Tracking CO_2 adsorption in a metal-organic framework (MOF) reactor. A micro-CT study

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1 Abstract

Atmospheric carbon dioxide (CO_2) levels reached records in 2024, committing the planet to further warming. Developing novel strategies to capture CO_2 is thus crucial to mitigating climate change and achieving net-zero emissions. In this work, X-ray computed tomography (XCT) is used to investigate non-destructively how CO_2 is absorbed in a metal organic framework (MOF)-based packed bed reactor. Both static and dynamic in-situ XCT measurements are performed to characterize the MOF's and packed bed's pore-structure and tracking the CO_2 uptake. It's shown that change in CO_2 concentration is detectable as a shift to higher gray values in the gray value distribution. It was found that pores become less interconnected further inside the particle, becoming less accessible to CO_2 gas. This observation suggests a more significant particle surface-level CO_2 uptake, here assessed through a developed image processing approach. This research helps to improve the uptake of CO_2 from the atmosphere and thereby to reduce the share of greenhouse gases.

Keywords: CO_2 adsorption, Metal-organic framework, X-ray computed tomography

Introduction

The increasing emission of greenhouse gases has surpassed the 400ppm threshold and continues to rise in 2025. This increase is a primary driver of global warming and climate change, prompting the development of new technologies to mitigate its effect [1]. Microporous metal–organic frameworks (MOFs) is a promising technology for carbon capture, offering high internal surface area (>1000 m^2/g), adjustable pore geometry and tuneable properties that make them highly effective for capturing CO_2 from industrial gas streams [2]. The size, shape and connectivity of the pores directly influence the gas uptake. Therefore, accurate characterisation of the complex MOFs pore structure is crucial to understand the CO_2 storage mechanisms. Current characterisation by scanning and transmission electron microscopy do not allow the quantification of the pore network of MOF materials and the three-dimensional (3D) visualisation. Moreover, they follow a destructive approach that destroys the structural integrity of the material and the evolution under load thus cannot be tracked. X-ray computed tomography (XCT) can offer a solution to this challenge [3]. In this work, XCT is used to investigate non-destructively how CO_2 is absorbed in a CO_2 fluidised packed bed reactor made of sorbent MOFs particles. The micron-scale pore structure of a single MOF particle is fully characterised from image data collected from a static XCT measurement. The CO_2 uptake on the surface and inside the MOFs particles was also tracked at reactor level, through time-lapse in-situ XCT measurements. Our findings provide better insight into the evaluation of CO_2 storage capacity in MOFs porous materials, thereby proving the XCT's suitability for designing better MOFs for carbon capture.

2 Experiment and Results

Commercial MOF particles type MOF-CZ from novoMOF, Zofingen, Switzerland (BET surface ~ 800 m^2/g) packed within a plastic inlet-controlled column (diameter 5 cm, height 25 cm) were considered in this work (cf. Fig. 2 a). The XCT experiments were conducted on a d2 XCT system from Diondo, Hattingen, Germany. A high-resolution scan (voxel size =3.9 μm) was initially performed to image the pore structure of single particle with optimised CT acquisition parameters (cf. Fig 1a). Afterwards, a sequence of XCT measurements were conducted after 15 min of CO_2 flow injection to the reactor, at a flow rate of 0.1 L/min. The collected image data was reconstructed and postprocessed using the X-AID, VGStudio MAX and Geodict2026 Software.

