Carbon Conversion:

Roles for Artificial Intelligence in Support of FECM RDD&D Priorities

February 2024

U.S. DEPARTMENT OF ENERGY

Fossil Energy and Carbon Management

Artificial intelligence (AI) holds the potential to accelerate the transition to a carbon-neutral economy and help achieve the technology research, development, demonstration, and deployment (RDD&D) goals set forth by the DOE Office of Fossil Energy and Carbon Management (FECM) in its *Strategic Vision*. FECM and the National Energy Technology Laboratory (NETL) continuously expand, maintain, and curate extensive scientific datasets and AI tools essential to carbon management, and they are now standing up a robust AI Multi-Cloud Infrastructure to enable the DOE research community to share and leverage a collection of tailored resources to expedite progress toward equitable and sustainable solutions.

As one step toward prioritizing AI development activities, FECM is exploring specific roles for AI in meeting the top RDD&D needs identified in the *Vision*. This document summarizes a series of discussions in which a range of specialists from FECM, NETL, and the DOE Office of Science suggested potential roles for AI in Carbon Conversion. This document should be viewed as a representative sample of the types of AI applications that may be needed; it is by no means a comprehensive list.

Cover image: AdobeStock #168274790

Contents

Potential Roles for AI in Carbon Conversion

The U.S. Department of Energy (DOE) Office of Fossil Energy and Carbon Management (FECM) and its partners are working to mitigate the climate crisis by developing new and improved technologies and conversion pathways for recycling carbon dioxide (CO_2) into value-added products. Ideally, these products will provide economic incentives for the conversion in addition to long-term storage for the incorporated carbon.

> **Carbon (CO_2) Conversion Vision Statement**
>
> Research, develop, and demonstrate a broad suite of technologies that convert CO_2 into environmentally responsible, equitable, and economically valuable products, and enable low-carbon supply chains to meet the goal of a decarbonized economy by 2050.
>
> *FECM Strategic Vision 2022*

Carbon conversion represents a key opportunity in the larger carbon capture and storage ecosystem, particularly where long-term storage is not available or where CO_2 sources are too distributed for centralized capture (FECM 2022). Conversion technologies can complement other CO_2-mitigation efforts, such as point source capture (PSC) and carbon dioxide removal (CDR) (FECM 2023a). While carbon-conversion approaches can be limited by the available markets for the products created, conversion technologies will be of particular interest in industry sectors that are hard to decarbonize by other methods.

FECM's Carbon Conversion Program invests in research, development, and demonstration (RD&D) projects to reduce carbon emissions by enabling the economic conversion of carbon oxides—including CO_2—into valuable products (FECM 2023a). The Carbon Conversion Program focuses on three main pathways (see Figure 1): catalytic conversion into fuels and chemicals, biological uptake into algae and bioproducts, and mineralization into inorganic materials. (A fourth pathway, Working Fluids, includes the direct use of CO_2 in more established processes such as enhanced oil recovery and is not a focus of FECM's Carbon Conversion Program.) Overall, a wide range of value-added materials can be created through the different types of carbon conversion—including pharmaceuticals, plastics, syngas, carbon nanotubes, and building materials.

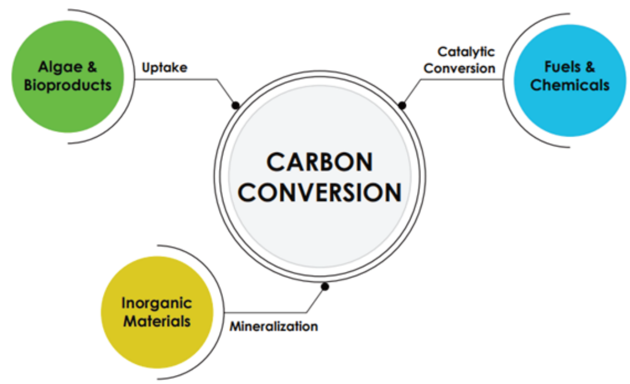

Figure 1. Key Carbon Conversion Approaches (Source: FECM 2023a)

To briefly introduce each of the three main pathways under consideration: **Catalytic Conversion** involves developing and evaluating novel catalysts that facilitate the carbon conversion process using less energy. The efficacy of a catalyst depends on its productivity in facilitating CO_2 reactions, its durability and ease of recyclability, and the energy and carbon intensity of producing it in the first place. **Biological Uptake** approaches take advantage of the CO_2 absorbed by algae-based systems during photosynthesis and use the resulting biomass to generate a range of chemicals, fuels, and other bioproducts. The cost-effectiveness of these technologies depends on the algae's rate of CO_2 uptake, the amount of energy needed to deliver CO_2 to the system, the duration of CO_2 storage, and other parameters. Lastly, **Mineralization** techniques make use of the way CO_2 exposed to an alkaline material reacts by permanently bonding with various calcium- or magnesium-based minerals to create carbonates—offering the potential to create building materials and other value-added products. While these reactions with alkaline materials occur naturally without added energy, the benefits of accelerated mineralization strategies depend significantly upon how effectively a mineral source reacts with CO_2 and how much commercial value is attached to the final product (Sandalow 2021). Figure 2 outlines these pathways and value-added products.

Converting CO_2 sources into economically viable products faces significant challenges. Viewed from a thermodynamic standpoint, CO_2 is a highly stable molecule, and significant energy, often achieved with a catalyst, is needed to convert it cost-effectively (Whang 2019). The various chemical pathways to create a desired product can be highly complex and interlinked. Optimal conversion opportunities may also depend on the local geography or other conditions specific to a particular factory or site. Overall, a complex range of factors may impact efforts to create a conversion system that can cost-effectively produce a valuable material from CO_2 at scale.

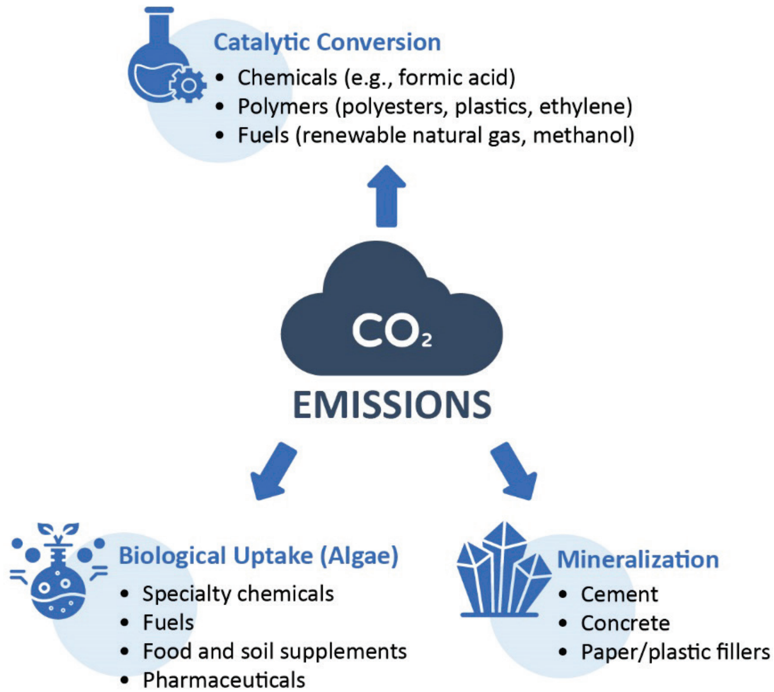

Figure 2: Key CO_2 Conversion Pathways and Products

As a result of these challenges, artificial intelligence (AI) can play a significant role in improving existing carbon-conversion technologies, exploring potential new conversion opportunities, and optimizing site performance and efficiency based on changing situations—to name a few possibilities. AI provides a wealth of opportunities to advance carbon-conversion approaches based on its capacity to quickly analyze and process large databases, manage interconnected systems, react to real-time feedback from smart sensors, and simulate or explore the vast potential of diverse catalyst chemistries and system designs.

FECM has identified numerous potential roles that AI can play in the RD&D of carbon conversion, as outlined in Figure 3. This figure extends across two pages and serves as a direct outline for the topics discussed in this document. Topics are categorized based on the three key aforementioned pathways—Catalytic Conversion, Biological Uptake, and Mineralization—along with a fourth section on Cross-Cutting Issues, which looks at how AI can help conversion approaches across the board.

Recent FECM solicitations and business opportunities in carbon conversion include the following:

- **BIL FOA 2829 - Carbon Utilization Procurement Grants**: provide up to $100 million to assist in purchasing products made from converted carbon emissions.
- **Lab Call - Core Laboratory Infrastructure for Market Readiness (CLIMR)**: supports accelerated stress testing capabilities for materials created from carbon conversion.

(FECM 2023b)

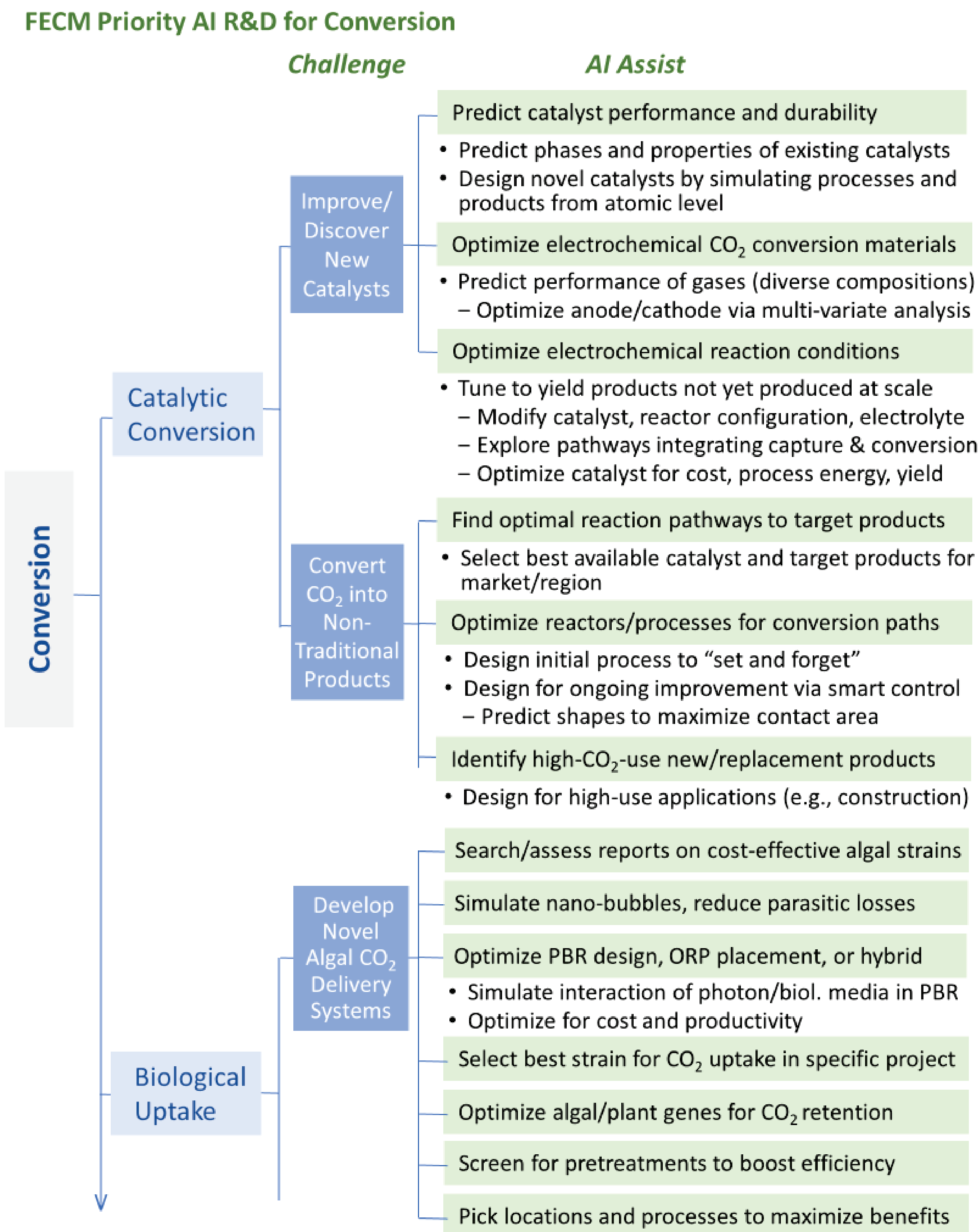

Figure 3: Summary of Potential AI Roles in Carbon Conversion (Note: Chart reflects document structure.)

