Point-Source Carbon Capture:

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 data sets 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 Point-Source Carbon Capture. 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.

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Potential Roles for AI in Point Source Carbon Capture

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 to capture carbon dioxide (CO_2) directly from large point sources in the power and industrial sectors. Once captured, this CO_2 is to be compressed, transported, and injected deep below ground for permanent geologic storage *or* incorporated into long-lived products.

Capture technologies on relatively high-purity industrial streams have supplied the food and beverage industry with CO_2 for nearly 100 years (Parker 2021). Technical advancements over recent decades now enable point source carbon capture (PSC) from more dilute CO_2 streams (see inset on CO_2 Concentrations)—producing CO_2 streams that are at least 90% pure by volume. PSC technology is still not in wide use today, mainly because of its high operating cost, water requirements, and capital equipment costs—as well as the challenges involved in separating low concentrations of CO_2 from other flue gas components that can adversely impact process efficiency, separation materials, capture systems, and materials of construction (De 2022).

PSC Vision Statement

Demonstrate first-of-a-kind carbon capture on power and industrial sectors coupled to dedicated and reliable carbon storage, that will lead to commercially viable nth-of-a-kind opportunities for widescale deployment and facilitate a carbon-free economy by 2050.

FECM Strategic Vision 2022

CO_2 Concentrations

Ambient air	~0.04% CO_2
Coal power plant	12-15% CO_2
NG power plant	3-5% CO_2
Industrial (process and combustion)	20->99% CO_2

The International Energy Administration (IEA) estimates that about 40 large-scale commercial facilities around the globe now apply carbon capture, utilization, and storage (CCUS) technologies to industrial processes, fuel transformation, and power generation to capture more than 45 million metric tons of CO_2 (45 $MtCO_2$) annually. Seven new, large-scale capture facilities have come online since 2022, and more than 50 more are projected to be completed by 2030. By that time, CCUS facilities are collectively expected to capture about 383 $MtCO_2$ per year. This growth reflects progress, but the pace is not on track to meet the 2050 goal of net-zero emissions (see large gap denoted by yellow bar in Figure 1). The United States has about 80 projects scheduled to become operational by 2030, which would increase national CO_2 capture capacity from over 20 $MtCO_2$ to more than 100 Mt CO_2 per year (IEA 2022). Cost-effective PSC is needed in the near and mid-term as demand for fossil-based power

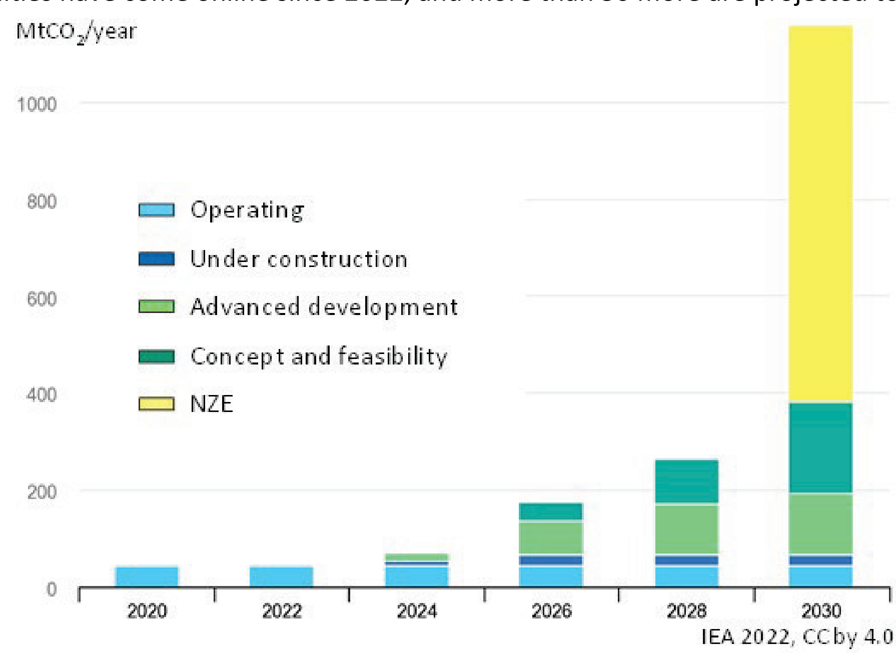

Figure 1. Current and planned global capacity of large-scale CO_2 capture projects, 2020-2030, is not on track to meet the Net Zero Scenario. (IEA, 2022, CC by 4.0)

will decline when reliable, long-term energy storage becomes available (Larson 2020), with the potential exception of hard-to-decarbonize industries (e.g., steel, cement).

FECM and its partners fund projects in research, development, demonstration, and deployment (RDD&D) to reduce the cost, increase the efficacy, and advance the deployment of commercial-scale PSC technologies in the power and industrial sectors (DOE/FECM 2022). The RDD&D will be closely coordinated with efforts to greatly expand U.S. carbon transport and storage capacity and to efficiently convert CO_2 into useful products that securely and durably contain the CO_2. The ramping up of CO_2 capture should parallel (not exceed) the pace of regional growth in long-term transport and storage capacity and in conversion facilities and markets. This coordination should enhance the economic feasibility and uptake of various PSC approaches (see Figure 2 and inset) and clarify the CO_2 purity levels required by emerging transport, storage, and conversion equipment and processes.

Given the need for rapid progress, the RDD&D follows a "learning by doing" approach—by which early investments in technology deployment should lead to cost reductions and encourage the deployment of lower-cost, nth-of-a-kind projects at scale. FECM's PSC RDD&D objectives include the following:

- Reduce capture costs for dilute (<20%) CO_2 sources.
- Transcend reliance on economies of scale by exploring R&D opportunities (e.g., modularization, process intensification, and advanced manufacturing).

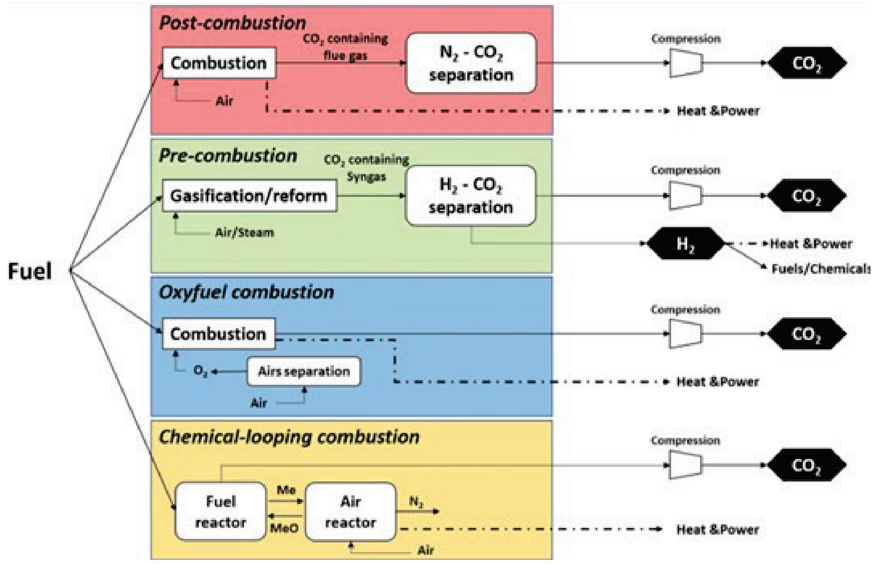

Figure 2. Approaches to point source carbon capture
Source: Raganati 2021, Energy Fuels 2021, 35,16, 12845-12868

Main Approaches to PSC

CO_2 generated by the power and industrial sectors is often mixed with nitrogen, water, and other gases. The CO_2 must be captured and purified prior to use or storage. Key approaches include:

Pre-combustion processes convert fuel into a gaseous mixture of hydrogen (H_2) and CO_2. The H_2 is separated and can be burned without producing any CO_2; the CO_2 can be compressed for transport and storage.

Post-combustion (or post-processing) processes separate CO_2 from exhaust gases. CO_2 can be captured using a liquid solvent or other separation methods. In an absorption-based approach, the CO_2 is absorbed by the solvent, then released by heating to form a high-purity CO_2 stream. This technology is the most mature and can be added to existing plants.

Oxy-fuel combustion processes use pure oxygen for combustion of fuel to produce an exhaust gas that is mainly water vapor and CO_2, which can be easily separated to produce a high-purity CO_2. The process avoids smog-forming nitrogen in the flue gas, but the pure oxygen adds to costs.

Inherent capture processes incorporate the capture of CO_2 into the inherent design of the process, never allowing produced CO_2 to be contaminated with other gases, keeping it in a high purity state (e.g., Allam cycle). *Global CCS 2022*

- Prepare flexible, commercial-scale technologies that can adjust to the evolving U.S. power grid.
- Demonstrate first-of-a-kind technologies.
- Conduct rigorous carbon accounting and environmental impacts analyses—and identify benefits.
- Coordinate and integrate with carbon transport, storage, conversion, and carbon dioxide reduction (CDR) technologies.[1]
- Ensure robust community engagement, particularly in communities previously harmed by fossil fuel projects.

