

# Materials and structural analysis solutions supporting carbon capture, utilization, and storage

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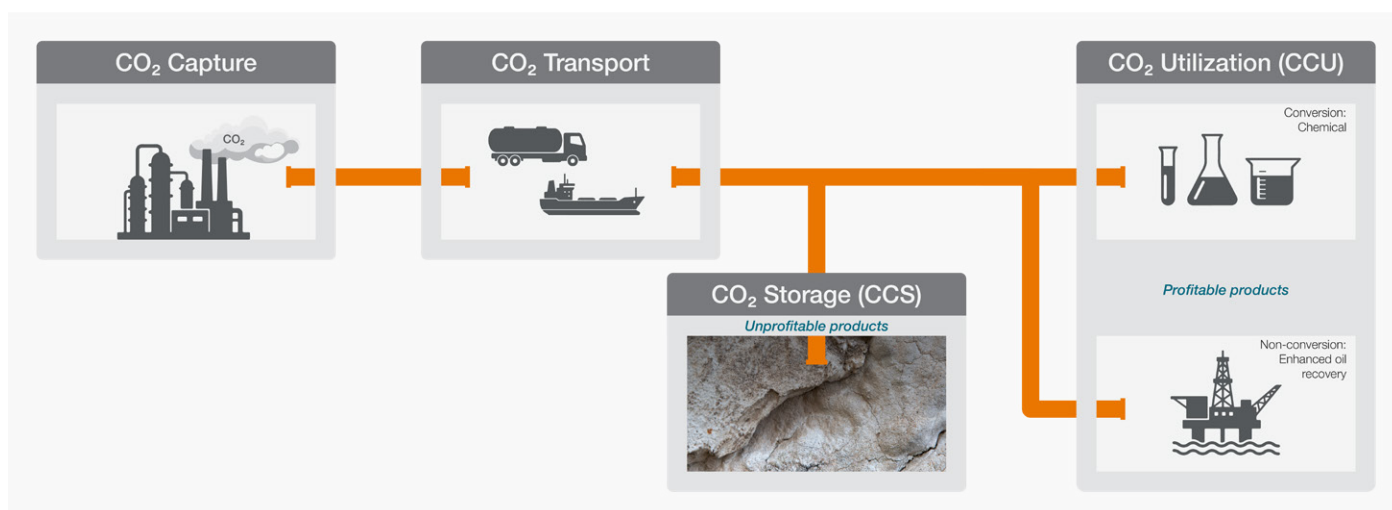


Figure 1. Schematic overview of the CCUS value chain, showing the four main stages; CO<sub>2</sub> capture, transport, utilization, and storage.

## Introduction

As industries work to reduce carbon (CO<sub>2</sub>) emissions, carbon capture, transport, utilization, and storage (CCUS) is becoming an increasingly important area of investment and innovation. The CCUS value chain includes four main steps: the capture of CO<sub>2</sub>, its transportation, followed by either its long-term storage or utilization in industrial applications (Figure 1).

CO<sub>2</sub> can be captured from industrial emissions, power plant exhaust, or even directly from the air. After this, it is transported, typically by pipeline or in containers, to either be stored underground in geological formations or used in other processes. As part of the utilization pathway, CO<sub>2</sub> may be converted into fuels, chemicals, and other materials; it can also be used directly in non-conversion applications such as enhanced oil recovery (EOR).

As investment in CCUS continues to grow, so does the need for analytical tools that improve our understanding of the materials, reactions, and structures involved across the value chain. Notably, the characterization of solid materials plays an especially important role in carbon capture, storage, and utilization; these will be explored in detail in this application note.

## Carbon capture: optimizing sorbent materials

There are several approaches to carbon capture; these are largely grouped depending on whether the capture occurs before or after combustion. In pre-combustion processes, fuel is converted into a gas mixture containing H<sub>2</sub> and CO. In oxy-fuel combustion, fuel is burned in pure O<sub>2</sub>. In post-combustion capture and direct air capture, however, CO<sub>2</sub> must be separated from a more dilute gas stream using sorbent or solvent materials (Figure 2). Because this process depends strongly on sorbent performance, the materials used must combine high capture efficiency, low cost, and long-term durability.