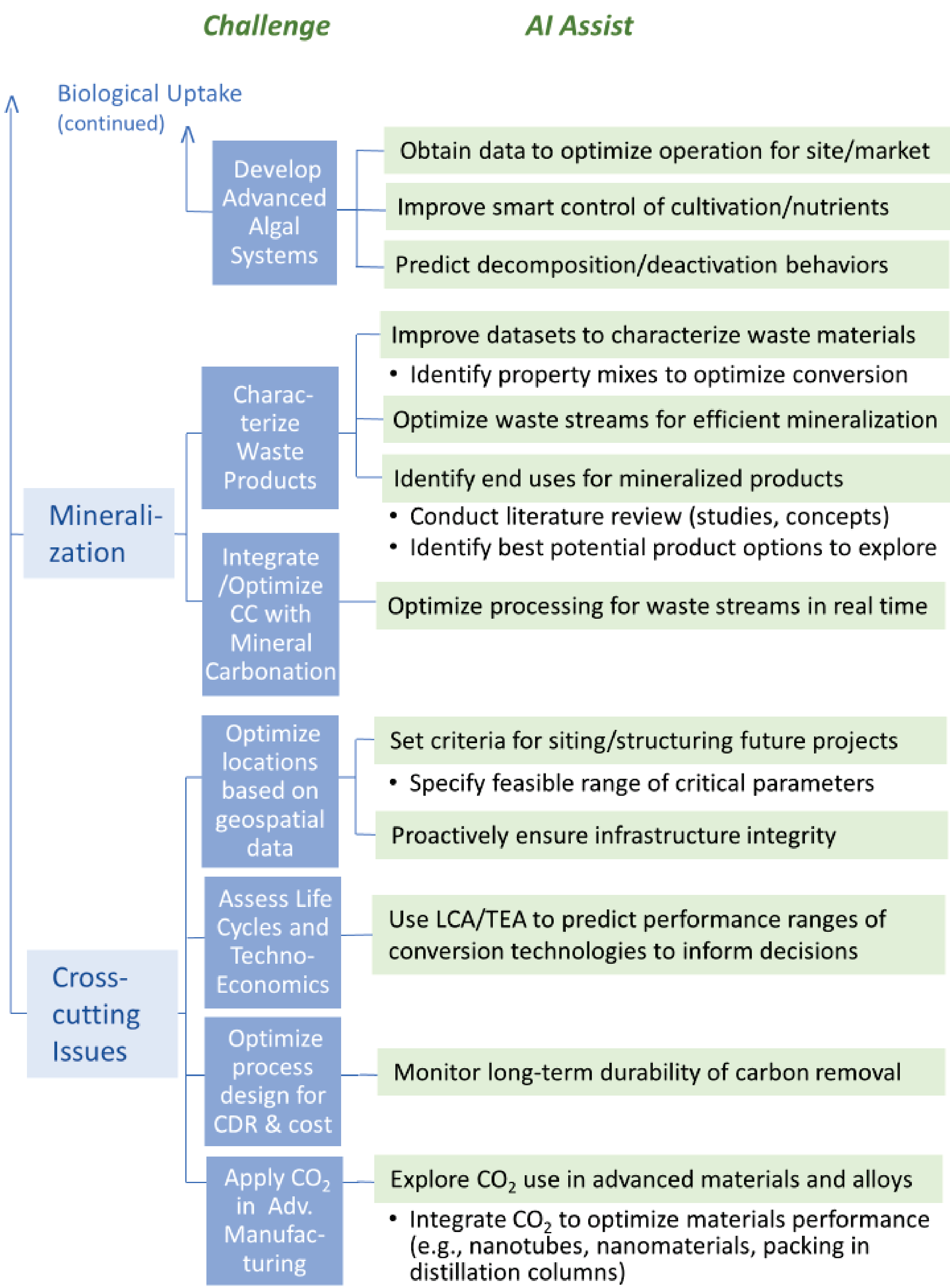

Figure 3. Summary of Potential AI Roles in Carbon Conversion (continued)
(Note: Chart reflects document structure.)

The FECM Carbon Conversion Program engages with a broad range of investment, consumer, governmental, and community stakeholders to develop cost-effective carbon-conversion methods and the required supporting infrastructure. The Program's RD&D portfolio includes public-private partnerships, university-based research grants, and agreements that leverage the resources and expertise of the national laboratories.

The National Energy Technology Laboratory's (NETL's) Research and Innovation Center helps implement FECM's portfolio of RD&D efforts, targeting key projects across each of the three previously mentioned technology pathways. The locations of currently funded projects relating to catalyst-, biologic-, and mineralization-based carbon conversion are shown in Figure 4, the NETL website provides project 3summaries and additional details (NETL 2023). The catalytic pathways target cost-effective CO_2 conversion into a broad selection of carbon-derived chemicals, polymers, and other products, including formic acid, ethylene, polyesters, plastics, and synthesized fuels. The biologic projects, which explore carbon uptake by algae, target cost-effective solutions that optimize CO_2 absorption while decreasing overall system energy needs, and the mineralization projects primarily focus on identifying the specific materials and conditions to maximize long-term CO_2 storage in widely used building supplies.

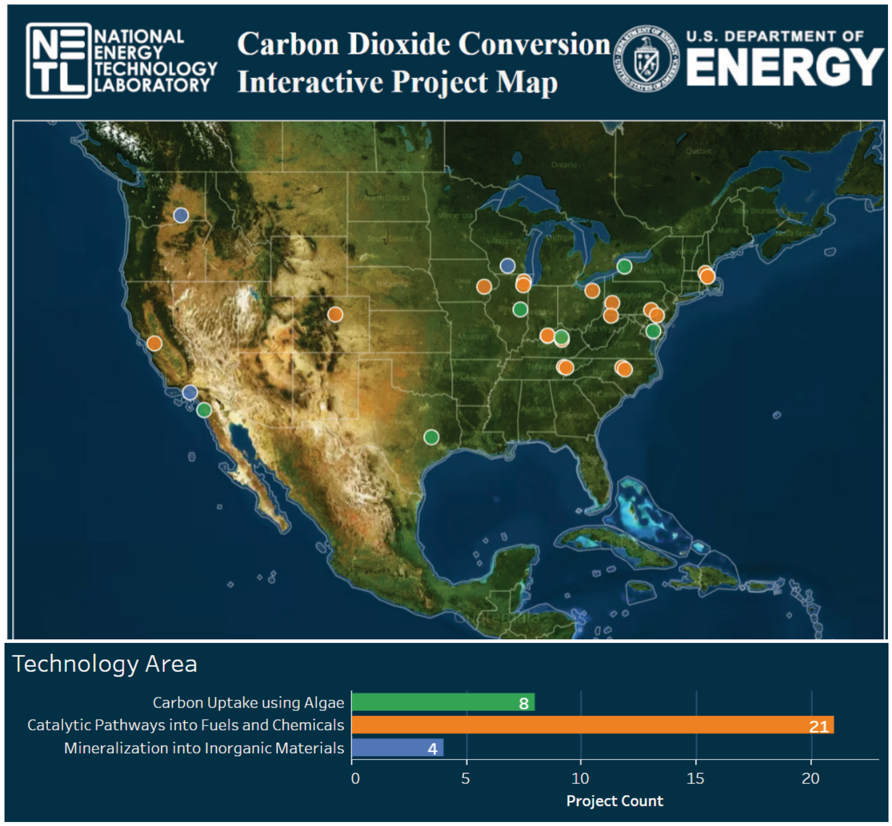

Figure 4. Current NETL-Administered CO_2 Conversion Projects
(Source: NETL 2023)

AI and machine-learning (ML) capabilities can expedite progress throughout these three core technology areas, and the following sections identify some of the key opportunities within each area. Decarbonization efforts across the nation are actively exploring carbon-conversion technologies, and AI/ML can assist in finding the approaches that are most cost-effective, optimized for a specific application, and beneficial in attaining U.S. carbon-reduction and sustainability goals. While the topics addressed below are by no means comprehensive in identifying the potential of AI/ML technologies in the carbon-conversion space, they are intended to highlight current opportunities and suggest broader ways in which AI/ML techniques may overcome hurdles to progress.

Catalytic Conversion

FECM's research into carbon conversion pursues the most cost-effective catalytic pathways to convert CO_2 into economically viable products. To reduce the energy input needed for CO_2 conversion, researchers seek catalysts that can attach themselves to CO_2 molecules just long enough to facilitate a reaction, then break away to serve this role again and again (Clark 2013)—improving conversion efficiency and cost-effectiveness. The Carbon Conversion Program specifically pursues catalyst-based research along four general tracks: thermochemical, electrochemical, plasma-mediated, and hybrid systems (FECM n.d.). A brief description of each track is provided in the accompanying sidebar.

The various types of catalytic reactions and diverse resulting products generate numerous conversion pathways for exploration. Currently funded FECM/NETL RD&D efforts include catalytic carbon conversion processes that create products like renewable natural gas, methanol, formic acid, dimethyl carbonate, bioplastics, carbon nanotubes, sodium bicarbonate, ethylene, propylene, propionic acid, syngas, ethylene, acetate, and recyclable polyester (NETL 2023). Integrated systems that include reactive capture and conversion processes enable the conversion of a dilute CO_2 stream into useful products without incurring the costs to purify or transport the CO_2 (FECM 2023b).

Beyond the wide array of potential catalytic reactions, chemical pathways, and end products, catalytic carbon conversion technologies confront challenges common to other fields undergoing significant innovation. Catalytic conversion is a highly dynamic RD&D space, with many possible conversion approaches currently at relatively low technology readiness levels (FECM n.d.). Future research will identify the most promising options for development toward commercial feasibility. Additional information on currently funded projects can be found on the NETL website.[1]

Key Catalytic Conversion Approaches

Catalysts can serve to selectively initiate and speed up different types of reactions. The four main catalytic-conversion approaches targeted by FECM are as follow:

Thermochemical: Energy is provided in the form of heat (and pressure), and the reaction is often driven by a catalyst.