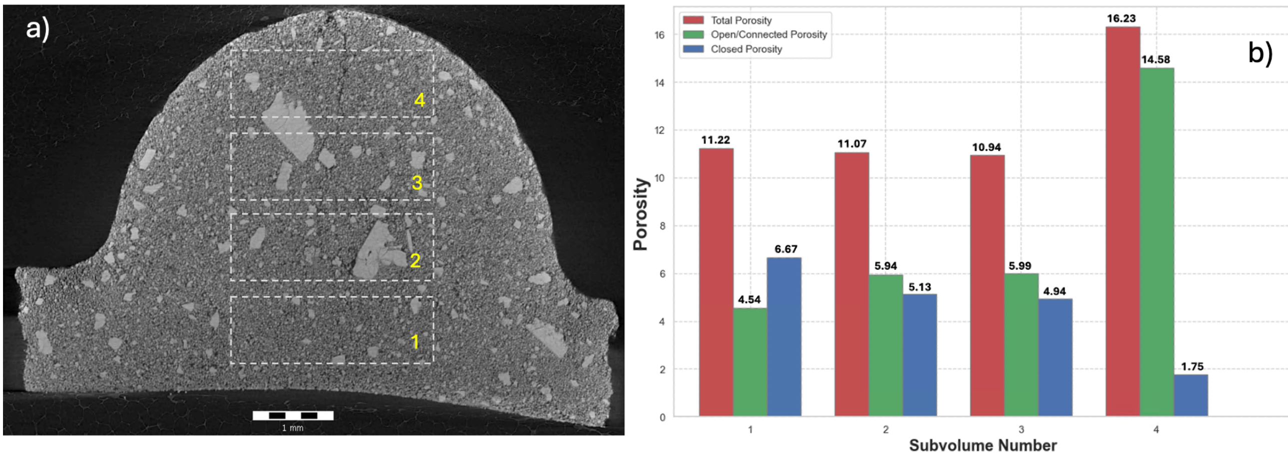

Fig. 1. High resolution XCT cross-section of a single MOF particle with highlighted sub-volumes (a) where porosity analysis was performed (b).

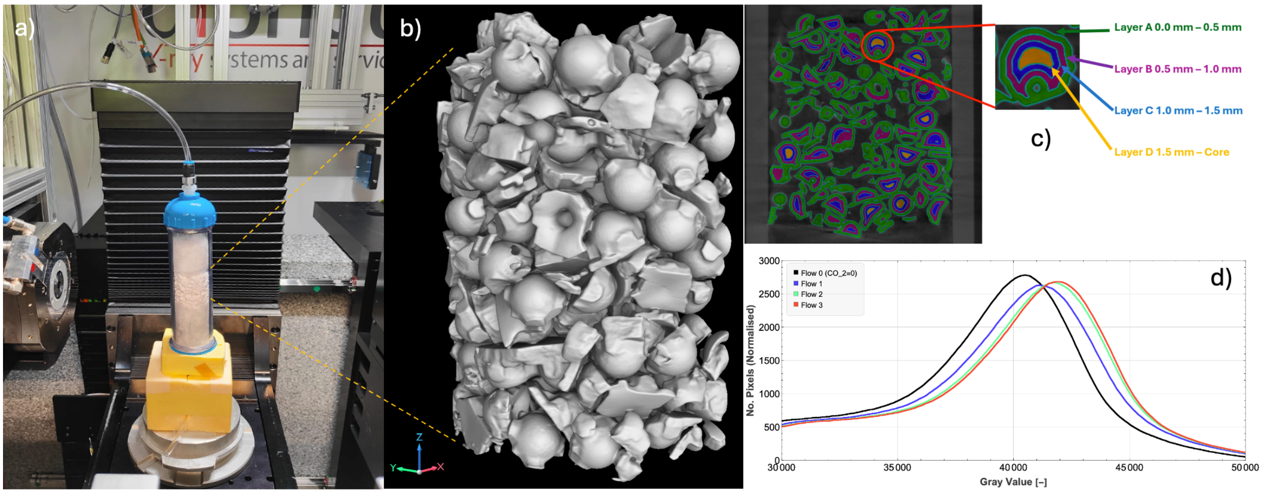

Fig. 2. (a) Snapshot of the experimental XCT setup. CO_2 is supplied from the top of the MOFs packed bed reactor located between the X-ray source (left) and the detector. (b) 3D rendering of the scanned packed bed. (c) XCT cross section showing the layered ROIs used in the analysis. (d) Voxel gray value distribution at the ROI closest to the particles surface (i.e., Layer A in (b)), at different CO2-flow injection times.

Pore structure analysis reveals that total porosity varies slowly from ~16% close to the surface to ~11% in inner regions. Bigger pores (4.28% larger diameters) were found close to the surface. In contrast, pore connectivity, varies strongly from ~15% in sub-volume 4 to ~4-5% in inner sub-volume (cf. Fig1b). This indicates the existence of larger surface area in the outer particle layers (Layer A Fig 2c) and therefore, a higher probability of interaction between the MOF particle and CO_2. To track changes on the CO_2 concentration, grey value distributions from the outer layer ROI of the MOF particles (layer A, Fig1c) were computed from XCT data collected at different CO_2-flow injection times. It was found that higher concentration of CO_2 leads to higher (brighter) voxel grey values, detected as a shift of the grey value distribution towards the right (cf. Fig. 2d). The higher the concentration (or density) of CO_2, the larger the shift of the peak distribution to the right, indicating a proportional relationship.

References

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