a logarithmic inset highlighting the low-concentration uptake, are shown in Fig 3.

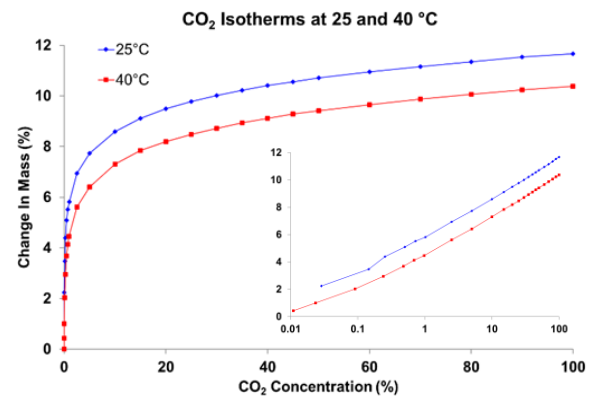


Figure 3: CO₂ isotherms for Lewatit® at 25 and 40 °C. Uptake vs CO₂ concentration on a logarithmic scale is shown in the insert in the bottom right corner.

The CO₂ isotherms confirm the high affinity of Lewatit® VP OC 1065 for CO₂, particularly at low concentrations relevant to DAC. The inset logarithmic plot highlights the steep initial slope of the isotherm, characteristic of amine-based chemisorption processes that favour adsorption even at very low partial pressures.

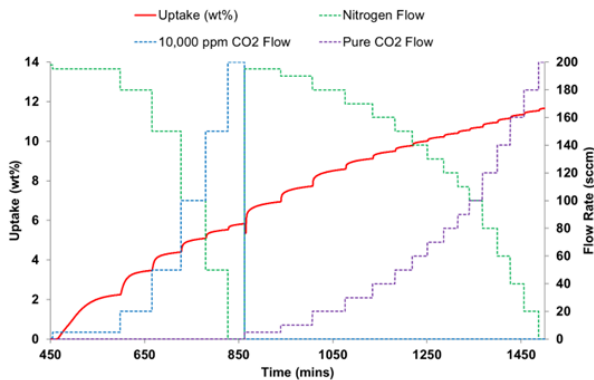


Figure 4: Time-resolved uptake data with various flow rates from different gas sources. This kinetic data was gathered from the 25 °C Isotherm experiment shown in Figure 2.

Fig 4 shows the time-resolved data from the 25 °C isotherm experiment from Fig 3. The change in mass (wt%) is plotted versus various flow rates from different mass flow controllers (MFCs). The three MFCs in use are connected to different gas sources: pure nitrogen, pure CO₂, and a pre-diluted cylinder containing 1% CO₂ in nitrogen, enabling the DVS to accurately control concentrations throughout the entire space. This method sought to maintain a total flow rate of 200 sccm while varying the ratio of the CO₂-containing gas stream to the carrier gas stream. The resulting CO₂ concentrations generated from this gas mixing were measured by an NDIR sensor (0-30,000 ppm CO₂) and the patented SMS Speed of Sound sensor (0.5-100% CO₂). This experiment was

performed in the DVS Carbon Advanced using the Advanced method type, where users define MFC flow rates of all six MFCs in the instrument.

The time-resolved data shows that Lewatit® was able to equilibrate quickly at all CO₂ concentration steps, even at the lower concentrations of 200 and 400 ppm, suggesting beneficial sorption kinetics at DAC-relevant conditions.

Gravimetric water sorption and co-sorption

Water sorption isotherms were measured at 25 °C in both an inert carrier gas (nitrogen) and a carrier gas containing CO₂ at 400 ppm and 10,000 ppm (1 vol%). Relative humidity was increased stepwise through a defined range, in a manner similar to the CO₂ isotherms, using the same equilibration criterion for all steps. The resulting data is displayed in Fig 5.

Fig 5a shows the total uptake at equilibrium as a function of relative humidity. Both experiments using 400 ppm and 10,000 ppm CO₂ carrier gas streams show their first isotherm equilibrium points at non-zero values at 0% relative humidity. This is due to CO₂ sorption prior to the introduction of humidity. Figure 5b is an adjusted plot of Fig 5a, where the baseline of the isotherm has been adjusted to account for this mass equilibration under the flow of the CO₂-containing carrier gas.