Electrochemical: Energy is provided in the form of electricity, and catalyzed reactions take place in an electrochemical cell.

Plasma-mediated: CO_2 is activated by energetic electrons instead of heat, and the reaction is often driven by a catalyst.

Hybrid Systems: These include biocatalysis, reactive capture, and conversion or systems that include a combination of thermochemical, electrochemical, or plasma-mediated approaches.

(FECM

Key engineering, technical, and financial parameters for down-selecting technologies for further research are still under development. Integrated field testing can help validate high-potential technologies, while Front-End Engineering Design (FEED) studies or operational demonstration projects can accelerate development of selected first-generation systems (FECM 2022). Associated needs include building the supply chains and other infrastructure to support these emerging catalytic-conversion systems. Future systems may integrate multiple advanced technologies, potentially incorporating CO_2 conversion approaches alongside hydrogen production.

For catalytic approaches, "All paths rely on high activity, high selectivity, and stable conversion catalysts" (Chen 2023a). Opportunities presented by catalyst-based conversion technologies remain largely in their infancy, and

[1] NETL Carbon Dioxide Conversion Program project: https://netl.doe.gov/carbon-management/carbon-conversion

emerging AI tools could deliver considerable benefit by identifying the most-promising chemical pathways and moving the resulting conversion technologies to commercialization quickly and effectively. Some of the main FECM-identified opportunities for AI in catalytic conversion are discussed in the following sections.

Improve/Discover New Catalysts

AI- and ML-driven methodologies are particularly well equipped to tackle the complex nature of catalytic reactions and the vast potential search space for cost-effective catalysts and reaction pathways (Zhang 2022). Finding and optimizing effective catalysts with ideal performance and durability characteristics are critical steps in developing carbon-conversion technologies that meet the needs of industry.

Predict Catalyst Performance and Durability

To effectively identify promising catalysts, thermodynamic simulation software (including packages that incorporate CALculation of PHAse Diagrams [CALPHAD] methods) can be used to predict the phases and properties (e.g., melting temperatures) of potential catalytic materials. The synthetic phase information generated by such thermodynamic software can then be coupled with density-functional theory (DFT) to predict catalyst performance. Such approaches can be used by AI to **predict the phases and properties of existing catalysts** and to generate sufficient synthetic data to help train AI models to find optimal solutions. An example of the iterative feedback loops used in supervised learning models is outlined in Figure 5.

Density-Functional Theory

"Density-functional theory (DFT) is a successful theory to calculate the electronic structure of atoms, molecules, and solids. Its goal is the quantitative understanding of material properties from the fundamental laws of quantum mechanics." (Kurth 2005)

An insufficient supply of up-to-date catalyst data can constitute a major hurdle in training a neural network. The volume of specialized data needed for effective ML frequently exceeds the amount that can be obtained experimentally. While data acquired through synthetic modeling may be computationally more expensive and quantitatively less accurate than measured data at the outset, it can be *qualitatively* valuable. Checking synthetic data through physical experimentation and validation—particularly using an iterative approach between modeling and selective real-world testing—can improve the effectiveness of such AI-driven efforts over time. An enormous quantity of synthetic data would be needed, and the AI training set would need to be rigorously verified. To properly train such models and ensure that they are effectively modeling reality often requires cooperative efforts by experienced electrochemists, data scientists, and AI experts.

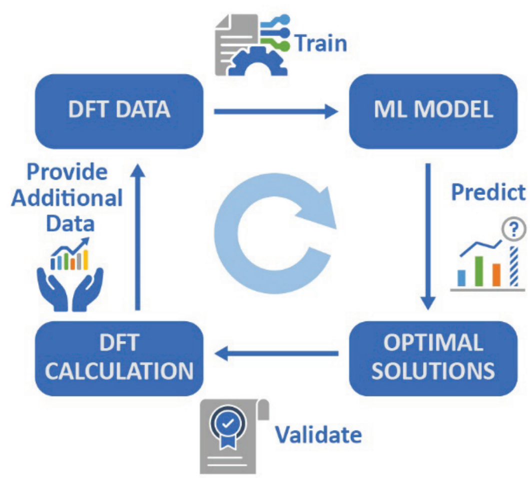

Figure 5: Example of Supervised Learning Approach Using Iterative Feedback Loops
(Source: modified from Chen 2023a)

Additional challenges in predicting catalyst performance include uncertainties regarding approximations resulting from the DFT predictions; projected material costs, stability, and CO_2-adsorption effects; and the "black box" nature of decision making in AI models (Zhang 2022). The last of these challenges is typical of AI/ML-based models that require significant accountability—as in the autonomous-vehicle segment, where the process for making situation-based decisions is critically important.

While AI must overcome numerous challenges when applied to exploring catalyst behavior, the potential rewards are significant. Coupling phase simulation software and DFT predictions (as described above) can help train neural networks that should ultimately be able to **design novel catalysts by simulating processes and products from an atomic level**. This capability could potentially save substantial cost and effort in experimental studies and accelerate the development of novel approaches to cost-effective carbon conversion.

Optimize Electrochemical CO_2 Conversion Materials

Ideally, electrochemical CO_2 conversion processes will use cost-effective catalysts and renewable electricity to convert CO_2 into value-added materials. Figure 6 shows a typical electrochemical schematic. The effectiveness of such conversion technologies depends upon numerous process efficiencies, including how much current/energy is required to power the reactions; how quickly these reactions occur; how effective the given catalysts and reactor setups are at generating the desired downstream products (i.e., “Faradaic efficiency”); and how long a system can continue operating before the catalysts deteriorate, become deactivated, or no longer function effectively (i.e., “durability”) (Overa 2022). Optimizing an electrochemical system’s catalysts, configuration, long-term durability, and other key parameters is crucial to creating a financially viable CO_2 conversion method.

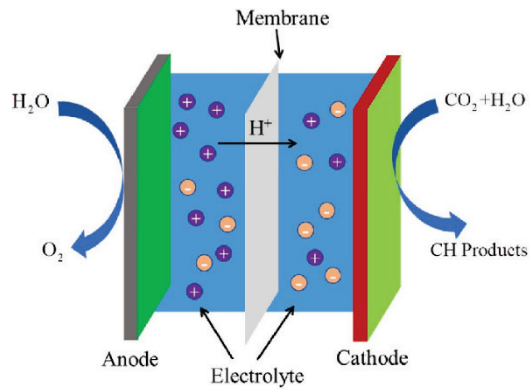

Figure 6: Example Schematic of Electro-chemical CO_2 Reduction Reaction

One challenge in understanding the performance of these systems is knowing precisely which chemical reactions are occurring within the electrochemical cell (Kempler 2023). This challenge applies specifically to the Faradaic efficiency mentioned above—i.e., what are the electrochemical reactions producing, and how much of from the supplied CO_2 is in the desired product(s)? For any given system, gases of various compositions will be present near the electrochemical cathodes and anodes, and simply measuring current between the electrodes does not provide a full understanding of system effectiveness (Kempler 2023).

Faradaic Efficiency

“Faradaic efficiency (FE) describes the overall selectivity of an electrochemical process and is defined as the amount (moles) of collected product relative to the amount that could be produced from the total charge passed, expressed as a fraction or a percent.”

(Kempler 2023)

A key optimization challenge, then, is to **predict the performance of diverse compositions of gases** within an electrochemical system. The focus here is on optimizing the anode and cathode elements, potentially using a simplified, one-dimensional model of the electrochemical device and synthetically providing it with device gases of various compositions, current densities, and overpotentials. Ultimately, the goal is to maximize the cell’s performance in terms of efficiency, conversion, waste heat generated, product output, etc.

Based on the literature, AI/ML techniques have not been widely applied in modeling electrochemical CO_2 conversion; however, researchers have used a chemoinformatics-based ML model to improve the prediction of CO_2 absorption by physical solvents. Precise descriptors (like chemical bond structures and thermodynamic factors) were fed to the ML neural network, which more accurately fit the properties of solvents to their CO_2 solubility (Li 2019). This success suggests that a similar approach, using ML and detailed data on the characteristics of various device gases, might potentially be applied to predict or possibly optimize the electrochemical conversion of CO_2. Similarly, key parameters such as chemical kinetics, Faradaic efficiencies, current densities, and other properties might help **optimize anode/cathode elements via multi-variate analysis,** enabling AI-based techniques to optimize system configuration and maximize electrochemical CO_2 conversion.

Optimize Electrochemical Reaction Conditions

AI systems might go beyond enhancing or optimizing the electrode configurations for electrochemical reactions (as discussed above) to optimize overall electrochemical systems. Specifically, AI can assist in scaling up the processes to a commercial scale—including optimizing the catalysts involved, analyzing potential reactor configurations, and fine-tuning process efficiencies.

One crucial application of AI is to **tune existing catalytic conversion approaches to yield products not yet produced at scale**. Reaction conditions for electrochemical conversions can be optimized to favor products that have not yet been made selectively or at sufficiently high rates, such as methanol and methane. Methanol, for example, is used as a primary feedstock for making a wide range of organic compounds and bulk chemicals. Decentralized, cost-effective production of this feedstock could yield diverse options for integrating this type of carbon conversion into current and future supply chains (Ganesh 2016).

Building on recent advances in density functional theory for predicting material properties, AI/ML approaches can help fine-tune existing catalytic conversion pathways to achieve full-scale commercialization. Improvements may include **modifying the catalyst, reactor configuration, or electrolyte**—essentially targeting any process-related components/characteristics that can be better tuned through advanced computing optimizations. Efforts could also **explore pathways integrating capture and conversion** by evaluating and optimizing different potential chemical pathways. Identifying catalysts that minimize methane production (in turn minimizing a system's need for methane purges) or tolerate high levels of oxygen impurity can improve the productivity and economic opportunities of certain carbon-conversion pathways (Cordero-Lanzac 2022).

AI-based analytics can further be used to **optimize catalysts to improve cost, process energy, and yield**. Complex lifecycle analyses, like those targeting net reductions of CO_2 emissions (including emissions from a catalyst's production and conversion processes), could also be considered in the optimization process. Catalyst deactivation behavior may also be better quantified, as catalysts gradually change over time and physical experiments to measure the degradation effects can take a long time to produce useful data.

In general, long-term electrode durability studies are in short supply relative to experiments emphasizing efficiency and performance (Nwabara 2020). AI/ML methods implemented in tandem with the aforementioned DFT analyses and thermodynamic software could help synthetically model these electrochemical conversion systems and improve current understanding of how they perform over extended periods—with reduced need for physical testing. Such efforts would improve our ability to determine system lifecycle impacts, which can be greatly affected by the longevity of catalysts and electrode materials.