In pursuing these objectives, the FECM PSC Program and its research partners will build upon a range of new and ongoing engineering-scale testing and front-end engineering design (FEED) studies of PSC technologies that can economically capture at least 95% of the CO_2 from natural gas-fired combined-cycle (NGCC) flue gases with high (95%) CO_2 purity (DOE/FECM 2021), as needed. These FEED studies use existing knowledge and equipment to guide development of engineering plans and cost estimates for major investment decisions.

"[Carbon capture, utilization, and storage (CCUS)] is a practical way to meet climate goals with available, tested technology that can maintain grid reliability. The Intergovernmental Panel on Climate Change points to carbon capture as an important tool to cut emissions in the near term, and the U.S. Inflation Reduction Act boosted financial incentives for CCUS…There is no need to wait for a perfect power generation technology before putting our best, current technology to use for today's needs."

Bowie and Oumansour 2023

Recent legislation has heightened interest in PSC at power plants. The Inflation Reduction Act, in particular, has stimulated an increased number of U.S. power plant applications for carbon capture—primarily at NGCC plants (Duffy and Thompson 2023). In addition, the Bipartisan Infrastructure Law[2] directs DOE to fund new studies of carbon capture and storage (CCS) demonstration projects (Duffy and Thompson 2023). In February 2023, DOE announced $2.5 billion in funding for the Carbon Capture Large-Scale Pilots and Carbon Capture Demonstration Projects Program—to significantly reduce CO_2 emissions from electricity generation and hard-to-abate industrial operations. In May 2023, DOE announced an additional $45 million in funding for technology development to lay the foundation for an integrated U.S. carbon capture, transport, and storage industry (NETL 2023d).

Artificial intelligence (AI) has the potential to assess massive data sets, discover new patterns, build predictive models, design improved materials, boost process efficiency, integrate systems, and more—to accelerate commercially deployable PSC solutions for diverse CO_2 emissions sources. As summarized in Figure 3, FECM has identified possible roles for AI in improving PSC technologies for use at power plants (i.e., natural gas combined cycle) or industrial facilities and in preparing CO_2 streams for transport and storage.

DOE is investing $38 million in 22 projects (awarded under the "Carbon Management" funding opportunity) to develop technologies that capture CO_2 from utility and industrial sources or directly from the atmosphere and transport it either for geologic storage or for conversion into valuable products.

Carbon Capture Newsletter, March 2023, NETL

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[1] Separate FECM programs administer RDD&D portfolios on Carbon Transport & Storage, Conversion, and CDR.

[2] Section 41004(b)

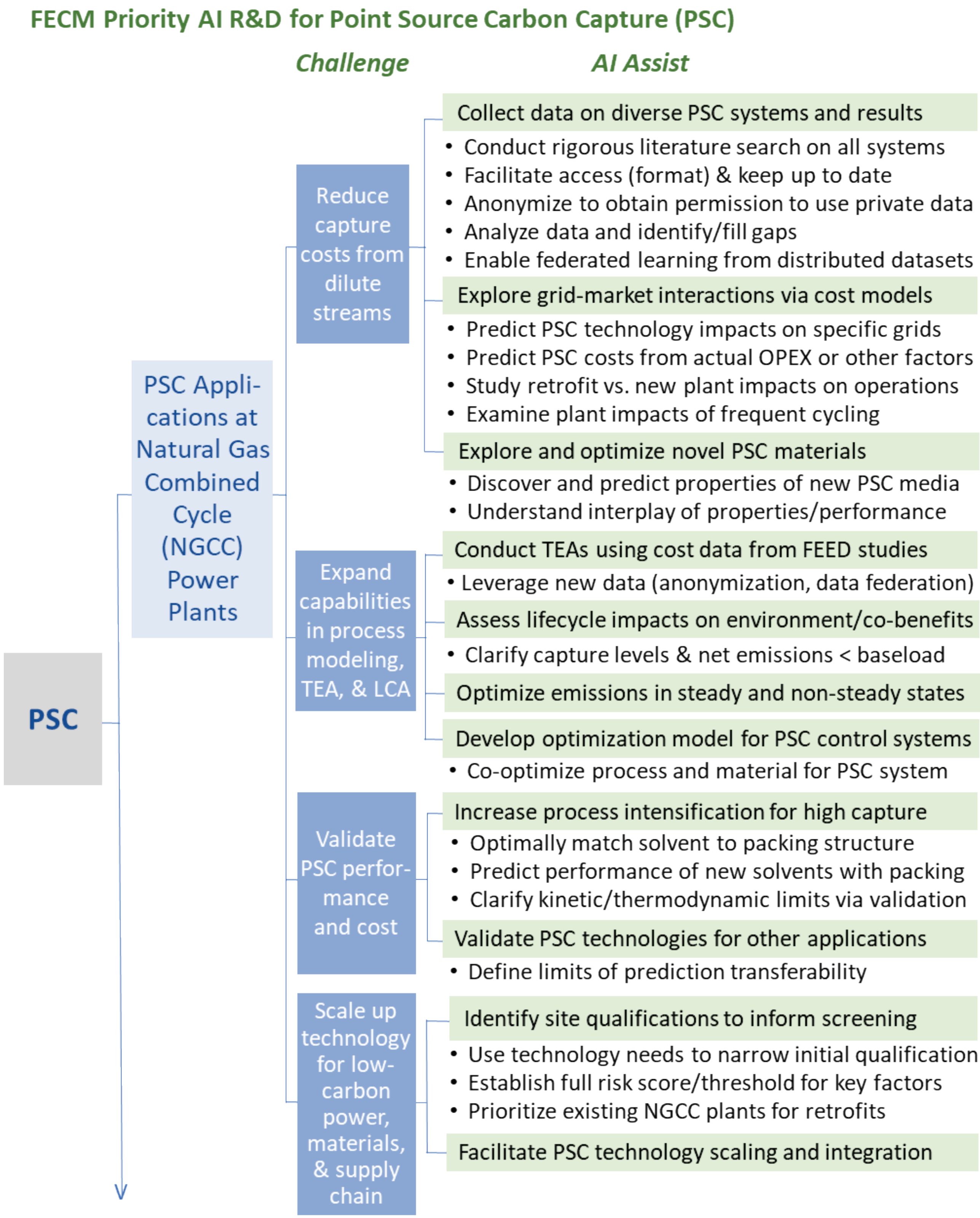

Figure 3. Summary of potential AI roles in PSC (Chart reflects document structure)

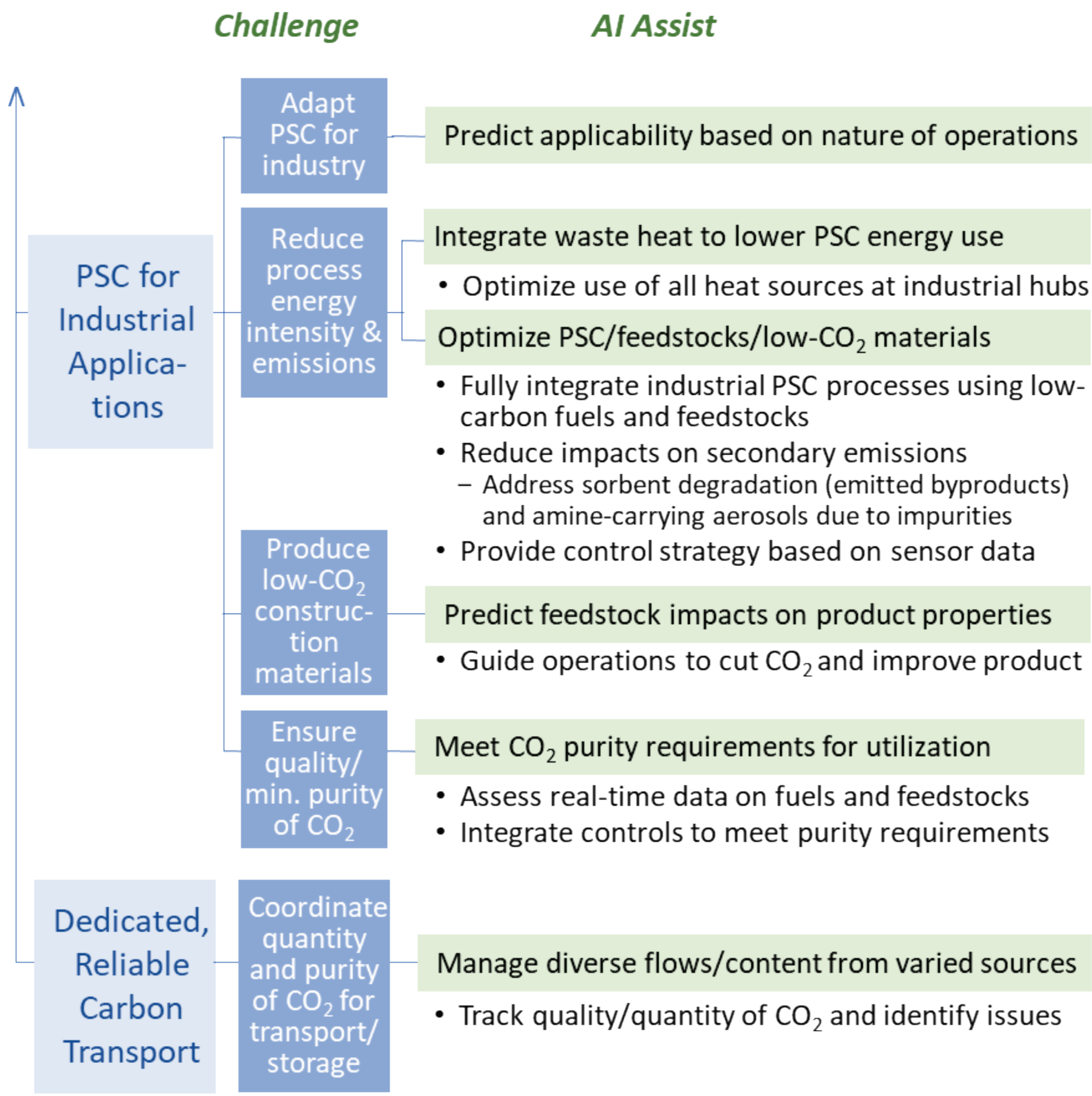

Figure 3. Summary of potential AI roles in PSC (continued) (Chart reflects document structure)