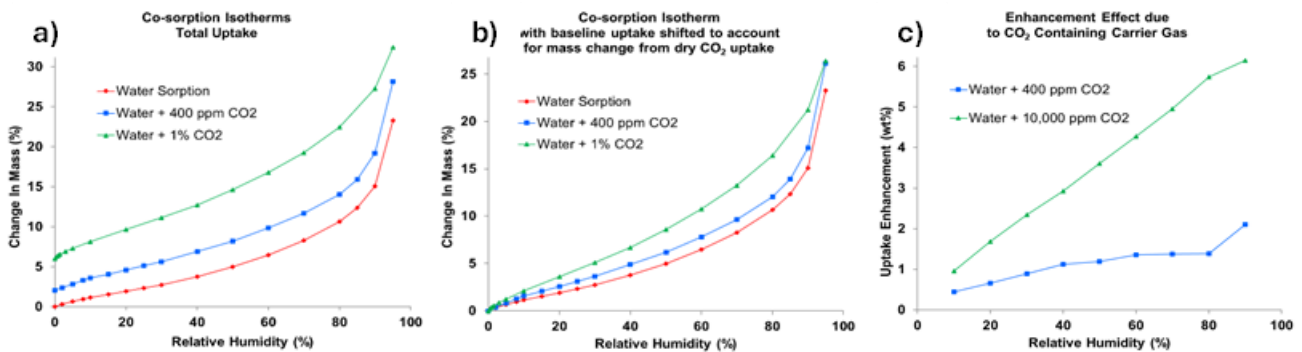


Figure 5: 5a) Co-sorption isotherms of water with various carrier gas streams, with total uptake plotted. 5b) The co-sorption isotherms shown in 5a, now with the change in mass reduced to account for the uptake measured from the CO₂-containing carrier gas under dry conditions. 5c) A plot of the enhancement effect, measured as the difference between the pure water sorption isotherm and the water sorption isotherms with a CO₂-containing carrier gas.



This was done by subtracting all equilibrium points across the entire isotherm from the equilibrium mass achieved under a flow of only dry ppm-level CO₂. Fig 5c shows the enhancement effect on total sorption for both co-sorption experiments. This was measured as the uptake difference between the pure water sorption isotherm and the adjusted co-sorption isotherms.

Total uptake was increased in both co-sorption experiments, and the extent of this enhancement appears to depend on the CO₂ concentration used. This enhancement in total uptake can be considered from two perspectives: water uptake was enhanced by CO₂, or CO₂ uptake was enhanced by water. It is likely that both scenarios are true in the case of Lewatit®.

Breakthrough Analysis and Synergistic CO₂-H₂O Interaction

To deconvolute the individual contributions of CO₂ and H₂O under humid conditions, fixed-bed breakthrough adsorption experiments were conducted (Figure 6a). After activation, adsorption measurements were conducted in two sequential stages. In Stage 1, the adsorbent was exposed to a dry feed of 1 vol% CO₂ in N₂ until saturation was achieved, as confirmed by the CO₂ concentration

measured at the column outlet reaching the inlet concentration. In Stage 2, the feed humidity was raised to 70% relative humidity (RH) and maintained until the adsorbent approached saturation under humid conditions. Following completion of both adsorption stages, the adsorbent bed was regenerated by heating to 110 °C under flowing N₂.

Under Stage 1 dry conditions with 1 vol% CO₂, a measurable CO₂ uptake capacity of 4.61 wt% was determined from the delayed breakthrough profile at the bed outlet, consistent with, though marginally lower than, the 5.82 wt% capacity observed in independent gravimetric measurements, a discrepancy attributable to differences in equilibration time and bed dynamics.

Upon introduction of humidity to a CO₂-saturated bed in Stage 2, a pronounced secondary depression in the outlet CO₂ concentration was observed prior to re-equilibration at a new steady state. This behavior constitutes direct experimental evidence of a synergistic CO₂-H₂O interaction, whereby moisture facilitates incremental CO₂ uptake on a sorbent that had already attained its nominal dry-state capacity. The additional CO₂ capacity gained upon humidification was 2.47 wt%, yielding a total CO₂ capacity of 7.08 wt%.