Convert CO_2 into Non-Traditional Products

In addition to improving upon established catalytic conversion pathways, AI techniques can help identify opportunities to convert CO_2 into other materials. Key examples include products with a substantial number of carbon–carbon bonds (e.g., carbon nanotubes, polymers, ethylene, etc.), raising the potential to cost-effectively manufacture a wide range of chemicals, pharmaceuticals, plastics, and more. Using CO_2 to produce polymers is of particular interest, as these can be made using relatively little energy, possess significant market value, and can incorporate CO_2 at rates above half of the resultant polymer's final mass (IEA 2019). The combined use of AI and chemoinformatics data is becoming increasingly common—particularly in areas such as analytical chemistry and pharmaceutical drug discovery (Saldívar-González 2020). A recent collaboration between Microsoft and Pacific Northwest National Laboratory used AI to greatly accelerate the discovery of new battery materials (Bolgar 2024). Such approaches might also find new catalytic conversion opportunities far more efficiently than through experimentation alone.

Find Optimal Reaction Pathways to Target Products

As different reaction pathways can lead to different optimizations or carbon–carbon bonds, AI technologies could prove particularly useful for determining optimum configurations and pathways for achieving targeted end products. Such approaches could help predict outcomes of varying thermodynamic and kinetic parameters based on different reaction temperatures, pressures, species ratios, catalytic surfaces, etc.—with the core goal of obtaining the highest species yield and CO_2 conversion for a specific end use. By using AI/ML approaches to explore a broad range of potential reaction pathways, the target end products (and perhaps the best available catalyst) might be selected in advance. For example, AI-based algorithms have helped screen catalysts for efficient reaction pathways to convert CO_2 into ethylene (Sexton 2020).

The Open Catalyst Project

One of the most frequent issues with creating AI/ML models is the lack of sufficiently large and accessible datasets to train such models. Generating the needed data exclusively from physical experiments can be incredibly difficult, if not impossible.

The Open Catalyst Project, a collaboration between Meta AI's Fundamental AI Research and Carnegie Mellon University's Department of Chemical Engineering, seeks to overcome this limitation by making large datasets of catalyst behavior publicly available (Open Catalyst Project 2023). The goal is to encourage the creation of low-cost catalysts to enable cost-effective renewable energy storage.

Currently available resources include one dataset with over 1.3 million molecular relaxations (characterizing catalyst reactions and resulting from over 260 million DFT calculations) and another set with 62,000 relaxations focused on oxide electrocatalysis (Nature 2022). Additional information on the project, including downloadable datasets and documentation, can be found at opencatalystproject.org.

Opportunities for cost-effective carbon conversion can depend heavily upon local and regional market considerations. It follows, therefore, that AI-based screenings utilizing localized inputs and nearby supply chains can help to **select the best available catalyst and target products for a given market/region**. Ultimately, this ability to pre-screen opportunities for a large number of locations can greatly enhance the targeting and efficacy of carbon-conversion programs.

For pre-screening approaches that use AI in tandem with methodologies such as chemoinformatics or DFT, it will be particularly important to ensure that simulated data sources match reality. Some identified opportunities may be overly idealistic or unachievable with the current state of a particular technology. Other opportunities simply might not offer a sufficiently large improvement in production or efficiency versus more established systems and reaction pathways. The accuracy of DFT, for instance, is not always well understood. It may turn out that interesting formulations and reaction conditions, when tested experimentally, simply highlight areas in which DFT makes poor predictions rather than something more interesting. Synthetic data will require experimentation and validation.

Optimize Reactors/Processes for Conversion Paths

AI/ML-based approaches for determining optimal reactors and processes for CO_2 conversion pathways can be used in tandem with supplemental models such as chemoinformatic datasets or computational fluid dynamics

(CFD). Such efforts can help optimize reactors and processes for various conversion pathways, potentially allowing developers to **design the initial process to "set and forget"** by incorporating such parameters as heat transfer requirements, contact areas, etc., into the system. Optimizing the conversion pathways would serve to lessen any required long-term maintenance, helping to drive down operating costs and improve overall cost-effectiveness.

> **Computational Fluid Dynamics**
>
> "Computational fluid dynamics (CFD) is a science that, with the help of digital computers, produces quantitative predictions of fluid-flow phenomena based on the conservation laws (conservation of mass, momentum, and energy) governing fluid motion."
>
> (Hu 2012)

The systems could additionally be **designed for ongoing improvement via smart control**, taking advantage of the improved monitoring capabilities afforded by AI-powered monitoring and control devices. Advanced smart sensors and responsive feedback systems can help to advance the above-mentioned "set and forget" approach, responding to any changing parameters that affect the conversion process in real time—and ultimately learning to improve such responses over time. Smart-manufacturing approaches have proven their ability to reduce energy use and emissions by 30%–50% in many cases, while smart grids using advanced onsite controls can cut electricity bills by 20% or more (Chen 2023b). Applying similar AI-based technologies to catalytic and other CO_2 conversion systems could help to realize comparable savings along with improved operations.

Advanced computing techniques can also be used to **predict reactor shapes that could maximize catalyst contact area** in these conversion systems, improving operational efficiencies. This framework of geometric optimization—synthetically testing out a broad selection of potential design shapes, without having to build actual prototypes for each—is particularly suited to the type of iterative optimization at which AI-based solutions excel. As one example of this approach, AI algorithms were recently used to evaluate the effectiveness of various system geometries in a direct air capture (DAC) reactor, helping to optimize the system's ability to capture CO_2 (Weber 2023).

Identify New/Replacement Products That Use High Amounts of CO_2

Other efforts to improve catalytic conversion of CO_2 using AI/ML methods could explore opportunities for new or replacement products that can be derived from CO_2. These non-traditional conversion pathways would ideally target high-intensity applications that would be able to incorporate large quantities of CO_2. Such efforts would **design products for high-use applications (e.g., construction).** AI approaches could be directed toward a specific application, product replacement, or novel material chemistries and product. For example, developers might target existing products for replacement by materials that store high levels of CO_2 for the long term.

A sizable portion of current research into novel, high-CO_2-use products is understandably directed at building materials for the construction industry—which require enormous amounts of base materials that typically need to be mined or pumped. Construction materials represent a huge potential long-term sink for CO_2. Current research efforts include using CO_2 to create concrete, paper, and plastic fillers (by combining CO_2 with magnesium and calcium from steelmaking by-products), and, to a lesser degree, high-value materials like carbon nanotubes and graphene (Cho 2019). As with all of these catalytic conversion processes, success will require improving process efficiencies and lifecycle costs to a degree that makes these CO_2-based products economically viable.

Biological Uptake

FECM's Carbon Conversion Program supports research into pathways for the biological uptake of CO_2 via algae-based systems and the subsequent conversion of the resulting biomass into cost-competitive products. Instead of using catalysts to lower the energy needs of CO_2 conversion, biological-uptake approaches utilize the highly efficient photosynthetic processes of micro- or blue-green algae (cyanobacteria) (NETL 2023). Microalgae use CO_2 as their main source of carbon, and some can incorporate CO_2 more than 100 times faster than terrestrial plants (Farooq 2022). The high growth rates and carbon-uptake capabilities of more than 3,000 identified strains of microalgae make them a highly promising route for carbon conversion (Fu 2019). AI can help to advance RD&D that leverages these algae-based biological uptake systems to mitigate CO_2 emissions.

Biological CO_2 conversion systems can produce a wide range of useful materials, including chemicals, food products, soil supplements, pharmaceuticals, and biofuels (FECM 2023a). Figure 7 highlights a selection of these products. The Bioenergy Technologies Office (BETO) within DOE's Office of Energy Efficiency and Renewable Energy (EERE) focuses on algae-to-fuel pathways, while FECM-led carbon conversion efforts focus on non-fuel algae-based products.

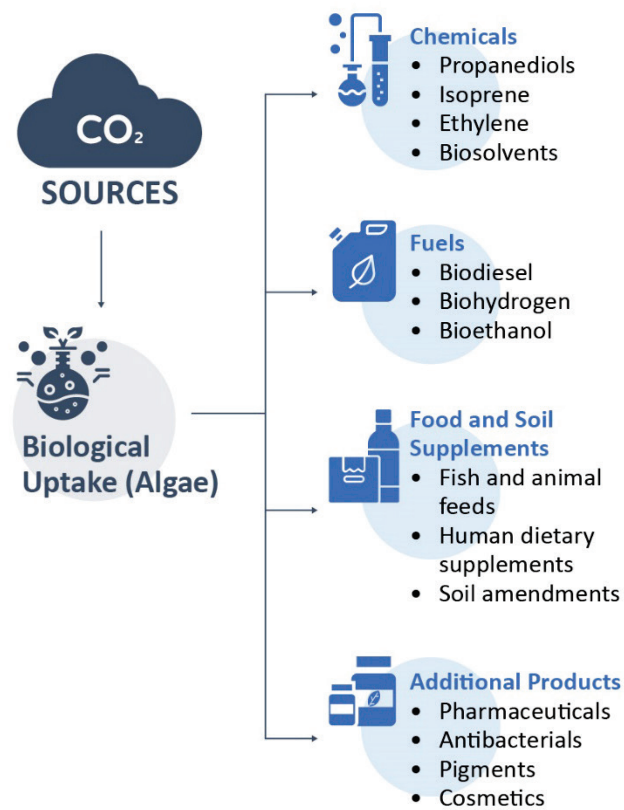

Figure 7: Key Materials Created by Algae-Based CO_2 Conversion Systems

(Data sources: Elst 2018, NETL n.d., Sun 2023)

Current research primarily focuses on microalgae or cyanobacteria cultivated in either photobioreactors (PBRs) or outdoor ponds (NETL 2023). Outdoor ponds (i.e., open raceway ponds) are discussed in more detail starting on page 16. PBR-based systems aerate the microalgae with CO_2 and replicate conditions (e.g., light, temperature, nutrients, pH, gas flow rate, etc.) deemed optimal for CO_2 uptake and algae growth (Fu 2019). These systems are typically enclosed and pass CO_2-enriched gas through an aerator before bubbling it into the microalgae. A key challenge in making these systems cost-effective is increasing the efficiencies with which CO_2 is delivered to the system and integrated into the algal biomass (Fu 2019). Research has explored numerous PBR geometries to find those that can most effectively generate valuable end products.

Algae generated from PBRs and outdoor pond systems can be broken into different biochemical fractions or components (e.g., proteins, carbohydrates, and a variety of different lipid classes), which can then be used to create diverse end products (Elst 2018). To date, product application values have tended to be inversely related to market size (Crocker 2017). The types and proportions of biochemical compounds generated depend on the particular strain(s) of microalgae used (Elst 2018) as well as the cultivation and production characteristics of the PBR (Crocker 2017).

As discussed below, improving the cost-effectiveness of biological-uptake conversion systems involves diverse strategies. Beyond fine-tuning system operating parameters (e.g., geometries, flow rates, and feedback loops), it requires minimizing energy use, maximizing carbon uptake, and optimizing production of the target biomass fractions. Ensuring efficient CO_2 uptake is a major consideration throughout. Other central concerns include choosing optimal algae strains for a given application to enable cost-effective operation.