PSC Applications at NGCC Power Plants

In the power sector, FECM focuses its PSC RDD&D on natural gas-fired generators, especially those that operate in a combined-cycle configuration. NGCC power plants are now the single largest source of electricity generation and electric-generating capacity in the United States (EIA 2022). These plants are cleaner and more efficient than coal-fired plants, and existing PSC technologies are generally able to capture at least 90% of the CO_2 emissions from an NGCC plant's flue gas or syngas stream. The goal is to widely deploy systems to capture at least 95% of the CO_2 and adjust CO_2 purity to meet the criteria for storage, transport, or conversion.

Efforts to improve the efficiency, flexibility, and economics of PSC technologies at NGCC plants face complex challenges. A key hurdle is to cost effectively separate the relatively dilute CO_2 (~4%) from other flue gas constituents, many of which are detrimental to separation materials, capture systems, materials of construction, and process and plant efficiency (NETL 2023a). Further challenges include control of byproduct emissions, energy-efficient sorbent regeneration, and more. FECM/PSC RDD&D directions include the following:

- Scale up PSC technologies at natural gas power plants integrated with long-duration carbon storage or CO_2 conversion, CDR (i.e., biomass carbon removal and storage), and energy storage.
- Develop PSC technologies that leverage low-carbon supply chains and produce low-carbon materials (e.g., cement, steel) coupled with advanced gas-fired power plants using lower-carbon fuels (e.g., hydrogen).
- Expand dynamic process modeling capabilities (CCS Knowledge, 2018), techno-economic assessment (TEA) and lifecycle analysis (LCA). (DOE/FECM 2022)

Reduce Capture Costs from Dilute Streams

To encourage wider use of advanced carbon capture technologies, the DOE PSC Program supports research to improve system performance and reduce costs (NETL 2023a). System costs tend to be lower for more concentrated CO_2 source streams and rise rapidly with CO_2 output streams above 95%.

CO_2 purity and pressurization requirements are largely determined by the planned CO_2 transport mode, storage option, and/or conversion technology, and these choices, in turn, depend on proximity to appropriate facilities and infrastructure. Many power plants today face high capture costs and limited affordable storage options, but costs can be reduced by developing advanced technologies, demonstrating and deploying carbon capture and transport hubs,[3] or generating offsetting revenues by converting the CO_2 into value-added products (McKinsey 2023). These variables complicate long-term predictions of capital and operating costs for capture systems, and the challenge is compounded by coming shifts in power plant operations as more renewable energy sources are added to the grid. Some first steps to lower the cost of carbon capture technology at NGCC plants[4] are to gather all available data and build more robust and flexible cost models.

Collect data on diverse PSC systems

AI requires massive amounts of data to learn and improve decision-making processes. A range of PSC technologies have been developed, demonstrated, and adopted at various fossil fuel-based power plants around the globe (primarily post-combustion technology), generating a trove of potentially useful data. DOE/FECM has already assembled a variety of data resources for PSC technologies (see inset), but additional data would likely enrich AI analyses and help improve model accuracy.

DOE Resources for PSC

The National Carbon Capture Center (NCCC) in Alabama, managed by Southern Company, provides a unique test bed to bridge the gap between laboratory research and large-scale demonstrations of cost-effective, technically viable carbon management technologies.

Point Source Carbon Capture Project Map: This interactive map provides information on active and completed projects managed under NETL's PSC and CDR Programs.

Carbon Capture Technology Compendium provides a summary of CO_2 capture technology R&D sponsored by Point Source Carbon Capture (PSCC) and Carbon Dioxide Removal (CDR) Programs at DOE/NETL.

Carbon Capture and Storage Database maintained by NETL provides interactive access to information on more than 75 carbon capture projects.

[3] Preliminary engineering design studies will consider how hubs will connect multiple CO_2transport modes to enable cost-efficient, long-term transportation options for all types of CO_2 sources (NETL 2023c).

[4] This configuration enables energy-efficient heat recovery while flue gas is cooled before entering the CO_2 capture system.

AI could help **conduct rigorous literature searches** to obtain as much information and data as possible about the full range of known PSC systems, including performance and costs.[5] AI tools offer intelligent search capabilities and can extract structured or unstructured data from approved online datasets. AI-powered automatic refresh can **continually update valuable data from online sources**. For off-line formats, natural language processing (NLP), optical character recognition (OCR), and other AI-based tools can collect or digitize records, then classify and sort them as needed. To convince private-sector organizations and test centers that their data can be shared safely, AI tools can **reliably "anonymize" proprietary datasets** and prevent data from being traced to its source. Alternatively, AI could **use a federated learning approach**, whereby an algorithm can be trained on raw data stored on a variety of distributed edge computing devices during multiple independent sessions. This approach can support development of machine learning (ML) models using a diverse range of heterogeneous data while providing data privacy and security (only aggregated data can be decrypted). Access to data across many organizations, locations, and PSC technologies would better position AI to **analyze data resources and identify existing gaps or predict emerging needs** to produce new insights and suggest new and more efficient technology approaches. At a minimum, AI data gathering can provide researchers with the latest news or trends in technology innovation and impacts.

Assembling useful datasets (performance, emissions, costs) from diverse carbon capture systems at NGCC plants is complicated by system variety and the interoperability of digital twins and other models. Even generating datasets from existing models could be problematic because those models are extremely complex and the data dense and fraught with uncertainty—hampering efforts to make meaningful comparisons or conclusions across systems. AI is thus valuable in identifying optimal data formats, quality objectives, and appropriate data models for diverse PSC systems.

Explore grid-market interactions using cost models.

AI has the potential to help utility planners, operators, and regulators predict the critical interactions of NGCC plants with carbon capture systems, grid operations, costs, and markets. The U.S. grid is already in the process of transitioning from its traditional, centralized, primarily single-energy-source (fossil) electricity generation model to a model that flexibly integrates a rising share of distributed, intermittent renewable energy sources—all while maintaining power quality, reliability, safety, affordability, and resilience. The sector must simultaneously adjust to a rapidly changing climate (disrupting historical power demand patterns and damaging infrastructure) and achieve zero carbon emissions by 2035, even as long-term storage solutions are still evolving. These fundamental shifts in sources and priorities signal the need for robust new planning and cost models.

Building reliable cost models to guide the grid during and after its transformation will require massive amounts of data, some of which is in limited supply today. For this reason, models may develop incrementally and improve as more and better data becomes available with the development, demonstration, and scale-up of new technologies. Power quality and reliability remain critical, and cost/benefit analyses must recognize the elevated importance of carbon capture.

To avoid adverse impacts, the power sector needs to understand how different capture technologies will affect power dispatch under diverse grid scenarios and at specific NGCC plants and grids. Tailored expansion planning models might help predict how the capacity mix for a specific grid is likely to change over time. This information

[5] In May 2023, the EPA published the technical support document *Greenhouse Gas Mitigation Measures: Carbon Capture and Storage for Combustion Turbines* (EPA 2023a), which estimates the cost of carbon capture systems at NGCC plants by extrapolating baseline data from a 2022 NETL study.

could then be combined with actual grid production costs[6] to show how various capacity mixes would dispatch in a specific market, but the equations and constraints in the model will heavily influence output. Drawing upon the full range of existing grid- and market-scale NGCC production models, AI might help **predict PSC technology cost impacts on specific grids.** The needed models may be complex and must be applied to actual plants to verify predictions.

Based on the traditional use of NGCC plants to supply base load power, past models assumed carbon capture costs could be predicted on the basis of plant capacity. Capacity may change significantly with the shift to more flexible operations (beyond steady state), and PSC costs may need to be based on other considerations, such as actual operating costs or expenditures (OPEX). With sufficient system, operating, and cost data, AI might generate new models to reliably **predict PSC costs from OPEX or other factors** under various scenarios. AI might also be used to optimize OPEX over a range of PSC designs, operating strategies, or capacity factors. Market signals can play an important role in the design process (Gooty 2023). PSC costs can also reflect external factors, such as tax incentives, regulations, fuel prices, and the mix of renewables.

ARPA-E's FLExible Carbon Capture and Storage

"FLECCS addresses a tension that will become more severe as electricity systems decarbonize: low-carbon resources such as CCS-equipped plants can reduce the cost of a net-zero carbon system, yet increasing penetration of highly variable renewable energy (VRE) sources such as wind and solar power complicate CCS design, operations, and commercialization potential.