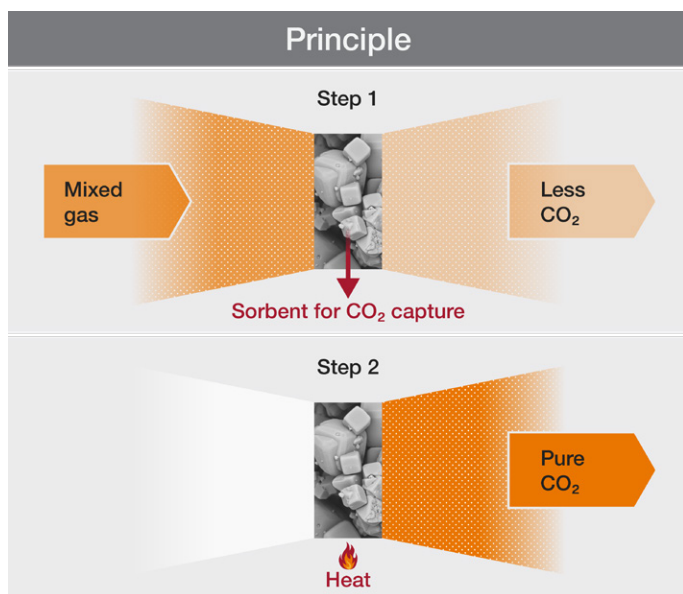


Figure 2. Schematic illustration of the sorbent-based carbon capture process. First, CO<sub>2</sub> is captured from a mixed gas stream by the sorbent material, reducing CO<sub>2</sub> concentration in the outlet gas. Heat is then applied to release and recover concentrated CO<sub>2</sub>.

Sorbent materials used for CO<sub>2</sub> capture include calcium carbonate, zeolites, and metal-organic frameworks (MOFs); these all have different structural and chemical characteristics that influence adsorption capacity, selectivity, and stability. To optimize their properties, researchers need analytical techniques that can connect material structure to capture behavior, including the material's morphology (size and porosity), crystallography, chemical composition, and chemical state. Thermo Fisher Scientific offers multi-technique approaches that can support this work, revealing the structure-property relationships that drive sorbent performance (Figure 3).

Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) can be used to examine particle morphology and pore structure; TEM also offers crystallographic information at high spatial resolution. Elemental composition can be revealed by the addition of energy-dispersive X-ray spectroscopy (EDX) to SEM or TEM, as well as through electron energy-loss spectroscopy (EELS) with TEM. X-ray photoelectron spectroscopy (XPS) and TEM-EELS can also elucidate chemical states and bonding environments, with TEM-EELS offering high spatial resolution.

Together, these techniques help researchers understand how sorbent materials function and how they can be optimized for improved carbon capture performance.

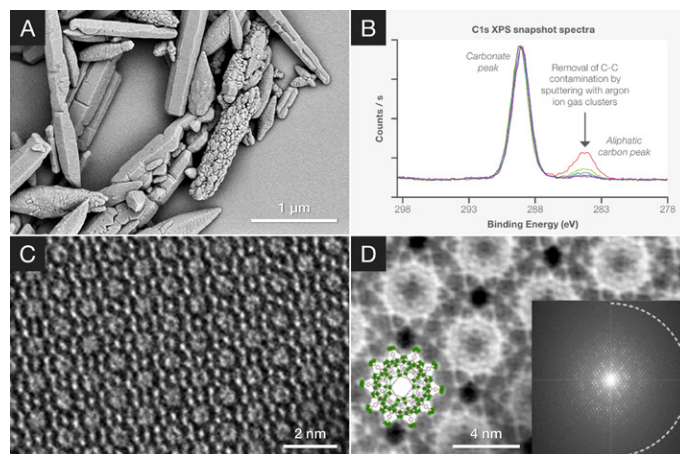


Figure 3. A) SEM image showing the porous morphology of calcium carbonate particles. B) XPS spectra showing surface chemical states consistent with carbonate species. C) TEM image of a zeolite sample obtained with a Thermo Scientific™ Talos™ TEM. D) IDPC-STEM image of a MoF, obtained with a Thermo Scientific™ Spectra™ TEM.<sup>1</sup>

## Carbon storage: understanding mineral reactions below the surface

In geological carbon storage, CO<sub>2</sub> is injected deep underground into suitable rock formations for long-term sequestration, typically at depths of 800 meters or more (Figure 4). While this concept seems relatively straightforward, the underlying science is highly complex. Geological storage does not depend on just one mechanism. Instead, CO<sub>2</sub> is kept underground through several trapping processes that improve storage security over time.

First, structural trapping keeps the injected CO<sub>2</sub> in place beneath an impermeable caprock, which acts as a seal above the reservoir. As the CO<sub>2</sub> moves through the porous rock, residual trapping leaves small droplets of CO<sub>2</sub> behind in the pore spaces. Over time, solubility trapping begins to occur, and the CO<sub>2</sub> dissolves into the salty groundwater that is present in the reservoir. Because this carbon-rich water is denser than the surrounding fluid, it sinks deeper into the formation, helping to reduce the risk of leakage. Finally, mineral trapping is the most permanent and longest-term mechanism, in which dissolved CO<sub>2</sub> reacts with the surrounding rock and forms stable carbonate minerals. Together, these mechanisms provide both immediate containment and increasingly permanent underground storage of CO<sub>2</sub>.