FECM's Carbon Conversion Program is addressing key challenges of algae-based systems by conducting RD&D to develop advanced algal concepts, field test and scale up emerging technologies, integrate novel technologies with existing commercial systems, and coordinate with other researchers on tool development (e.g., the Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies [GREET] Model). Currently funded projects through NETL's Carbon Dioxide Conversion Program include various efforts to improve system efficiencies and potential revenue, lower energy needs, and streamline CO_2 delivery and uptake. Further information about these projects can be found through NETL's program website.[2]

Develop Novel Algal CO_2 Delivery Systems

As noted above, DOE's work on algae-based conversion systems emphasizes the ability to cost-effectively capture, deliver, and utilize CO_2 in value-added products. One of the largest energy losses in these systems arises from compressing the sourced CO_2 to create the bubbles that help deliver it to the algae. Potential CO_2 sources include ambient air, flue gas, and commercially purified CO_2. Various approaches currently deliver this gas to the system, including direct bubbling, micro or nanobubbles, and porous or non-porous membranes (Zheng 2018). CO_2 can account for over half of a system's raw material costs; however, depending on the system, over half of the CO_2 delivered may fail to be taken up by the microalgae (Zheng 2018)—underscoring the critical importance of optimizing CO_2 delivery in these technologies.

The following sections outline key opportunities for AI/ML techniques to address these challenges.

Search/Assess Reports on Cost-Effective Algal Strains

Given the importance of cost-effectiveness and the challenges of attaining it, algae-based systems are still typically at the phase of bench-scale or pilot testing (Rafa 2021). A key opportunity at this point is to use AI-driven search tools or natural-language processing (NLP) models to evaluate the existing literature on cost-effective algal strains for high-volume CO_2 conversion. Such efforts could include reviewing the literature to compile useful parameters and metrics for identifying promising algal strains or analyzing scientific research studies to identify key gaps or overlaps in the current RD&D landscape.

Analyzing current RD&D publications, patent trends, and similar resources could potentially help direct research funds more effectively. Using a combination of learning models and science-based rules, AI tools might efficiently comb through copious volumes of existing research to enable an industry-wide analysis of research opportunities (Chen 2023a).

Simulate Nanobubbles To Reduce Parasitic Losses

Nanobubble technology, which typically involves generating miniscule gas bubbles (diameters of no more than a few hundred nanometers), has proven a promising approach for improving gas uptake in gas–liquid systems (Patel 2021). CO_2 uptake levels are a major limiting factor in algae conversion systems, and studies have shown that nanobubbles can exhibit lifespans of more than a month while enabling greater overall biomass growth and significantly increasing the percentage of introduced CO_2 that these systems can utilize (Patel 2021). Ultimately,

[2] NETL Carbon Dioxide Conversion Program: https://netl.doe.gov/carbon-management/carbon-conversion

these benefits help offset the parasitic losses that result from bubbling in the CO_2 that is not taken up by the algae.

AI/ML techniques could help explore and answer two key questions in this space: (1) what is the most efficient way to create nanobubbles and (2) how do nanobubbles interact with the microalgae?

The first problem may be more of a computational challenge: how to best generate and distribute these CO_2 nanobubbles within the system. Nanometer-scale bubbles help to maximize the surface-area-to-volume ratio of CO_2 that is available for biological uptake. Maximizing the availability of CO_2 translates into less work and pressure needed for gas delivery. Again, this part of the process helps lower the associated parasitic energy losses from nanobubble production.

The second problem is more immediately amenable to an AI-based approach and is based on the huge physical size differences between nanobubbles (measured in nanometers) and the microalgae (typically at the micrometer scale). This vast difference in scale (nano versus micro) means that it can be especially difficult to model the relatively massive number of nanobubbles that would interact with the algae at any reasonable model size. It is not entirely clear whether these large numbers of interactions would be best modeled through fluid dynamics simulations or direct numerical simulations (with the latter approach being more computationally expensive). AI techniques could help to generate and refine the synthetic data needed to model the numerous and complex interactions that occur between the CO_2 nanobubbles and the much larger algae. Such an approach may also help researchers better link algae growth rates to CO_2 uptake across the cell membrane.

Optimize PBR Design, ORP Placement, or Hybrid Designs

Photobioreactors (PBRs) and open raceway ponds (ORPs) are the two main types of configurations used by algae-based CO_2 conversion systems. Figure 8 shows some examples of the various configurations in use. PBRs, in particular, have been made in a wide variety of designs intended to optimize CO_2 uptake as well as the photosynthetic activity of the enclosed microalgae. Some PBR examples include stirred-tank, flat-panel, tubular, bag, pyramidal, and hybrid designs. Each of these approaches offers benefits and drawbacks in terms of light exposure, ease of cultivation, scalability, space requirements, cost, and ease of control (Chanquia 2021). ORP systems can be more cost-effective but tend to be less efficient and controlled because they are often exposed to ambient air and, therefore, more variable conditions. A hybrid approach to PBR/ORP systems is another route for research, potentially offering the benefits of both types (Crocker 2017).

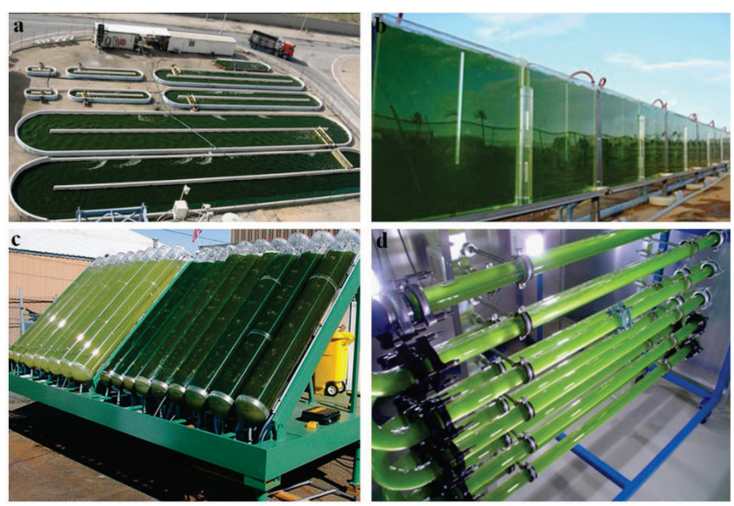

Figure 8: Different approaches to algae-based conversion systems: (a) open raceway pond (ORP), (b) flat-plate photobioreactor (PBR), (c) inclined tubular PBR, and (d) horizontal/continuous PBR.

Algae-based CO_2 conversion systems are highly dependent on CO_2 flow rates, nutrient transmissions, temperature, sunlight availability, and other variable conditions that affect the algae's photosynthetic processes (Fu 2019). AI/ML methods can be used to explore and optimize these systems, including **simulating the**

interactions of photons and biological media in PBR designs, potentially using digital twins or simulation-based training. To take such considerations from a computational approach to an AI-based one, optimization efforts might include an iterative series of PBR or ORP designs that take advantage of transfer-learning techniques—using previously trained models for these systems in subsequent design efforts to explore a broad design space and gradually improve performance. Such efforts might proceed along lines similar to those discussed earlier in optimizing design shapes for catalyst-based systems. An iterative methodology could also be applied to **optimize system designs for cost and productivity**.

Select Best Strain for CO_2 Uptake in a Specific Project

Along with CO_2 bubble size, light availability, pH, and other key system characteristics, the particular strain of microalgae used in a biological uptake system will have a significant effect on the amount of CO_2 that can be incorporated (Thawechai 2016). Identifying an ideal strain among the 3,000+ known varieties of microalgae presents a considerable optimization challenge. Selecting the most important variables to optimize (e.g., CO_2 fixation rate, system energy costs, biomass generated, etc.) will also be crucial (Thawechai 2016). Similar to the preceding discussion about optimal PBR design, AI-based techniques can be used to help determine an optimal algae strain for CO_2 uptake in a specific project given parameters like feed source, weather, and geography.

Optimize Algal/Plant Genes for CO_2 Retention

The optimization of gene sequencing through ML and deep-learning techniques is the focus of numerous ongoing AI-based initiatives (Buvailo 2023). These tools can scour an enormous amount of genetic data, helping to efficiently generate synthetic gene sequences that are tuned to effectively perform specific biological activities (Buvailo 2023). By applying these AI methods to the criteria of carbon-conversion systems, the genes of algae strains and plants could be tweaked to increase CO_2 retention as well as produce specific, high-value biological products. Potentially, multiple optimization efforts could be performed simultaneously—optimizing PBR design and strain selection.

Screen for Pretreatment Approaches to Boost Efficiency of Photosynthesis

As previously noted, a system's specific algae strain and cultivation parameters will influence its photosynthetic efficiency as well as the balance of biological compounds produced by the algae (including proteins, lipids, carbohydrates, etc.) (Elst 2018). The types and amounts of nutrients provided within a system can enhance system efficiency, as can the overexpression of certain types of enzymes, among other factors (Vermaas 2021). Numerous factors play into optimizing the long-term operation of a conversion system, and an AI-expedited search of existing literature could help identify both algae pretreatment strategies and system nutrients that can enhance photosynthetic efficiency.

Pick Locations and Processes to Maximize Benefits

Ultimately, AI-supported approaches can help tune system performance across numerous potential optimization parameters, such as: best locations and algal processes for a given system type; ideal environmental and social impacts; lowest costs (transportation, energy, capital, operating, etc.); optimal usage of low-cost/low-carbon energy, land, and water; and, especially, highest CO_2 capture rates. Large-scale analyses of this sort could also help address challenges in measuring, monitoring, and crediting carbon removal.

> "The CO_2 solubility and uptake efficiency can be enhanced by controlling the bubble size, design of the photobioreactor, proper selection of microalgae strain, and selecting appropriate operating conditions, such as flow rate, the concentration of CO_2, and pH." (Farooq 2022)

Implementing AI-based smart controls in a system can enhance long-term performance and efficiency, helping ensure that the desired performance metrics are achieved.

Develop Advanced Algal Systems

The following sections briefly address advanced, system-wide opportunities for putting AI technologies to work to improve algal-based conversion systems. Whereas preceding sections emphasized CO_2 delivery and optimizing its uptake by the microalgae or cyanobacteria strain, the following discussions build upon that emphasis to target system-wide, long-term optimization of cost and performance.

Obtain Data to Optimize Operations for Site/Market

System performance can be fine-tuned by selecting operating characteristics (e.g., CO_2 gas quality, sunlight utilization, algal species, PBR/ORP design, and other parameters) that align with site- and market-specific data. Site data (such as energy sources and weather conditions) could support optimal energy-saving decisions, and market data (biochemical products in demand by accessible manufacturing facilities or markets) could influence the selection of a particular algal species. Incorporating transfer-learning techniques could prove useful to iterate on promising system optimizations and ensure that projected annual benefits outweigh any weather-related or operational setbacks a system is likely to encounter. Using AI to optimize a microalgae system based on site-specific weather conditions, for example, has been shown to improve profitability and could be widely applicable to these types of systems (Jayaraman 2015).