Changing market signals are resulting in operational challenges such as increased ramping of electricity generators. Such frequent ramping has several disadvantages, including reduced capacity factor, increased operations and maintenance costs, reduced power generator efficiency, and the potential for increased CO_2 emissions during ramping even if integrated with a CCS plant. Given these trends, CCS processes and redesign should be reconsidered to ensure they can contribute to a low-cost, net-zero carbon electricity system, even if a given CCS process itself is not net-zero."

The program will use "capacity expansion models to identify optimal portfolios of grid resources given certain cost and performance characteristics, to understand whether the processes developed in FLECCS will be valuable in a future grid."

ARPA-E FLECCS website

Planners also need a better understanding of how PSC systems will affect operations when they are installed on existing NGCC plants—and how those operations and costs will differ from those of new plants that are designed for PSC systems and the modern grid. To clarify answers to these retrofit-versus-greenfield questions, researchers will need detailed operations and cost data on PSC retrofits and new plant systems (see examples in inset on next page) and on a growing array of capture media. With reliable operations and cost data from these projects, AI might **assess retrofit vs. new plant impacts on operations**, predict costs, and potentially **show how different types of PSC systems and materials respond to projected grid operating profiles**.

Explore and optimize novel PSC materials

Cost is the most commonly cited barrier to wider adoption of PSC systems. Material-based costs may be incurred at multiple points, including procuring the capital equipment, manufacturing the capture media, using energy (heat or pressure) and water (steam) to regenerate the media, and replacing media that can degrade from exposure to high temperatures and impurities in the flue gas. The choice of PSC capture material may also

[6] The cost of operations is different for every plant due to variations in taxes, debt-equity ratios, $ index year, the cost of debt, etc., and evolving grid management needs may render today's costs irrelevant for new and future systems.

adversely affect plant equipment, reduce plant efficiency, generate secondary emissions, or limit options for CO_2 transport or utilization. The strengths and weaknesses of common PSC capture media (see inset on following page) are summarized briefly in the Appendix.

AI methods may be implemented to design PSC systems that enable CO_2 separation with a minimum energy penalty and cost. These methods can be applied at the molecular level, focusing on materials discovery and property prediction, and at the process-level. AI could also play an expanded role in predicting the properties of potential capture media,[7] identifying promising novel capture media, matching media to specific system requirements, predicting material performance under projected changes in plant operations, and maximizing media flexibility to handle evolving operating scenarios.

AI and ML methods can assist in the **discovery of materials and in predicting/optimizing properties of solvents and sorbents** for CO_2 capture. Several ML models have been employed to predict thermodynamic properties such as the solubility of CO_2 in capture solvents (e.g., amine-based solvents and ionic liquids) and to maximize absorption capacity as a function of specified operating conditions such as inlet CO_2 concentration, pressure, and temperature (Chen 2015, Abooali 2019, Ghazani 2018). In addition, AI methods have been applied to predict physical properties of solvents, such as viscosity, surface tension, and thermal stability, all of which can help to optimize the performance of PSC systems.

AI approaches have also been shown to enable the design of new sorbents. Due to the ease with which sorbent molecules can be tuned, an infinite number of structures are possible. In the case of metal organic frameworks (MOFs), for example, AI tools can screen the thousands of materials structures in existing databases to identify the best candidates for CO_2 capture—considering such parameters as CO_2 uptake, ease of synthesis, stability (to moisture), and cost (Abdi 2021, Gheytanzadeh 2021, Dureckova 2019). ML methods may also help establish structure-property relationships to drive the discovery of new adsorbents with optimized functionalities.

PSC Projects at U.S. Natural Gas Plants

- **Net Power**, Odessa, TX: This plant plans to inherently capture nearly all of the plant's emissions from burning natural gas with oxygen. It is expected to go online in 2026. (Occidental, Baker Hughes, Constellation)

Start-up dates uncertain:

- **Efficient**, Edwardsport, IN: CCS to be added to a combined cycle power plant that enables flexibility of fuels including syngas gasified from coal, natural gas, or blends of the two. Expects to use Honeywell UOP's technology to capture about 3.6 million tonnes per year. (Duke Energy Indiana)
- **Lake Charles Power Station**, Westlake, LA: The proposed NGCC plant would use Mitsubishi Heavy Industries technology to capture at least 95% of CO_2 emissions of about 2.4 million tonnes/yr. (Entergy)
- **Cypress Carbon Capture**, Hahnville, LA: Project would add CCS to the Taft natural gas plant. It would separate and prepare to store up to 3 million tonnes of CO_2 per year, or at least 90% of the emissions.
- **Polk Power Station**, Mulberry, FL: The project would add ION Clean Energy's CCS technology at the natural gas plant. It plans to capture at least 95% of CO_2 emissions equating to nearly 3.7 tonnes per year to be stored in geological deposits.

Reuters, "Factbox: Emerging carbon capture projects at U.S. power plants," May 12, 2023.

[7] For an overview of some pros and cons of various carbon capture materials, see Table 1 at https://link.springer.com/article/10.1557/s43577-022-00364-9/tables/1 (Ozkan 2021).

ML has been less frequently applied to membranes and other novel materials for CO_2 capture, but opportunities have been identified in these areas. Prospects include correlating structure-property relationships to enable the design of highly selective, permeable, and cost-effective membranes and designing electrochemical cell configurations to improve capture performance. Ultimately, AI might enable a suite of sophisticated models supported by agile, automated data streams about the key properties of candidate materials as a means to **fill critical knowledge gaps in the complex interplay among materials, processing, properties, and performance**—potentially creating a virtual PSC material foundry (credit concept to McDannald et al. 2022).

Expand Capabilities for Process Modeling, Technoeconomic Analysis, and Lifecycle Analysis

Evolving conditions and priorities underscore the need for better and more robust models to help the power sector provide sustainable, efficient, safe, dependable, affordable, and flexible power generation facilities for the coming decades. Past models emphasized cost-efficient base load operations to meet regulatory requirements for reliability and power quality as well as limits on GHGs, criteria air pollutants, and water use.

Models must now identify the most cost-effective routes to zero emission systems that can flexibly adapt to rapid cycling and shifts in demand patterns (e.g., air conditioning during extreme heat events) and perform reliably (or provide resilience) despite growing climate impacts (rising air and water temperatures, decreased water availability, increasingly frequent and more severe weather events). Additional factors to be integrated may include coordination with new energy storage capacity and meeting the requirements of new carbon utilization or transport and storage facilities.

Developing and validating models that effectively integrate these diverse factors will require extensive data that may be difficult to attain and assess. ML and AI could help to obtain and synthesize the massive amounts of data (see page 6) needed to develop comprehensive models that use technoeconomic analysis (TEA) and lifecycle analysis (LCA) to predict the best carbon capture technology and operating conditions for a given NGCC plant design.

Common PSC Capture Media

Point source carbon capture (PSC) R&D leverages diverse capture media and one or more of the following approaches:

Solvents involve the chemical or physical absorption of CO_2 into a liquid carrier.

Sorbents chemically or physically adsorb the CO_2 on the solid sorbent surface.

Membranes separate CO_2 from the bulk gas using variations in molecular permeation rates through porous material based on the distinct molecular structure of CO_2.

Cryogenic processes use the difference in boiling points of gasses to separate them via condensation (EPA 2023a).

Novel concepts are alternative technologies like electrochemical membranes or additive manufacturing of system components.

Hybrid systems leverage material synergies.

Enabling technologies are concepts that could improve multiple materials.

NETL 2023b

Please see the Appendix for additional information.

Currently, rigorous process modeling and techno-economic analyses for emerging carbon capture technologies are limited (Jiang 2023). As summarized below, components of model development might address TEAs, LCAs (including co-benefits and potential liabilities), effective carbon capture and net emissions at less than baseload operation, ways to optimize emissions control across operating profiles, and PSC system optimization overall.

Conduct technoeconomic analyses (TEAs) using cost data from FEED studies

Robust TEAs using simulated carbon capture technologies for NGCC plants will require large datasets with detailed technical and economic data. Completed and ongoing DOE FEED studies of post-combustion PSC options are a potentially rich source of accurate data. A useful ML tool might incorporate data from FEED studies targeting emerging carbon capture systems at new or retrofit domestic gas-fired power plants. As noted above, some published studies omit relevant financial data (page 7), and this may be true of some FEED studies as well. For cases in which data owners consider the data proprietary, AI tools may be leveraged to **obtain access through data anonymization or federated learning**, which can avoid compromising the integrity or security of their data.

> **CCUS Supports Power Sector Flexibility**
>
> "Flexibility to deal with short-term and seasonal variability of electricity demand and supply is critical to ensure the stable and reliable operation of power systems. Coal and gas-fired power plants, which can adjust their power output on demand, have traditionally been the main sources of flexibility."
>
> "Although there are a wide range of low-carbon alternatives available for power generation, CCUS is projected to play an important role for three key reasons:
>
> - CCUS can help to avoid the "lock-in" of emissions from the vast fleet of existing fossil-fueled power plants through retrofits.
> - CCUS enables the sector to become net-negative though biomass-fueled power plants with CCS (BECCS).
> - CCUS can help to meet the growing need for system flexibility as the share of variable renewable energy technologies in generation and the need for "dispatchable" capacity increases."
>
> IEA 2020, *Special Report on CCUS*

Assess lifecycle impacts of emissions on the environment and co-benefits

Lifecycle analyses should address the full range of emissions (types and amounts) that can be expected when NGCCs with PSC technologies operate at non-steady states. Beyond predicting CO_2 capture levels and net emissions, AI may assist in predicting the compounds released with the component breakdown of capture media. Data on these emissions is currently scarce, and the chemistries of sorbents are often considered proprietary. Similarly, the chemistries of capture media used in FEED studies are not always disclosed. AI might assist by reviewing the literature and obtaining data via owner-approved anonymization or federated learning.