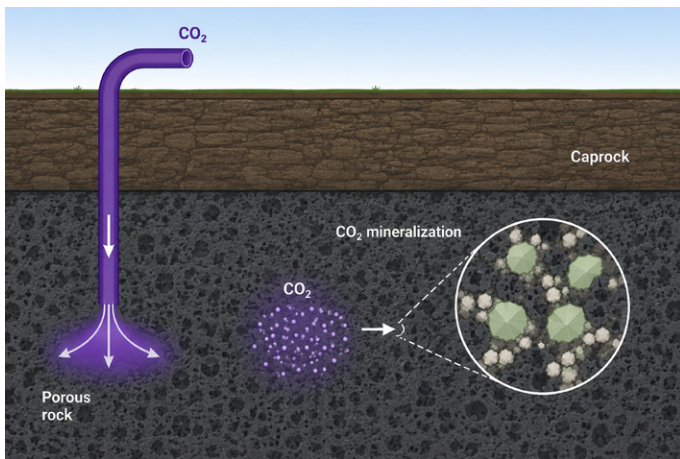


Figure 4. Illustration of underground CO<sub>2</sub> mineralization, in which injected CO<sub>2</sub> reacts with the host rock and is stabilized in the form of solid carbonate minerals.

To better identify suitable geological sites, and monitor potential leakage issues, researchers need to understand how CO<sub>2</sub> interacts with minerals in the subsurface. A multi-technique approach is valuable because no single method can fully describe how carbon storage systems evolve during carbon mineralization.<sup>2</sup> SEM-EDX can be used to examine pore morphology and chemical composition, while micro-computed tomography (micro-CT) and focused ion beam SEM (FIB-SEM) support 3D analysis of porosity and connectivity. *Ex-situ* and *in-situ* electron microscopy can provide high-resolution insight into mineral transformations and CO<sub>2</sub>-mineral reactions during carbon mineralization, while surface-sensitive techniques, such as XPS, can help characterize the chemical state changes of mineral oxides. These instruments are supported by a range of specialized software solutions, including Thermo Scientific™ Maps Min and Avizo™ Software, which can greatly facilitate the characterization of these complex mineral systems.

Figure 5 shows an example of 2D mineral characterization with SEM-EDX and Maps Min Software. In SEM, the backscattered electron (BSE) image reveals grains with compositional contrast. Heavier elements, such as metals, reflect more electrons and therefore appear brighter, while lighter elements, such as carbon or oxygen, reflect fewer and appear darker. For compounds, such as mineral phases, the average atomic number of the phase determines its BSE greyscale, with higher average atomic number phases appearing brighter. Maps Min Software combines BSE imaging with EDX mapping during data acquisition, automatically identifying the mineral phases present through a classification algorithm. From these mineral maps, quantitative data on mineral and rock composition can be generated along with textural characteristics. Understanding the mineralogical and textural properties of a geological feature, such as its pore-mineral associations, can greatly elucidate its potential for mineral trapping.

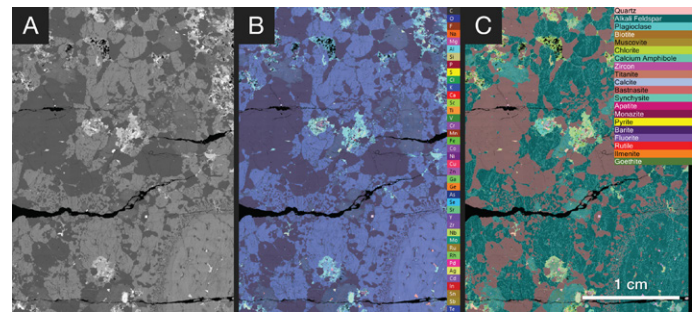


Figure 5. 2D mineral characterization with SEM-EDX and Maps Min Software. A) SEM-BSE image showing grains with compositional contrast. B) EDX contributes elemental characterization, aligned with the SEM data. C) Maps Min Software uses the SEM-EDX data to automatically identify mineral phases and quantify their compositions, abundances, associations, and grain sizes.

When combined with FIB-SEM, this 2D analysis can be extended into three dimensions (Figure 6). Avizo Software is used to analyze this data, quantifying pore characteristics such as size, shape, and ratio.