Improve Smart Control of Cultivation/Nutrients

Incorporating smart controls with AI could significantly improve the effectiveness of added nutrients and cultivation efficiency in a conversion system. Algae growth rates are directly affected by a system's pH, temperature, substrate, and light availability (Penn State n.d.), so feedback loops that monitor and trigger appropriate system responses to real-time conditions can improve algae growth and overall yield. A recent study developed a predictive kinetic model for the addition of nutrients (nitrogen and phosphorus), and the experimental results demonstrated increased yields of both starches (+270%) and lipids (+74%) (Figueroa-Torres 2021).

Predict Decomposition/Deactivation Behaviors

Finally, as discussed for catalytic conversion, AI coupled with smart sensors and controls can help to monitor and ultimately predict decomposition/deactivation behaviors in algae-based systems. Microalgae can be susceptible to bacteria, fungus, and parasites. Particularly in flue-gas and open-system applications, these and other contaminants could interact with the biomass in a way that diminishes system productivity and CO_2 uptake. These deactivation effects can have a major, adverse impact on the long-term productivity and effectiveness of these systems. AI-based controls can help to identify the causes of such degradation behaviors, the potential effects on end-product quality, and the point at which a system will cease to produce effectively.

Mineralization

FECM's Carbon Conversion Program supports RD&D into pathways to accelerate and improve carbon mineralization—a natural process by which CO_2 is bound into rock as a solid carbonate mineral. This process occurs when CO_2 reacts with alkaline materials (like magnesium or calcium) exposed in crushed rock generated by a range of industrial processes such as mining or steelmaking (Sandalow 2021).

Whereas the previous section focuses on using CO_2 to grow microalgae for conversion into *organic* value-added products, this section focuses on reacting CO_2 with alkaline materials to create *inorganic* value-added products. CO_2 will react with these materials without added energy—a major benefit to these approaches. Furthermore, the products of mineralization can be used in building materials like cement, concrete, and paper/plastic fillers, which have huge potential markets and offer long-term CO_2 storage (FECM 2023a). This section addresses ways in which AI technologies can potentially support RD&D efforts to make mineralization systems more efficient.

Despite the clear benefits, mineralization approaches face numerous challenges: the process tends to occur slowly, the best mineral resources for mineralization are not fully understood, the products (e.g., building materials) tend to be of relatively low commercial value, and most mineralization efforts to date have operated on a small scale (Sandalow 2021).

FECM's Carbon Conversion Program supports key RD&D efforts to address challenges in mineralization. These efforts include lab- and bench-scale testing and validation of carbonation rates and other critical factors, demonstrating emerging mineralization technologies that complement other carbon-capture approaches, and field-testing novel mineralization systems (FECM 2022). Currently funded CO_2 mineralization initiatives through NETL's Carbon Dioxide Conversion Program aim to accelerate the speed of mineralization, increase the amount of CO_2 converted, develop and scale up novel pathways or processes, and enhance the commercial end products (NETL 2023). Further information about current projects can be found on NETL's program website.[3]

> "With strong and sustained policy support from governments around the world, carbon mineralization processes could remove 1 $GtCO_2$ from the atmosphere per year by 2035 and 10 $GtCO_2$ per year by 2050. More research is needed to test this hypothesis and define conditions under which carbon mineralization could achieve this potential."
>
> (Sandalow 2021)

Characterize Waste Products

For CO_2 conversion systems using enhanced mineralization reactions, the needed alkaline materials can come from many sources, including mining activities; concrete, cement, and fertilizer facilities; and processes incorporating coal combustion (Sandalow 2021). AI/ML-based techniques could help clarify the performance of these diverse resources to make CO_2 mineralization systems more effective at carbon mitigation.

Improve Datasets to Characterize Waste Materials

Waste products can be highly heterogenous, varying widely in physical, chemical, and biological characteristics. A range of geological surveys could characterize and map the available resources (Sandalow 2021) to overcome the challenge this variability could pose to enhanced mineralization processes. Robust datasets would support the use of AI to **identify the specific property mixes of alkaline materials that optimize conversion**. Using AI to collect better data on waste materials and their characteristics could also potentially increase the availability of suitable resources for these mineralization systems.

Building such datasets may require significant time and effort—as will learning to characterize waste products using emergent AI technologies. Depending on the waste streams and processes, reliably predicting the composition of certain waste products may prove difficult.

[3] NETL Carbon Dioxide Conversion Program: https://netl.doe.gov/carbon-management/carbon-conversion

Optimize Waste Streams for Efficient Mineralization

AI technologies could further improve the utilization of identified alkaline waste streams. Smart sensors and controls could help optimize the generation and composition of waste products for use in mineralization systems, improve collection and sorting, and monitor storage conditions in real time. Given that waste streams are frequently not homogeneous and can be part of complex supply chains, AI could potentially maximize resource usage while adjusting processes in response to the changing availability and chemical makeup of waste products.

Identify End Uses for Mineralized Products

Successful mineralization processes will identify value-added end products that can optimally leverage nationwide opportunities and also take advantage of local or regional resources. For example, facilities could be located and processes fine-tuned to exploit nearby alkaline resources as well as markets for the end products. To better assess and optimize these opportunities, AI could be used to **conduct a literature review (e.g., studies and concepts)** of key mineralization properties and potential end uses/markets from existing literature and data sources. These efforts could potentially find higher-value product opportunities for mineralization systems or identify novel mineralization pathways and opportunities for converting CO_2 into value-added materials. AI-based research efforts incorporating a literature review and key regional parameters could help focus initial design efforts and **identify the best potential product options to explore** for a given site location.

As an example, mineralization systems currently tend to offer calcium-based end products. This is unsurprising given that calcium oxide bonds more readily to CO_2 than magnesium oxide, and industrial waste products are more likely to contain high amounts of calcium than magnesium. However, significant amounts of magnesium-based alkaline materials are available from natural minerals and brines, and these might become more widely utilized as technologies advance (Woodall 2019).

Analyses of products and their applications should consider the longevity of CO_2 storage (avoiding those that would readily release the CO_2 back into the atmosphere). Figure 9 identifies some of the most common industrial uses of calcium- and magnesium-based carbonate materials, such as fertilizers, refractory metals, pharmaceuticals, and building materials. Of these, the construction industry currently offers the largest and most promising long-term CO_2 storage solutions (Woodall 2019). To reliably determine how long converted carbon remains sequestered by mineralization, smart sensors could monitor and compare the degradation of concrete and other end products.

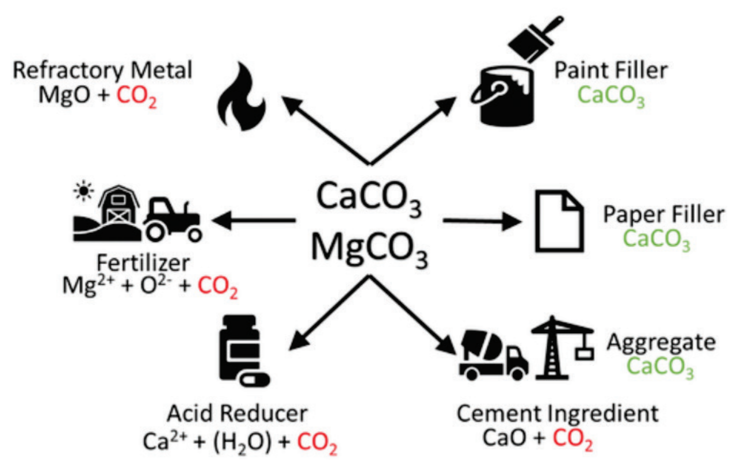

Figure 9: Typical Uses of Calcium and Magnesium Carbonates
(© Woodall 2019, Creative Commons Attribution 4.0 International)

Integrate/Optimize Carbon Capture with Mineral Carbonation

AI/ML-based analysis can further support the integration of mineralization techniques with other carbon capture and carbon removal methodologies. Specifically, AI-enhanced tools and smart controls could help optimize the integration and operation of these complex systems over time. In cement and concrete production, for instance, mineralization techniques could be used in combination with point-source carbon capture and other mitigation measures to further reduce the emissions of these processes (Sandalow 2021).

Optimize Processing for Waste Streams in Real Time

> "AI algorithms can be used to analyze and identify different types of materials in waste streams, enabling automated sorting and separation." (BIS Research 2023)

AI can expedite the processing of various waste streams in real time, smartly managing the available alkaline materials while optimizing the operating parameters of the mineralization process. These smart processing systems might combine AI with a multi-physics simulation model to determine ideal operating conditions based on the characteristics of the incoming waste streams (which may be under partial control) and the desired properties of the end products. Smart controls could provide real-time feedback (and apply analyses of historical data on material properties/product quality) to optimize system operations for current resources. In a parallel concept, AI is already applied to advanced recycling processes to efficiently handle complex waste streams, elevate sorting capabilities, reduce contamination, and optimize diverse supply chains (BIS Research 2023).

Cross-Cutting Issues

Beyond the challenges and opportunities for applying AI specifically to catalytic conversion, biological uptake, and mineralization (discussed above), AI/ML-based methodologies hold the potential to improve CO_2 conversion systems more broadly. This section highlights some of these cross-cutting areas, including optimizing conversion locations, developing lifecycle and techno-economic analyses to validate system benefits, optimizing designs to maximize affordable CO_2 uptake, and integrating CO_2 utilization into advanced manufacturing.

Optimize Locations Based on Geospatial Data

Successful CO_2 conversion systems must be properly matched with the resources available in a given region. This synchronization is commonly referred to as the "tri-location challenge," allowing access to reliable CO_2 sources, inexpensive renewable electricity, and favorable commercial markets for the end products (FECM 2022). Two key applications of AI technologies to establish effective CO_2 conversion operations are to (1) set up proper location-based criteria for site selection and (2) conduct smart monitoring of critical infrastructure to ensure successful long-term operation.

Set Criteria for Siting/Structuring Future Projects

Regardless of the specific type(s) of carbon conversion system being considered, AI could assist in identifying the best locations for potential projects and in fine-tuning system operations to leverage resources in a particular region. Key considerations may include proximity to metropolitan areas with viable markets or ready access to favorable transportation networks. For example, defining maximum haul distances, based on factors like expected fuel prices or required transportation modes to markets, might help refine economic analyses. Similarly important site considerations may include long-term access to CO_2 emissions sources or pipelines and the costs and carbon intensities of available energy sources. Project planning efforts will benefit from careful data management and prioritization of critical factors.

Ultimately, being able to **specify a feasible range of critical parameters** for AI optimization can improve the efficiency and effectiveness of project identification efforts. While decision makers must remain aware of variables that could change significantly over the lifetime of a project, an informed and streamlined screening of initial options can expedite planning and avoid lengthy delays associated with the need to evaluate the vastly complex and interrelated criteria at many potential sites.

Proactively Ensure Infrastructure Integrity

Proactive maintenance can help to ensure the long-term integrity of infrastructure. AI combined with smart sensors can monitor the condition of pipelines, wellbores, and other utilities so that proactive repairs or timely maintenance activities can minimize disruption to operations. AI control systems that react appropriately to input from sensors that monitor diverse conditions (e.g., CO_2 pipeline stress) could require significant upfront training and will improve with feedback-based learning.