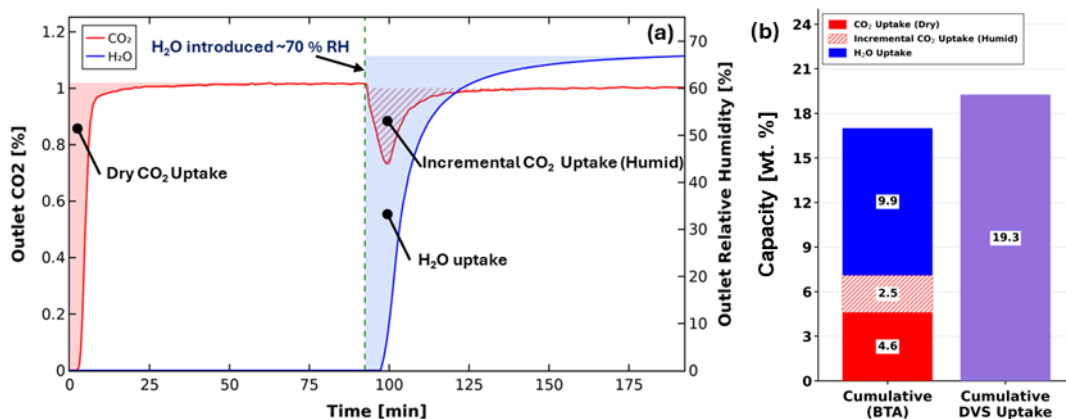


Figure 6: (a) CO₂ (red) and H₂O (blue) breakthrough curves. The light red region indicates CO₂ uptake under dry conditions, the patterned red region shows the incremental uptake under humid conditions, and the light blue region represents H₂O uptake. H₂O (70% RH) was introduced in Stage 2 at 92.39 minutes, as indicated by the dotted green line. (b) Calculated capacities derived from the breakthrough curves, expressed in wt % and compared with the cumulative DVS uptake at 70 % RH and 1 % CO₂.



This represents approximately a 54% enhancement relative to dry conditions. The corresponding H₂O uptake capacity at 70% RH was determined to be 9.91 wt%, a value that may be marginally underestimated given that full saturation had not been achieved by the experiment's end (Figure 6b). Nonetheless, this value exceeds that obtained from single-component gravimetric experiments (8.27 wt%), confirming that both CO₂ and H₂O adsorption capacities are mutually enhanced under co-sorption conditions.

Mechanistic Interpretations: Reaction pathways

Lewatit® VP OC 1065 is known to exhibit enhanced CO₂ sorption capacity in the presence of humidity relative to dry conditions. Under moist gas streams, CO₂ uptake is thought to increase due to the formation of additional chemically bound species, resulting in higher working capacities within DAC-relevant concentration ranges. Fig 7 shows the possible reaction pathway under dry conditions, in which two primary amine groups react with one CO₂ molecule to form an ammonium ion and a carbamate ion. In humid conditions, a single amine group reacts with one CO₂ and one H₂O molecule to form one ammonium ion and one bicarbonate. Under humid conditions, the ratio of amine groups:CO₂ is 1:1; in dry conditions, this ratio is 2:1, meaning the CO₂ capacity is theoretically doubled by the presence of humidity [3].

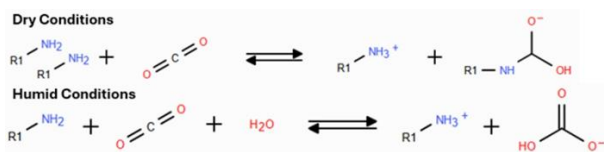


Figure 7: Reaction pathway of CO₂ on primary amines under dry and humid conditions.

The enhancement effect measured in amine-functionalised sorbents has commonly been attributed to this additional bicarbonate ion formation [4]. However, this assumption may hold for liquid amines with mobile functional groups, allowing easy coordination of 2 amine groups. Lewatit® consists of primary amine groups, which

are bound to the co-polymer backbone, heavily restricting their mobility. Coordination of multiple primary amine groups requires interaction between polymer chains; therefore, the enhancement of CO₂ capture may not be directly linked to bicarbonate formation at low CO₂ concentrations and could instead be caused by swelling of the sorbent and pore opening [5].

Swelling of Lewatit® Beads from Humidity

To examine swelling of the material under humid conditions, pictures of the Lewatit® beads were taken under a dry nitrogen flow at 0% RH and at 90% RH. The picture of the sample under these conditions is shown in Fig. 8. The beads exhibited an average increase in diameter of 4% under humid conditions compared to dry conditions. The introduction of water into the macropores and between the polymer chains causes expansion of the bead. Water adsorption onto flexible, porous materials can both enhance and impede access to certain adsorption sites, depending on swelling-induced changes in the sorbent's structure [6].