Once the full scope of potential emissions from a specific PSC technology /media option have been identified, a further analysis will be needed to fully understand the fate, duration, and potential GHG effects of those emissions over time. AI may assist in conducting lifecycle analyses to **clarify the net environmental impacts of each technology/media approach, projecting CO_2 capture levels and the net impacts of emissions over time**. This information would be a valuable input in helping the power sector and members of affected communities make informed choices as to the best PSC technology for a specified NGCC power plant.

> **Data To Support Environmental & Social Justice**
>
> "NETL is leveraging publicly available datasets and environmental and social justice findings within the context of CCS systems to develop an integrated database that will support the efficiency and integrity of CS stakeholder needs for a range of commercial, regulatory, and research applications. This is an evolving project and application will be updated periodically with new datasets and information."
>
> Maneesh 2023, NETL *CCS-EJ-SJ* Database

Optimize emissions in steady/non-steady states

AI may help in optimizing PSC technologies to minimize emissions first under various scenarios for steady-state operations, and then for non-steady-state conditions.

This will help define a system's true flexibility to respond to changing grid conditions. Reinforcement learning may be used with older surrogate process control models to fine-tune more advanced control of carbon capture systems without modifying a plant's existing control scheme. Concerns remain that some of the existing control technologies that are effective during baseload operations may become far less effective when plants operate below base load—as expected during increased cycling on the modern grid. AI/ML can account for the uncertainty of dispatch scenarios by performing (stochastic) optimization to design a system that will deliver the most robust performance across the defined range of operating uncertainties.

AI could be leveraged to model emission profiles associated with capture materials degradation in both steady-state and non-steady state conditions. Additionally, AI might help mitigate these emissions by optimizing control measures, such as sparging, water and acid washes, or corrosion inhibitors, given plant operating conditions.

Develop robust optimization model for PSC control systems

Operating conditions are likely to remain uncertain as NGCC power plants adapt to growing amounts of intermittent renewable energy sources on the grid. AI might assist in designing a PSC system that delivers robust performance despite the uncertainties of deployment. Full physics models may be too complex or expensive to optimize these systems, so surrogate ML models could be beneficial—as long as developers have access to sufficiently accurate data for model training and validation. AI developers might begin by optimizing such models at the lowest level of operation. Instead of prioritizing the lowest cost of carbon capture for an assumed capacity, a system and controls might be designed to deliver some level of profit (not maximized) across a broad range of potential dispatch scenarios.

Another approach might be to **co-optimize the capture material *and* process** for a PSC system. AI surrogate models might be developed to design the capture material (starting from the chemical structure and prediction of properties) and simultaneously optimize the process for that material. This work may involve the extension of existing, complex, computational models to predict the chemical properties of a carbon capture media based on its atomic structure. AI models might then predict how the properties of many candidate systems would work for different PSC processes and conditions to help identify the best candidate material/process pairs. This approach might enable, for example, the synergistic design of sorbents and adsorption processes (Asgari 2021, Burns 2020).

AI can also be used to identify the best process configurations and parameters to reduce the energy penalty and maximize the CO_2 capture rate under various operating conditions, such as inlet flue gas temperature, CO_2 fraction, and flow rate (Sipöcz 2011, Shalaby 2021, Li 2015). Specifically, AI might reduce the computational complexity traditionally involved in solving the systems of nonlinear partial differential equations that govern absorption and adsorption models.

Validate PSC Performance and Cost

As discussed, surrogate ML models have the potential to improve upon engineering models that simulate the performance of PSC systems. A critical hurdle is the lack of real-world data on how PSC systems will affect the performance of these power plants when the plants undergo increased cycling. The lack of commercial-scale data on plant performance under these future conditions could hinder model validation and add uncertainty.

A recent study evaluated five ML algorithms trained on data generated by engineering models in building an ML surrogate model to estimate reboiler energy consumption at a post-combustion PSC-equipped plant under current (not future) conditions. The study concludes that surrogate ML models are a promising technique to supplement or replace engineering models as they offer fast run times, robust predictions, and the ability to predict energy performance with aging components while requiring less data and understanding of the system. The authors caution that the amount and nature of available data may affect model accuracy, and technical and statistical nuances of ML models may obscure some opportunities for improvement (Aliyon 2023).

AI models that simulate PSC systems on NGCC plants allow researchers to explore the potential performance impacts of various processing and design variations without making changes to operating power plants (not permitted by regulatory agencies). This approach may be particularly valuable in evaluating opportunities to further intensify processes (e.g., alternative packing structures) and expand technology applications.

CCUS Retrofit Costs Depend on the Plant

"In general, the cost of CO_2 capture is inversely proportional to the CO_2 purity of the emission stream. But even within the same industry, several factors meaningfully impact the cost of capture, including facility design [number of capture units], separation technology used in the capture process, local energy prices, emissions volumes, flue gas temperature and pressure, and the presence of emissions stream contaminants.

Because of these project-specific factors, estimates can vary widely for current and projected costs. In general, capture costs are the most expensive component in the CCUS value chain, but economies of scale, learning by doing, modularization and standardization, and novel capture technologies could all yield significant cost improvements."

Pathways to Commercial Liftoff: Carbon Management, DOE, 2023

Increase process intensification to improve carbon capture efficiency

Process intensification efforts to improve CO_2 carbon capture tend to focus on reducing equipment size and improving process dynamics to enhance mixing and mass/heat transfer—leading to greater selectivity, energy efficiency, and sustainability (Wang 2017). Researchers are exploring alternative packing structures/materials and other ways to maximize solvent exposure to flue gases as a means to increase carbon capture.

More efficient packing structures could reduce the required amount of packing and make it possible to reduce the size of the absorber columns and reduce costs (Thompson 2022). Researchers are lifting the design constraints imposed by conventional steel packing structures by using 3D printers to make custom-designed polymer (or metal) structures that enhance liquid/gas contact and increase CO_2 mass transfer (Sarmah 2023). Smaller, more efficient columns might perform the same function at a lower capital cost. Smaller-diameter distillation columns might also reduce heat integration needs, energy demand, and the amount of liquid required, which could lower operating costs (Chamchan 2017, Riese 2022).

The challenge is that 3D printing and other innovations enable virtually limitless packing structure geometries with varied channel sizes and levels of intricacy. ML and AI could potentially help to **match a specific solvent with the best packing structure to optimize system performance and affordability**. Drawing on data from a broad portfolio of projects that have used different absorbers/packing materials and structures, ML might generate algorithms to rapidly screen a large number of potential packing structures for use with new solvents. Alternatively, AI might help **predict the performance of new solvents in combination with a range of packing materials and structures**.

To design PSC systems for optimal performance and economy, researchers need to **better understand the kinetic and thermodynamic limitations** of new and existing solvents and their interactions with PSC system components. Progress in this area may require complex computational fluid dynamics (CFD) models that bridge geometries, and high-fidelity, physics-based models could be validated with data from bench-scale systems. Gaining a deeper understanding of system limitations could lead to the design of more efficient gas-liquid reactors employing new principles and technologies for CO_2 capture. AI might then uncover patterns in the data to steer the research in new and productive directions (e.g., hybrid superstructure optimization). [See inset on related work by the CCSI^2 Initiative to support industry in scaling up new capture technology and maximizing learning at every stage of modeling and system development.]

> "In addition to technology improvements, different trends could further improve the techno-economic performance of CO_2 capture. Examples include modularisation of capture systems within self-contained, plug-in systems (with the potential to reduce land footprint, costs and lead times of capture retrofits across applications) and hybridisation of different capture technologies within capture systems (to increase capture rates while reducing costs and/or energy penalty)."
>
> IEA 2023

CCSI^2 Explores Advanced PSC Modeling

The Carbon Capture Simulation for Industry Impact (CCSI^2) is a partnership among national laboratories, industry, and academic institutions that applies cutting-edge computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies from discovery to development, demonstration, and ultimately deployment to hundreds of power plants. The CCSI^2 initiative will apply the advanced simulation tools developed by its predecessor project, CCSI.

The CCSI Computational Toolset is an integrated, comprehensive suite of validated science-based computational models, the use of which will increase confidence in equipment and process designs, thereby reducing the risk associated with incorporating multiple innovative technologies into new carbon capture solutions. The scientific underpinnings encoded in the models will also help maximize learning at every stage of the modeling and development efforts.

www.acceleratecarboncapture.org/

Validate PSC technologies for other applications

Experts must carefully validate AI models to ascertain that they reliably obey the laws of physics, and model predictions need to be verified by testing (another data-intensive step). Hybrid models offer a way to effectively combine first principle-based models with ML models in a joint architecture (Kurz 2022). Once AI models can be shown to successfully simulate PSC systems at NGCC power plants and can accurately predict their performance, interest will be high in using these models in related yet distinct applications. Anticipating this eventuality, AI might help **define the limits of prediction transferability**, particularly given the infinite variety of capture media (e.g., geometries, channel sizes, chemistries). Some pilot-scale results may be transferable to predict impacts in comparable applications that would not change substantially with scale, requiring minimal additional training data. In the absence of clear guidelines, however, access to these models might lead some users to extend application beyond a reasonable scope, whereas others might needlessly cling to high-fidelity physics models when the AI could save considerable time and money. Ideally, the new models would answer questions such as the following: What are the limits of extrapolation supported by the current model? Is the model applicable to a system in which specified parameters are within a certain range? What additional training data and validation is required for a defined amount of change in key parameters? What is the recommended process to validate transfer learning from a similar full-scale system?