Assess Life Cycles and Techno-Economics

Properly quantifying project impacts will help ensure that carbon conversion efforts lead to positive outcomes. Lifecycle analysis (LCA), techno-economic analysis (TEA), and other types of studies look at the various energy and economic resources input to these systems as well as the resultant benefits, including the amount of CO_2 converted and storage duration. However, significant work is needed to accurately quantify and standardize LCA and TEA considerations in the context of CO_2 conversion systems—particularly as such analyses help guide governmental procurement and regulations to improve the overall effectiveness of these systems (FECM 2022).

Use LCA/TEA to Predict Performance Ranges of Conversion Technologies to Inform Decisions

Given the typical complexity of LCA/TEA evaluations when applied to CO_2 conversion systems, AI-based methods could help gather and summarize the primary data for analysis. More accurate and detailed data might provide better initial LCA/TEA estimates for systems in development. In practice, these efforts would likely share similarities with the aforementioned AI-assisted literature reviews.

LCAs and TEAs depend on numerous variables, suggesting that the results may best be regarded as a response surface rather a single value to inform decisions. Some of these variables (e.g., catalyst durability) are directly related to a specific conversion process, while others (e.g., future fuel costs or the financial competitiveness of other carbon management methods) are generally independent of the process under consideration. AI-enhanced approaches may help to both conduct these complex analyses and optimize project designs based on the defined priorities. These studies would likely need to account for hard-to-predict factors like future carbon-management technologies and the mix of electricity generation (fossil/renewable) sources.

Optimize Process Design for CDR and Cost

Regardless of system type, AI methods could be used to simultaneously optimize the carbon uptake and cost-effectiveness of conversion processes. This approach fundamentally differs from optimizing project designs based on cost alone and may involve tuning operations to maximize CO_2 abatement while producing end products at a price point that markets will accept. This AI-based design optimization could be ongoing—responding to real-time prices, resources, and other variables.

Monitor Long-Term Durability of Carbon Removal

A critical measure of any CO_2 conversion system is how long the resulting materials provide effective carbon removal, which is tied to product use profiles and durability. Concrete and synthetic aggregates tend to afford particularly long-term storage opportunities for CO_2, and AI-based smart sensors could help measure and monitor the durability of these and other end products to better quantify CDR benefits. Long-term monitoring could further improve how these materials are produced in the first place and how they are combined with other materials to maximize the carbon management benefits.

Apply CO_2 in Advanced Manufacturing

Novel manufacturing techniques could be developed to incorporate captured CO_2 into advanced materials that offer superior properties. Ideally, large markets would place a high value on such materials, which, in the case of stronger and lighter structural materials, might further reduce CO_2 emissions during the use of these materials (Mission Innovation 2017). AI tools might assist in converting CO_2 for use in additive manufacturing (i.e., 3D industrial printing) or 3D design to improve performance.

Explore CO_2 Use in Advanced Materials and Alloys

Carbon-based composite materials like nanotubes and nanofibers are currently targeted as potential end products of CO_2 conversion systems. These products offer relatively high commercial value but can be difficult to manufacture in large quantities (Kim 2020). Computation-based optimization of 3D designs have proven highly successful over the years. An early example would be the CFD-based simulations that Oak Ridge National Laboratory used to improve designs for distillation columns (Eldridge 2005). AI tools could take design innovation to a new level.

> "Crosscut activities will enable new and improved materials, processes, and systems across supply chains and product lifecycles. Advanced Manufacturing is critical for a transformation of the national and global energy systems to meet our climate goals, and create a competitive, resilient, agile manufacturing sector."
>
> (DOE n.d.)

Current AI-driven technologies can streamline design by requiring fewer experiments and might more effectively incorporate CO_2 into complex composite materials like nanotubes. CO_2 could further be incorporated in additive manufacturing technologies and alloys, helping to identify opportunities using non-traditional shapes or optimizing the amount of CO_2 that can be incorporated into a design to achieve certain performance criteria.

AI tools can ultimately help to effectively **integrate CO_2 to optimize materials performance (e.g., nanotubes, nanomaterials, and packing in distillation columns)** while improving the range and value of potential end products. AI-based solutions might also help conversion systems adapt to changing conditions and available materials to ensure material quality. As with preceding discussions involving CFD and other physics-based simulations, real-world testing and verification will be necessary to properly verify promising results.

Sources

BIS Research 2023. BIS Research. 2023. "Implementing AI in Advanced Recycling: A Solution for Turning Trash into Treasure." LinkedIn. www.linkedin.com/pulse/implementing-ai-advanced-recycling-solution-turning-trash. Accessed January 16, 2024.

Bolgar 2024. Bolgar, Catherine. 2024. "Discoveries in weeks, not years: How AI and high-performance computing are speeding up scientific discovery." Microsoft. https://news.microsoft.com/source/features/sustainability/how-ai-and-hpc-are-speeding-up-scientific-discovery/. Accessed January 26, 2024.

Buvailo 2023. Buvailo, Andrii. 2023. "From Gene Editing to Pathway Design: How AI is Transforming Synthetic Biology." TeselaGen Biotechnology. https://teselagen.com/in-the-news/ai-is-transforming-synthetic-biology/. Accessed January 8, 2024.

Chang 2022. Chang, Fangfang, Meiling Xiao, Ruifang Miao, Yongpeng Liu, Mengyn Ren, Zhichao Jia, Dandan Han, Yang Yuan, et al. 2022. "Copper-Based Catalysts for Electrochemical Carbon Dioxide Reduction to Multicarbon Products." *Electrochemical Energy Reviews* 5(3). http://dx.doi.org/10.1007/s41918-022-00139-5.

Chanquia 2021. Chanquia, Santiago N., Guillem Vernet, and Selin Kara. 2021. "Photobioreactors for cultivation and synthesis: Specifications, challenges, and perspectives." *Engineering in Life Sciences (Special Issue: Emerging Biotechnologies Viewed by Emerging Bioengineers – Volume 2)* Vol. 22, Issue 12 (December 2022), 712–724. https://doi.org/10.1002/elsc.202100070.

Chen 2023a. Chen, Honghao, Yingzhe Zheng, Jiali Li, Lanyu Li, and Xiaonan Wang. 2023. "AI for Nanomaterials Development in Clean Energy and Carbon Capture, Utilization and Storage (CCUS)." *ACS Nano* 2023, 17, 11, 9763–9792. https://doi.org/10.1021/acsnano.3c01062.

Chen 2023b. Chen, Lin, Zhonghao Chen, Yubing Zhang, Yunfei Liu, Ahmed I. Osman, Mohamed Farghali, Jianmin Hua, et al. 2023. "Artificial intelligence-based solutions for climate change: a review." *Environmental Chemistry Letters*, Vol. 21 (2023), 2525–2557. https://doi.org/10.1007/s10311-023-01617-y.

Cho 2019. Cho, Renee. 2019. "Capturing Carbon's Potential: These Companies Are Turning CO2 into Profits." Columbia Climate School. https://news.climate.columbia.edu/2019/05/29/co2-utilization-profits/. Accessed January 3, 2024.

Clark 2013. Clark, Jim. 2013. "1. An Introduction to Types of Catalysis." *LibreTexts Chemistry*. https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplemental_Modules_and_Websites_(Inorganic_Chemistry)/Catalysis/Examples/Examples_of_Catalysis/1._An_Introduction_to_Types_of_Catalysis. Accessed November 20, 2023.

Cordero-Lanzac 2022. Cordero-Lanzac, Tomas, Adrian Ramirez, Alberto Navajas, Lieven Gevers, Sirio Brunialti, Luis M. Gandía, Andrés T. Aguayo, S. Mani Sarathy, and Jorge Gascon. 2022. "A techno-economic and life cycle assessment for the production of green methanol from CO_2: catalyst and process bottlenecks." *Journal of Energy Chemistry*, Vol. 68 (May 2022), 255–266. https://doi.org/10.1016/j.jechem.2021.09.045.

Creative Commons n.d. (no date). "Licenses List." https://creativecommons.org/licenses/list.en. Accessed January 15, 2024.

Crocker 2017. Crocker, Mark. 2017. “CO_2 to Bioplastics: Beneficial Re-use of Carbon Emissions from Coal-Fired Power Plants Using Microalgae.” Presentation on DOE-funded project at the University of Kentucky. www.netl.doe.gov/sites/default/files/2017-11/Project-Kickoff-Meeting-29623.pdf.

DOE n.d. U.S. Department of Energy (DOE). n.d. *Department of Energy Crosscuts Overview – FY 2023 Congressional Budget Justification*. www.energy.gov/sites/default/files/2022-05/doe-fy2023-budget-volume-2-crosscutting.pdf.

Du 2020. Du, Yunze. 2020. “A Comprehensive Analysis on the Future of Algae Biofuels in China.” *IOP Conference Series: Earth and Environmental Science* 615(1), 012048. http://dx.doi.org/10.1088/1755-1315/615/1/012048.

ECO Magazine 2023. ECO Magazine. 2023. “Carbon Capture Study at the Largest Artificial Reef Pushes Past Half-Way Mark, Early Data is Promising.” Environmental Coastal & Offshore (ECO). www.ecomagazine.com/news/coastal/carbon-capture-study-at-the-largest-artificial-reef-pushes-past-half-way-mark-early-data-is-promising. Accessed January 16, 2024.

Eldridge 2005. Eldridge, R. Bruce, Valmor de Almeida, Tyler Thompson, Pat Au-Yeung, Christian Green, Mike Lockett, Mark Pilling, Ahmad Haidari, et al. 2005. “Final Report - Advanced Hydraulic and Mass Transfer Models for Distillation Column Optimization and Design.” *The University of Texas at Austin and Oak Ridge National Laboratory*. https://digital.library.unt.edu/ark:/67531/metadc885992/.

Elst 2018. Elst, Kathy, Miranda Maesen, Griet Jacobs, Leen Bastiaens, Stefan Voorspoels, and Kelly Servaes. 2018. “Supercritical CO_2 Extraction of *Nannochloropsis* sp.: A Lipidomic Study on the Influence of Pretreatment on Yield and Composition.” *Molecules* 2018, 23(8), 1854. https://doi.org/10.3390/molecules23081854.

Farooq 2022. Farooq, Wasif. 2022. “Maximizing Energy Content and CO_2 Bio-fixation Efficiency of an Indigenous Isolated Microalga *Parachlorella kessleri* HY-6 Through Nutrient Optimization and Water Recycling During Cultivation.” *Frontiers in Bioengineering and Biotechnology* Vol. 9 (February 10, 2022). https://doi.org/10.3389/fbioe.2021.804608.

FECM 2022. U.S. Department of Energy Office of Fossil Energy and Carbon Management. 2022. *Strategic Vision: The Role of Fossil Energy and Carbon Management in Achieving Net-Zero Greenhouse Gas Emissions.* www.energy.gov/sites/default/files/2022-04/2022-Strategic-Vision-The-Role-of-Fossil-Energy-and-Carbon-Management-in-Achieving-Net-Zero-Greenhouse-Gas-Emissions_Updated-4.28.22.pdf.

FECM 2023a. U.S. Department of Energy Office of Fossil Energy and Carbon Management. 2023. “Carbon Conversion: Office of Fossil Energy and Carbon Management.” www.energy.gov/fecm/carbon-conversion. Accessed November 28, 2023.