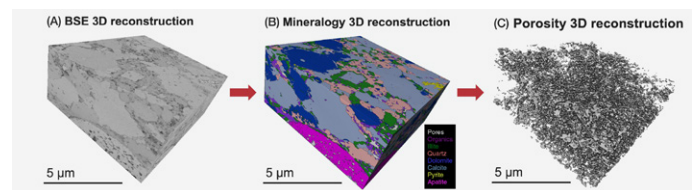


Figure 6. 3D mineral characterization using SEM-EDX and FIB-SEM with Maps Min and Avizo Software. A) BSE-based 3D reconstruction showing bulk morphology. B) Quantitative mineral analysis with Maps Min Software. C) 3D porosity reconstruction with Avizo Software.

Note that, although the specimens shown in Figures 5-6 are not from a carbon storage reservoir, similar workflows can be applied to reservoir samples to better understand their mineral distributions and pore networks.

Academic researchers have also used TEM to investigate fine structural details and to better understand carbon mineralization processes. For example, scientists at PNNL have used TEM and EDX to study layered microstructures in carbonate materials<sup>3</sup> as well as environmental TEM to monitor carbon mineralization *in-situ*.<sup>4</sup>

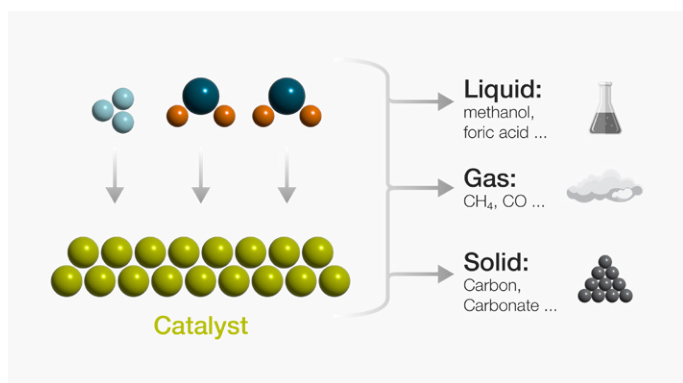
Together, these techniques can improve our understanding of how CO<sub>2</sub> interacts with subsurface minerals, supporting both fundamental research and the development of more reliable geological storage strategies.

## Carbon utilization: characterization of catalysts and synthesized materials

Captured CO<sub>2</sub> is used in a range of industrial pathways, from biological and chemical conversion to non-conversion applications such as enhanced oil recovery and direct use. Among these pathways, chemical conversion benefits especially from materials characterization because CO<sub>2</sub> is transformed into new materials such as fuels, chemicals, plastics, and carbon-based solids (Figure 7), which makes a multi-modal characterization workflow particularly relevant.

Key analytical needs in this segment include morphology, chemical composition, chemical state, and *in-situ* analysis. Because catalysts are often nanoscale materials, TEM is especially valuable here, as it can reveal catalyst structure and track structural changes during reactions.

Scientists have also used XPS to study catalyst surface chemistry,<sup>5</sup> SEM to examine catalyst morphology,<sup>6</sup> and STEM-EELS to investigate the fine structural and chemical features of nanoscale catalysts.<sup>7</sup> Specialized TEM approaches, leveraging *in-situ* holders<sup>8</sup> or environmental TEM (ETEM), have also been used to monitor the structural changes undergone by catalysts during various reactions.



**Figure 7. Schematic illustration of catalyst-assisted CO<sub>2</sub> chemical conversion into different product types.**

Characterization can also extend beyond the catalyst itself to the products formed by these reactions. SEM-EDX has been used to characterize carbonate products,<sup>9</sup> while TEM-EDX has been used to analyze carbon nanofibers formed during CO<sub>2</sub> conversion.<sup>10</sup> By combining catalyst characterization with product analysis, researchers can gain a more complete understanding of how CO<sub>2</sub> is converted and how these systems can be further optimized.

## Summary

The growing demand for CCUS is creating a pressing need for the characterization of solid materials and their transformations across capture, storage, and utilization processes. Thermo Fisher Scientific offers a range of analytical technologies and workflows that are primed to support CCUS, including TEM, SEM, FIB-SEM, and XPS instrumentation. These can support the development of solid sorbent materials for carbon capture, reveal mineral distributions and pore networks critical for carbon mineralization and storage, and can characterize catalysts as well as the solid products formed during CO<sub>2</sub> re-utilization. By combining these complementary techniques across multiple length scales, materials characterization can connect structure, chemistry, and performance, helping researchers advance more efficient, reliable, and scalable CCUS solutions.

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