Scale Up PSC Technology for Low-Carbon Power, Materials, and Supply Chain

DOE seeks to develop and scale up of PSC technologies at advanced NGCC power plants that use lower-carbon fuels,[8] leverage low-carbon supply chains, and generate low-carbon construction materials (e.g., cement, concrete, steel). AI might inform investments in PSC development and scaling by helping to screen candidate sites, clarifying requirements for affordable hydrogen production, and ranking existing NGCC plants in terms of suitability to be retrofit with PSC systems.

Identify site qualifications to inform screening

Strategic siting of CCS facilities could minimize financial and logistical barriers to technology adoption (GAO 2022). To meet U.S. climate goals, future, large-scale PSC projects and commercial-scale demonstrations would benefit from access to a variety of CCS hub functions, such as the following (Hancu 2022):

- High CO_2 capture efficiencies (>95%)
- Reduced carbon capture CAPEX/OPEX under a wide range of feed conditions
- Maximized co-benefit pollutant removal
- Access to conversion or transport/storage systems
- Low-carbon supply chains.

The technologies selected to serve some of these functions require a range of supporting resources, underscoring the need to thoroughly understand the characteristics of strong candidate sites (DOE/FECM 2022). Some site characteristics may make or break the long-term sustainability of specific PSC projects and their ability to scale successfully (e.g., insufficient water resources, lack of existing controls).

DOE has collected large amounts of data from its completed and ongoing CCS FEED and pre-FEED studies across the country. AI might draw upon this data to assess the most important site characteristics for determining site feasibility. Specifically, the AI might identify minimum site characteristics required to meet planned objectives as a means to **narrow initial qualification of proposed sites**. Requirements would vary with the system technology, but minimum needs would likely include factors such as the following: access to low-carbon materials of construction; land, water, and utility requirements; high-level CAPEX/OPEX information; existing environmental controls on the plant (upstream controls may add to costs); and proximity to industrial markets for carbon converted to products.

Not all key system data or site factors may be readily available [see AI capabilities to enrich datasets on pages 6-7], but AI may be able to assess the pivotal requirements by system type and **establish a risk score or thresholds for key factors.** DOE has already developed the Carbon Capture Retrofit Database (CCRD spreadsheet), which contains basic information on each plant, but AI could build on that foundation. Ultimately, AI might set minimum thresholds or produce a risk score (or a matrix of scores) to assist in site selection. Similarly, AI could assess detailed information on all existing NGCC plants to **prioritize existing plants for PSC retrofit** (solvent-based, post-combustion capture is currently the most mature technology for NGCC power plant retrofit).

[8] Lower-carbon fuels include hydrogen and natural gas with renewable natural gas (i.e., biogas) produced from various biomass sources through a biochemical process like anaerobic digestion or through thermochemical means, such as gasification. With minor cleanup, biogas can be used to generate electricity and heat and is used as a replacement for traditional natural gas to generate combined electricity and heating for power plants (DOE AFDC).

Facilitate PSC technology scale-up and integration with markets

In planned hub environments, NGCC power plants are expected to take advantage of access to low-carbon fuel options and potential markets. The mix of available fuels and markets could potentially increase PSC system performance and offset costs, but the mix of options for PSC systems, energy resources, and markets will vary widely for each plant and site. Scaling up a PSC technology already holds challenges, but making sure that a PSC NGCC system can take full advantage of available resources without costly pretreatments and can deliver captured emissions to proximate markets or pipelines at the required level of purity and pressure makes the undertaking far more complex. For each segment (input, process, materials, output) to be integrated into a larger system, AI would require extensive data from test centers, FEED studies, bench- or pilot-scale demonstrations, or related industrial processes. Ultimately AI might provide guidelines on the best mix of resources, PSC systems, and products to deliver the best performance (carbon capture and secure storage) and lowest costs for a particular plant and site.

Even when decoupled from the markets, it is difficult to develop process-scale models that accurately reflect process interactions. Models to successfully optimize processes and their integration with specific markets are apt to be complex and will require intensive scrutiny, testing, and validation. Advances in explainable AI may facilitate this essential process.

PSC for Industrial Applications

The industrial sector produces an enormous range of products and generates about 30% of U.S. GHG emissions through multiple, distributed, small emission streams with varied compositions. Cost effectively decarbonizing these emissions streams will require affordable PSC technologies that are compatible with industry processes and priorities (DOE/FECM 2022).

> "The majority of industrial sector emission sources are numerous but smaller and therefore lose the "economy of scale" benefit realized by the power sector. Leveraging the multi-party hub concept can spread the cost of the transport and storage component of CCS to multiple parties, decreasing the overall cost.
>
> *FECM Strategic Vision* (DOE/FECM 2022)

The complexity of capturing CO_2 from industrial sources varies across the sector as CO_2 concentrations differ widely by industry and by the specific stream targeted for CO_2 capture. Carbon abatement is particularly challenging in industries that rely on high-temperature processes that are hard to electrify or that rely on CO_2-producing chemical reactions not involving fossil fuel combustion (DOE/FECM 2022). Five of these hard-to-decarbonize industries (chemical processing, refining, iron and steel manufacturing, food and beverages, and cement and lime) collectively represent approximately 51% of energy-related CO_2 emissions in the U.S. industrial sector and 15% of total U.S. CO_2 emissions (DOE 2022). As described in the DOE *Industrial Decarbonization Roadmap,* decarbonization will require a combination of the following approaches:

- Improved energy efficiency
- Industrial electrification
- Low-carbon fuels, feedstocks, and energy sources
- CCUS
- Alternate approaches, including negative emissions technologies (e.g., BECCS and CDR)

Of these five approaches, the first three could reduce 40% of the targeted emissions; however, as shown in Figure 4, CCUS is predicted to bring about the largest reduction in carbon emissions in the long term (DOE 2022).

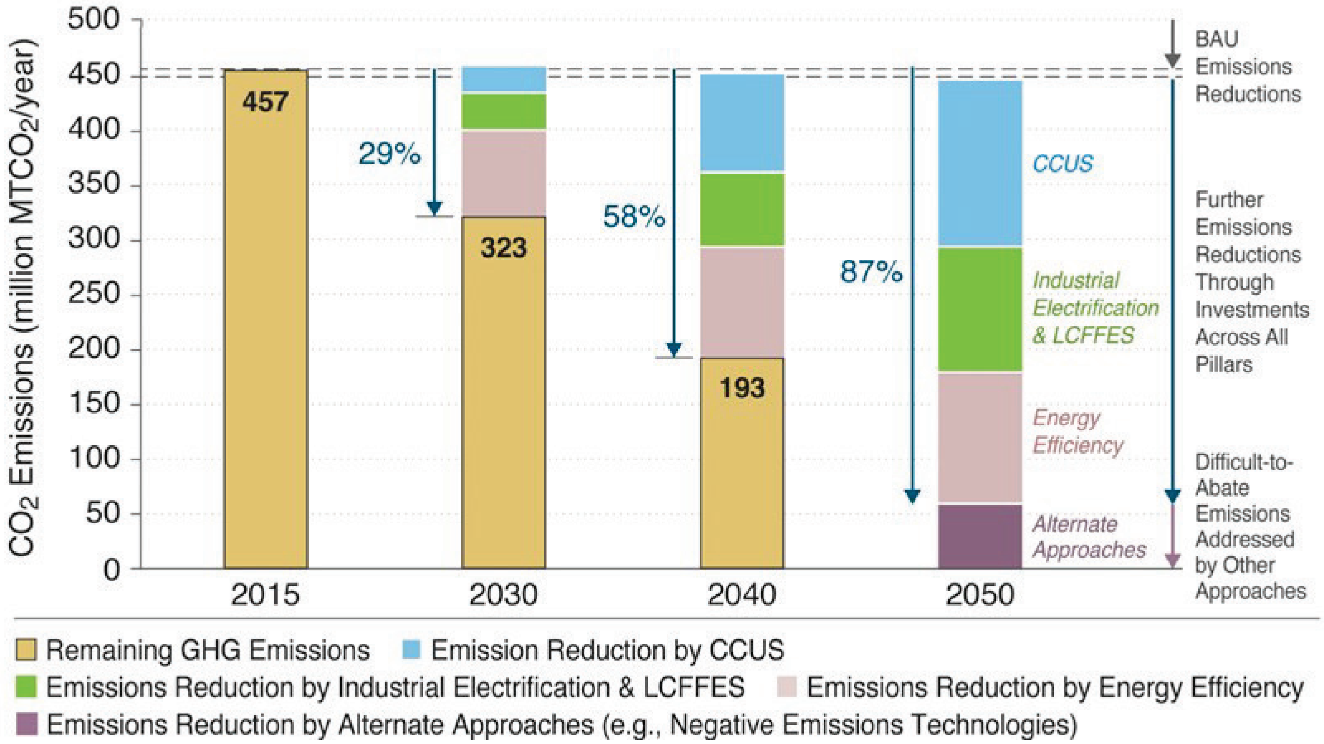

Figure 4. The Path to Net-Zero Industrial CO2 Emissions in the United States (million MT/year) for Five Carbon-Intensive Industrial Subsectors, 2015–2050. (DOE 2022) Industrial Decarbonization Roadmap

Adapting PSC technology originally developed for fossil fuel-based power plants for use by industrial systems is widely viewed as the fastest route to industrial decarbonization, but diverse industrial subsectors will require significant adaptation to accommodate industrial operations, reduce energy and carbon intensity, ensure product quality, enhance control of secondary emissions, and meet purity requirements for secure CO_2 utilization or transport and storage.