FECM 2023b. U.S. Department of Energy Office of Fossil Energy and Carbon Management. 2023. “Solicitations and Business Opportunities.” www.energy.gov/fecm/solicitations-and-business-opportunities. Accessed November 29, 2023.

FECM n.d. U.S. Department of Energy Office of Fossil Energy and Carbon Management. n.d. “Catalytic Conversion Pathway.” www.energy.gov/fecm/catalytic-conversion-pathway. Accessed December 15, 2023.

Figueroa-Torres 2021. Figueroa-Torres, Gonzalo M., Jon K. Pittman, and Constantinos Theodoropoulos. 2021. “Optimisation of microalgal cultivation via nutrient-enhanced strategies: the biorefinery paradigm.” *Biotechnology for Biofuels* 14, 64 (2021). https://doi.org/10.1186/s13068-021-01912-2.

Fu 2019. Fu, Jingwei, Yun Huang, Qiang Liao, Ao Xia, Qian Fu, and Xun Zhu. 2019. “Photo-bioreactor design for microalgae: A review from the aspect of CO_2 transfer and conversion.” *Bioresource Technology* Vol. 292, 121947. https://doi.org/10.1016/j.biortech.2019.121947.

Ganesh 2016. Ganesh, Ibram. 2016. “Electrochemical conversion of carbon dioxide into renewable fuel chemicals – The role of nanomaterials and the commercialization.” *Renewable and Sustainable Energy Reviews*, Vol. 59 (June 2016), 1269–1297. https://doi.org/10.1016/j.rser.2016.01.026.

Hu 2012. Hu, Howard H. 2012. “Chapter 10 – Computational Fluid Dynamics.” In *Fluid Mechanics (Fifth Edition)*, edited by Pijush K. Kundu, Ira M. Cohen, and David R. Dowling, 421–472. Academic Press. https://doi.org/10.1016/B978-0-12-382100-3.10010-1.

IEA 2019. International Energy Agency (IEA). 2019. “Putting CO2 to Use: Creating value from emissions.” Paris: IEA. www.iea.org/reports/putting-co2-to-use. Accessed January 3, 2024.

Jayaraman 2015. Jayaraman, Suresh K., and R. Russell Rhinehart. 2015. “Modeling and Optimization of Algae Growth.” *Industrial & Engineering Chemistry Research* 54(33), 8063–8071. https://doi.org/10.1021/acs.iecr.5b01635.

Kempler 2023. Kempler, Paul A., and Adam C. Nielander. 2023. “Reliable reporting of Faradaic efficiencies for electrocatalysis research.” *Nature Communications* 14, 1158 (2023). https://doi.org/10.1038/s41467-023-36880-8.

Kim 2020. Kim, Gi Mihn, Won-Gwang Lim, Dohyung Kang, Jae Hyun Park, Hyunjoo Lee, Jinwoo Lee, and Jae W. Lee. 2020. “Transformation of carbon dioxide into carbon nanotubes for enhanced ion transport and energy storage.” *Nanoscale* 12, 7822–7833. https://doi.org/10.1039/C9NR10552B.

Kurth 2005. Kurth, S., M.A.L. Marques, and E.K.U. Gross. 2005. “Density-Functional Theory.” In *Encyclopedia of Condensed Matter Physics*, edited by Franco Bassani, Gerald L. Liedl, and Peter Wyder, 395–402. Elsevier. https://doi.org/10.1016/B0-12-369401-9/00445-9.

Li 2019. Li, Hao, Dan Yan, Zhien Zhang, and Eric Lichtfouse. 2019. “Prediction of CO_2 absorption by physical solvents using a chemoinformatics-based machine learning model.” *Environmental Chemistry Letters* 17(3), 1397–1404. https://doi.org/10.1007/s10311-019-00874-0.

Mission Innovation 2017. Mission Innovation. 2017. *Accelerating Breakthrough Innovation in Carbon Capture, Utilization, and Storage: Report of the Mission Innovation Carbon Capture, Utilization, and Storage Experts’ Workshop*. U.S. Department of Energy and Kingdom of Saudi Arabia’s Ministry of Energy, Industry & Mineral Resources, 3-46. https://mission-innovation.net/wp-content/uploads/2018/09/Accelerating-Breakthrough-Innovation-in-Carbon-Capture-Utilization-and-Storage-_0.pdf.

Nature 2022. Nature.com. “Achieving net zero emissions with machine learning: the challenge ahead.” *Nature Machine Intelligence* 4, 661–662 (2022). https://doi.org/10.1038/s42256-022-00529-w. Accessed January 2, 2024.

NETL 2023. U.S. Department of Energy National Energy Technology Laboratory. 2023. "Carbon Dioxide Conversion Program." https://netl.doe.gov/carbon-management/carbon-conversion. Accessed November 28, 2023.

NOAA Research 2023. NOAA Research. 2023. "New system uses seawater to capture and store CO_2." https://research.noaa.gov/2023/09/08/new-system-uses-seawater-to-capture-and-store-co2/. Accessed January 16, 2023.

Nwabara 2020. Nwabara, Uzoma O., Emiliana R. Cofell, Sumit Verma, Emanuela Negro, and Paul J. A. Kenis. 2020. "Durable Cathodes and Electrolyzers for the Efficient Aqueous Electrochemical Reduction of CO_2." *ChemSusChem* 2020, Vol. 13, 855–875. https://kenis-group.chbe.illinois.edu/Publications/2020/nwabara_2020_durability.pdf.

Open Catalyst Project 2023. Open Catalyst Project. 2023. "Open Catalyst Project." Meta AI and Carnegie Mellon University. https://opencatalystproject.org/. Accessed December 21, 2023.

Overa 2022. Overa, Sean, Byung Hee Ko, Yaran Zhao, and Feng Jiao. 2022. "Electrochemical Approaches for CO_2 Conversion to Chemicals: A Journey toward Practical Applications." *Accounts of Chemical Research* 55(5), 638–648. https://doi.org/10.1021/acs.accounts.1c00674.

Patel 2021. Patel, Anil Kumar, Reeta Rani Singhania, Chiu-Wen Chen, Yi-Sheng Tseng, Chia-Hung Kuo, Chien-Hui Wu, and Cheng Di Dong. 2021. "Advances in micro- and nano bubbles technology for application in biochemical processes." *Environmental Technology & Innovation* Vol. 23 (August 2021), 101729. https://doi.org/10.1016/j.eti.2021.101729.

Penn State n.d. Penn State College of Earth and Mineral Sciences. n.d. "EGEE 439: Alternative Fuels from Biomass Sources – 9.4 Design of Algae Farms." www.e-education.psu.edu/egee439/node/695. Accessed January 9, 2024.

Rafa 2021. Rafa, Nazifa, Shams Forruque Ahmed, Irfan Anjum Badruddin, M. Mofijur, and Sarfaraz Kamangar. 2021. "Strategies to Produce Cost-Effective Third-Generation Biofuel From Microalgae." *Frontiers in Energy Research* Vol. 9 (September 7, 2021). https://doi.org/10.3389/fenrg.2021.749968.

Saldívar-González 2020. Saldívar-González, Fernanda I., José L. Medina-Franco. 2020. "Chapter 3 - Chemoinformatics approaches to assess chemical diversity and complexity of small molecules." In *Small Molecule Drug Discovery: Methods, Molecules and Applications*, edited by Andrea Trabocchi and Elena Lenci, 83–102. Elsevier. https://doi.org/10.1016/B978-0-12-818349-6.00003-0.

Sandalow 2021. Sandalow, D., R. Aines, J. Friedmann, P. Kelemen, C. McCormick, I. Power, B. Schmidt, and S. Wilson. 2021. *Carbon Mineralization Roadmap Draft October 2021*. Lawrence Livermore National Laboratory. www.osti.gov/biblio/1829577.

Sexton 2020. Sexton, Chrissy. "AI used to find new catalyst for CO2 conversion." Earth.com. www.earth.com/news/machine-learning-pinpointed-a-catalyst-for-co2-conversion/. Accessed January 3, 2024.

Sun 2023. Sun, Zhongliang, Hui Chen, Liqin Sun, and Qiang Wang. 2023. "Converting carbon dioxide to high value-added products: Microalgae-based green biomanufacturing." *GCB Bioenergy* 15(4), 386–398. https://doi.org/10.1111/gcbb.13031.

Thawechai 2016. Thawechai T., Cheirsilp B, Louhasakul Y, Boonsawang P, Prasertsan P. (2014). Mitigation of Carbon Dioxide by Oleaginous Microalgae for Lipids and Pigments Production: Effect of Light Illumination and Carbon Dioxide Feeding Strategies. Bioresour. Technol. 2016 Nov; 219:139-149. doi: 10.1016/j.biortech.2016.07.109. Epub 2016 Jul 27. PMID: 27484670. [PubMed]

Vermaas 2021. Vermaas, Wim. 2021. "Multi-pronged approach to improving carbon utilization by cyanobacterial cultures." Presentation at the DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review, March 23, 2021. www.energy.gov/sites/default/files/2021-04/beto-35-peer-review-2021-algae-vermaas.pdf.

Weber 2023. Weber, Justin, Jarrett Riley, Steven Rowan, and Ronald Breault. 2023. "The Development of an NETL DAC Reactor: Optimization of Direct Air Capture (DAC) Reactor Configuration Using Artificial Intelligence (AI) Inverse Engineering Techniques." Presentation at the 2023 FECM / NETL Carbon Management Research Project Review Meeting - Carbon Dioxide Removal, August 29, 2023. https://netl.doe.gov/sites/default/files/netl-file/23CM_CDR29_Weber.pdf.

Whang 2019. Whang, Ho Seok, Jinkyu Lim, Min Suk Choi, Jonghyeok Lee, and Hyunjoo Lee. "Heterogeneous catalysts for catalytic CO_2 conversion into value-added chemicals." *BMC Chemical Engineering* 1, article no. 9 (2019). CC 4.0. https://bmcchemeng.biomedcentral.com/articles/10.1186/s42480-019-0007-7

Woodall 2019. Woodall, Caleb M., Noah McQueen, Hélène Pilorgé, and Jennifer Wilcox. 2019. "Utilization of mineral carbonation products: current state and potential." *Greenhouse Gases: Science and Technology* 9(6): 1096–1113. https://doi.org/10.1002/ghg.1940.

Zhang 2022. Zhang, Zhen, Yun Zheng, Lanting Qian, Dan Luo, Haozhen Dou, Guobin Wen, Aiping Yu, and Zhongwei Chen. 2022. "Emerging Trends in Sustainable CO_2-Management Materials." *Advanced Materials* 34, Issue 29, 2201547. https://doi.org/10.1002/adma.202201547.

Zheng 2018. Zheng, Qi, Xiaoyin Xu, Gregory J.O. Martin, and Sandra E. Kentish. 2018. "Critical review of strategies for CO_2 delivery to large-scale microalgae cultures." *Chinese Journal of Chemical Engineering* Vol. 26, Issue 11 (November 2018), 2219–2228. https://doi.org/10.1016/j.cjche.2018.07.013.