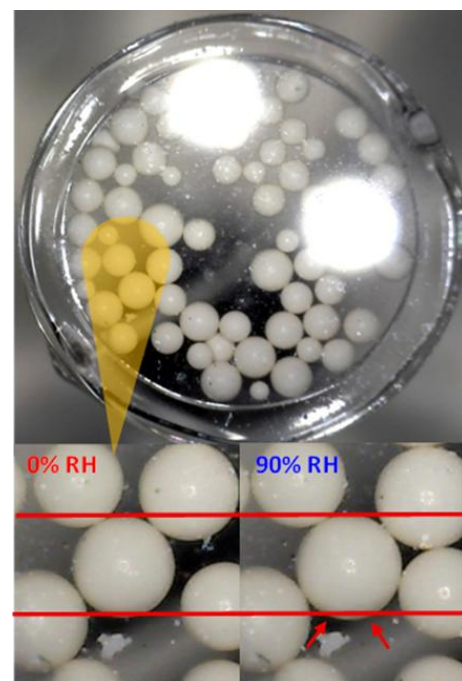


Figure 6: Picture of Lewatit® beads on a quartz pan taken from the camera accessory at 0% RH and 90% RH to determine the extent of swelling.



Co-sorption Cycling and Stability

Finally, a multi-cycle co-sorption experiment was performed at 25 °C to evaluate the stability of Lewatit® under repeated exposure to CO₂ and H₂O. Each cycle consisted of exposure to dry 10% CO₂ followed by the introduction of 50% RH, with regeneration between cycles achieved by flowing dry nitrogen at ambient temperature. Uptakes in each segment are presented both as a cycling plot (Fig 9) and as a table of uptake values (Table 1).

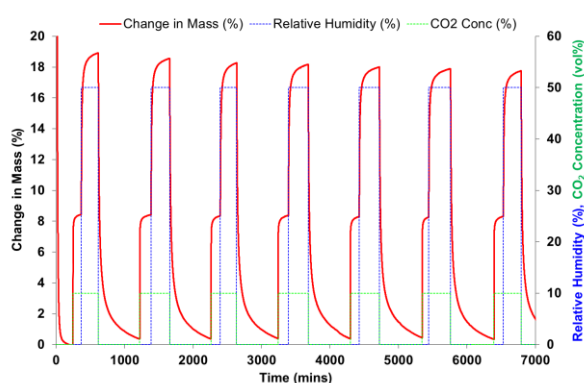


Figure 7: Cycling performance of Lewatit over multiple co-sorption steps. First, 10% CO₂ was introduced, then 10% CO₂ + 50% H₂O for 7 cycles.

The uptakes show that over seven consecutive cycles, CO₂ uptake in the 10% CO₂ step remains in a narrow range around 8.3–8.4 wt%, while uptake in the 10% CO₂ + 50% RH step remains close to 18–19 wt%, with modest declines across cycles. This indicates acceptable short-term stability of the resin; however, sorption performance may continue to decrease over a longer experimental timeframe.

Conclusion

Taken together, the CO₂ isotherms, kinetic profiles, water sorption, co-sorption cycling experiments, and breakthrough analysis demonstrate that amine-functionalised sorbents like Lewatit® VP OC 1065 remain a strong candidate material for DAC applications under both dry and humid conditions. The material shows high affinity and significant capacity at low CO₂ concentrations, fast sorption

kinetics, humidity-enhanced CO₂ uptake, and acceptable short-term stability under repeated co-sorption cycles without aggressive regeneration.

From a process design standpoint, the observed synergy between water and CO₂ suggests that DAC cycles could be tailored to operate at controlled humidity levels that maximize working capacity while keeping regeneration energy acceptable.

This study underscores the value of the complementary analysis from DVS Carbon, DVS Carbon Advanced and BTA Frontier platforms for characterizing advanced sorbents for carbon capture under realistic conditions. Independent multicomponent control enables experiments that would be difficult or impossible to perform on conventional single-component gravimetric or volumetric instruments, including precise mapping of CO₂/H₂O co-sorption, cycling under programmable gas compositions, and systematic variation of temperature and flow while monitoring real-time mass and concentration changes.

References

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