Adapt Power Plant PSC Technology for Industry

To maintain and enhance U.S. industrial competitiveness, PSC technologies for use by the industrial sector must avoid adversely affecting the quality or cost of the end products. In addition, PSC technologies originally developed for the power sector may need to be optimized for a variety of highly specific flue gas conditions (including a broad range of CO_2 concentrations and impurities) present in industrial manufacturing processes. Other issues to be solved in adapting PSC to industrial processes include industry's frequent use of batch versus continuous operations and the dynamic changes in feedstocks and operations.

Predict PSC system applicability based on the nature of an industry operation

AI might help to predict the best PSC system for a specific industrial operation using the composition of CO_2 flue gases or process operating conditions. AI models might assist in selecting the most cost-effective PSC technologies for a specific process, site, or market. More sophisticated AI models could potentially anticipate a diverse range of operations to inform the development of flexible PSC technologies that would be suitable for a broad range of industrial applications.

Reduce Process Energy Intensity and Emissions

Potential pathways to lower industrial PSC costs include integrating the abundant waste heat sources from industrial processes to drive the PSC and combining similar CO_2 streams. Leveraging these pathways will require a deeper understanding of diverse batch operations in the base plants, particularly the impacts of changes in feedstocks on the concentrations of CO_2 and the potential for impurities in the flue gas—which can increase secondary emissions and product quality.

Integrate waste heat to reduce PSC energy use

Many industries use a range of cost-saving waste heat recovery systems (specific to low-, medium-, or high-temperature heat grades) to reduce fuel consumption, lower harmful emissions, and improve production efficiency (Jouhara 2018). High-quality residual or waste heat from many industrial processes (e.g., chemicals, glass making) could help lower the energy costs of heat for PSC systems.

> "Of all the measures that will be required to curb greenhouse gas emissions, transforming the way we produce and consume heat in industry and buildings is one of the largest and most intractable."
>
> McKinsey Sustainability Blog, 2022

Some large, heat-intensive plants already combine different process heat streams of the same grade to optimize benefits from a recovery technology for the specific grade(s) of heat. In some cases, the recovered heat is used to supply district heating, which produces clear energy and efficiency benefits. In a hub scenario, high-quality heat from multiple processes and co-located companies might potentially be combined to drive cost-effective district heating *and* PSC systems. The specific cost of capture will naturally depend on the heat profile and capture plant configuration, but a recent analysis has shown that low capture costs can be achieved when excess heat is available during a long period of the year or if there is a high peak amount of heat (Eliasson 2022). A case study at an integrated steel mill in Sweden found that emissions could be reduced 36% when the CO_2 capture plant is prioritized over district heating (Eliasson 2022).

AI could help to **explore the potential to productively utilize all available heat sources** to lower PSC system costs across large plants, industrial hubs, or anywhere appropriate streams are available. Given the many available and emerging heat recovery technologies, AI models might recommend the most effective recovery system or mix of systems for the provided heat requirements. In the future, AI might monitor excess heat data from various systems in real time and automatically route the various heat streams for optimal recovery, efficiency, and cost benefits.

Optimize PSC systems for low-carbon feedstocks and production of low-CO_2 materials

Industrial PSC systems will increasingly need the flexibility to effectively capture emissions generated from industry uptake of sustainable feedstocks while continuing to provide CO_2 streams for products that store CO_2 for the long term, including materials of construction. Biomass is a feedstock of particular interest because of the way plants convert CO_2 into oxygen as they grow, offering the potential for net negative emissions.

Industries may increasingly take advantage of sustainable biomass, particularly in the form of processed waste (e.g., sawmill wastes, nutshells, industrial wood waste), processed fuel (e.g., biogas, densified biomass, charcoal waste, methanol, ethanol), or woody biomass (e.g., wood waste, forest floor, sweepings). Other options may include subsets of municipal solid waste (MSW). Levels of available biomass and other alternative fuels and feedstocks typically vary over the year, introducing additional issues for PSC technology. The issue is that biomass and other sustainable fuel sources (e.g., MSW, tires) take a variety of forms, some of which may create challenges for PSC technology.

AI may be able to help industries **fully integrate industrial PSC processes to effectively use low-carbon fuels and feedstocks**. A key part of this AI-facilitated integration may involve continuous sampling and monitoring of the feedstocks (mix and content) to optimize PSC operations and effectiveness. Although the biomass may reduce net CO_2 emissions, it could introduce new variables that produce GHGs or other harmful emissions at the stack. For example, biomass impurities could increase solvent degradation, increasing the release of toxic byproducts. Biomass or other feedstocks might also generate tiny particles or aerosols that would absorb amines and carry them out of the stack. Since many industrial processes are inherently batch (e.g., steel electric arc furnaces), the levels of flue gas and concentrations within the flue gas may vary widely from one batch to the next. AI might help develop effective engineering controls to monitor and optimally manage those rapid transitions between widely divergent steady states to **reduce adverse impacts on secondary emissions.**

At a larger scale, AI might **provide a control strategy to optimize overall PSC system operations** based on real-time sensor data. In addition to rapidly adjusting controls to optimize cost-efficient capture of GHG emissions in the presence of rapidly fluctuating feedstock mixes, AI could potentially perform strategic stream integration. In an exceptionally large plant or a hub-like environment, multiple feedstock streams might feed different combustors and AI could potentially divert materials from one stream to another (or route some problematic streams to temporary storage) to keep impurities to manageable levels and improve PSC effectiveness.

Produce Low-CO_2 Products/Construction Materials

Monetary incentives and public demand for products that durably sequester CO_2 could drive further industry investment in new CO_2 utilization technologies. Through 2030, the outlook for industrial CO_2 utilization capacity remains far smaller than for CO_2 storage. Beyond 2030, technology innovations and more supportive policies and regulatory frameworks could change captured CO_2 from a cost (storage) to a useful material, potentially expanding future markets (Biniek 2020).

"CO_2 use does not necessarily lead to emissions reduction. Climate benefits associated with a given CO_2 use depend on the source of the CO_2 (natural, fossil, biogenic, or air-captured), the product or service the CO_2-based product is displacing, the carbon intensity of the energy used for the conversion process, and how long the CO_2 is retained in the product."

Tracking CO_2 Capture and Utilisation, IEA 2023

Many products can potentially be made from CO_2. As highlighted in the *FECM Strategic Vision*, building materials are a promising way to turn the CO_2 captured from industrial flue gases into a value-added product that can prevent the CO_2 from returning to the atmosphere over the long term. The *Vision* targets near-term development of technologies to improve CO_2 curing in building materials. Concrete, which is made by adding sand and gravel to cement, then mixing it with water, is a valuable material for climate-resilient construction. CO_2 may also be injected directly into the concrete, where the CO_2 reacts with calcium ions in the cement to make more calcium carbonate, potentially improving the strength of the concrete. This represents an attractive solution to the cement industry's enormous carbon footprint, which represents about 8% of global CO_2 emissions (Nature 2021). Other future uses of interest include carbon fiber, green polyurethane, biochar, and aviation fuels (Biniek 2020).

Predict feedstock impacts on product properties

As mentioned above, using CO_2 in industrial products must not adversely affect product quality. Cement that incorporates CO_2 captured from industrial processes that increasingly use biomass or other fuels could raise some issues. For example, if impurities like chlorine (or degraded solvent byproducts) were to find their way into the captured CO_2 stream, the quality of the cement might suffer, which is unacceptable. AI might help detect and remove these impurities before they enter the PSC system or **guide operations to cut CO_2 and improve the product**. The optimal placement of sensors and controls to handle dynamic impurity issues will depend upon the plant design for retrofits and should be considered in new plant design.

Ensure Quality and Minimum Purity of Captured CO_2

Underground storage represents the most promising option to permanently store very large volumes of captured CO_2, but industry utilization is an attractive way to offset capture costs. Some high-purity CO_2 produced as a byproduct of certain industrial processes (e.g., ammonia production) is currently used in a variety of industries (e.g., medical, chemical, food, and beverage), and innovative new pathways are under development.

Whatever the planned final disposition of a captured CO_2 stream, to address the climate crisis, the CO_2 must not be released to the atmosphere for an extended period. In addition, the CO_2 stream must meet appropriate standards and best practices for safe and secure transport, storage, and utilization. A recent report from the National Academies of Sciences, Engineering, and Medicine contains tables that provide both an Overview of Recommended Maximum Impurity Limits for CO_2 Transport in Pipelines and Shipping and an Overview of Impurities of Concern by CO_2 Utilization Routes (NASEM 2023).

> "CO_2-emitting industries hesitate to deploy capture technologies if there is no infrastructure to transport and store the captured CO_2, but development of such infrastructure is risky if industry is not already capturing CO_2. It can take years to plan, permit, and build infrastructure for capturing, transporting, and storing CO_2. Developing this infrastructure in parallel rather than in sequence could accelerate deployment of the CCUS industry as a whole, according to stakeholders."
>
> *Decarbonization* (GAO 2022)

Meet purity requirements for utilization

Impurities in a CO_2 stream not only affect the PSC process and environment (as noted above), impurities affect how the stream can be utilized. A key challenge in capturing CO_2 from a broader range of industrial processes is making sure that each stream meets the specific minimum purity requirements for the target use—even as the mix of feedstocks changes suddenly. Even the types of impurities present in minute quantities in high-purity CO_2 streams can make a big difference, depending upon the application. For example, gas impurities can reduce the speed and quality of cuts by powerful industrial lasers and reduce the energy efficiency and stability of welds (CO2Meter 2023).

As new CO_2 utilization technologies become available for lower-quality captured CO_2 streams and the developers clearly define the minimum CO_2 purity standards for each, CO_2-generating/capturing industrial facilities may need AI to continuously **assess real-time data on fuels and feedstocks** to anticipate shifts in potential contaminants and take action to assure compliance. AI might help to develop and **run integrated controls to meet purity requirements** (minimize downstream impurities) by altering the mix of feedstocks for different processes, adjusting PSC operating parameters, or recombining output CO_2 streams from different processes/feedstocks. If applicable, AI-run analysis and controls may reroute streams to prevent particular impurities from reaching utilization systems with known sensitivities.

Dedicated, Reliable Carbon Transport and Storage

Achieving America's goal of a net-zero carbon economy by 2050 will require developing an expansive new carbon transport and storage industry and robust supporting infrastructure. The needed infrastructure must be deployed at an unprecedented pace and scale nationally and globally. A recent study estimates that by 2030 the U.S. infrastructure for carbon storage (both on and offshore) will need to accommodate at least 65 million tonnes of CO_2 per year—roughly the amount used by today's CO_2-enhanced oil recovery (EOR) industry—to meet the 2050 goal (Larson 2020).

Coordinate Quantity and Purity of CO_2 for Transport and Storage

The widespread deployment of PSC systems needs to proceed at a pace that matches the simultaneous development and deployments of a robust CO_2 transport and storage industry and infrastructure. Essentially, the CO_2-capture facilities must coordinate carefully with pipeline (or other transportation modes) and storage facility developers to make sure the captured CO_2 meets all applicable standards and requirements so that all of it can be handled safely and securely by the supporting infrastructure—without exceeding capacities.

> "A national or regional audit of the emissions associated with industrial clusters—including the age and type of facilities—together with an assessment of CO_2 storage options and opportunities for using the CO_2 is needed to inform the planning and development of infrastructure. Early planning and co-ordination can promote more efficient investment decisions in the long term... Governments can play a leading role in this planning and co-ordination across regions and industries."
>
> *Special Report on Carbon Capture Utilisation and Storage* (IEA 2020)

As in the case of utilization, different types of impurities (either already in the CO_2 stream or formed when the CO_2 comes in contact with other materials or conditions) can lead to major issues in the phase behavior of CO_2 streams, which can affect the design and operation of pipelines and injection wells (Razak 2023) or increase the risk of leaks. Cross-sector coordination can help to identify the potential ways in which captured streams and their impurities could change chemically or physically when in contact with the transport equipment and materials or natural elements within subsurface storage caverns. Transport equipment and materials include pumps, sensors, pipelines, barges, tank cars, and ships, though pipelines are the most common mode.

Manage diverse flows/content from varied sources

Industry-generated CO_2 streams must be carefully managed both to provide a continuous flow (often from batch or flexible operations) and to optimally mix or sort the diverse streams by critical characteristics/contents (e.g., temperature, pressure, purity, contaminants). Similar to the proposed AI role in managing the purity of captured CO_2 streams for specific utilization schemes, AI might help to closely monitor and optimize the various CO_2 streams and contents within a large industrial facility or hub environment to gain maximum utility from the flows and avoid issues.

AI systems could be developed to **track the quantity and quality of CO_2 and identify any issues** to avoid mismatches between the CO_2 stream and the transport and storage infrastructure. As suggested in Figure 5, a more sophisticated version of this capability might use AI and real-time sampling to automatically optimize upstream operations, shift feedstocks, or reroute/remix sub-standard CO_2 streams to avert problems and bring them into compliance. Conceivably, if the AI in a fully integrated system were to detect a significant drop in impurities in one or more streams, it could signal a time-limited acceptance of higher impurity limits in other streams.

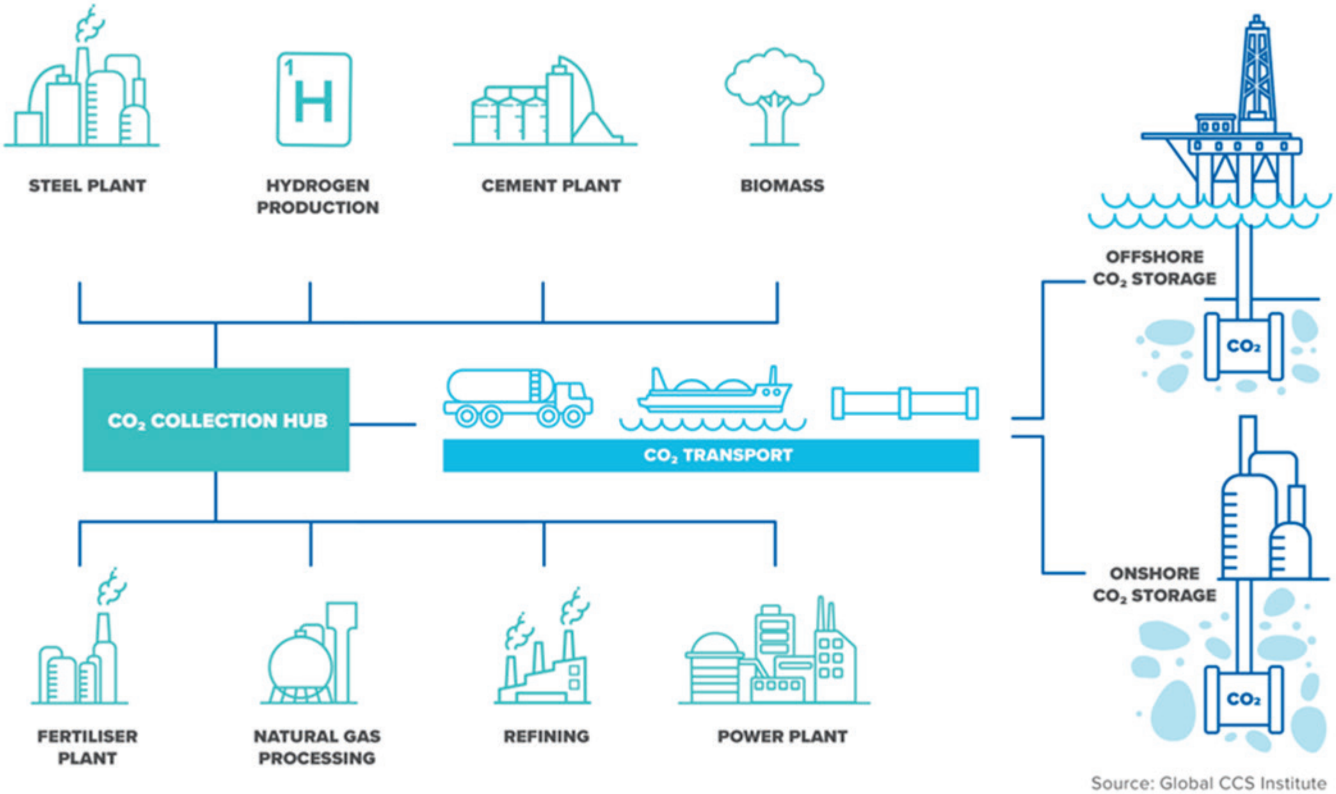

Figure 5. Within extremely large industrial plants or regional hubs, AI might proactively adjust operations so that incoming captured CO_2 streams can be properly treated to meet required transport or utilization standards.
(Image: Global CCS Institute)

Appendix: Strengths and Weaknesses of Common Capture Media

- ***Solvents.*** The most mature carbon capture process, liquid absorption, bubbles the flue gas up through a liquid solvent that selectively absorbs the CO_2. This process often uses amines—volatile and often toxic chemicals (Ozkan 2022) that react strongly with CO_2. The gas that departs the “absorber” is largely CO_2-free, and the liquid (with amine and trapped CO_2) is pumped to a separate tower known as a “CO_2 stripper.” There, the solution (water, amine, and CO_2) is generally heated (other options include pressure or electrical potential swing) to force the amine to release its CO_2. The regenerated liquid amine-water (20–50% amine) is then returned to the absorber to trap more CO_2 (Global CCS 2022). Potential disadvantages of liquid solvents include the high energy demand for regeneration, low absorption and desorption rates, amine losses to evaporation (Raganati 2021), high emissions of volatile solvents (Elmobarak 2023), and corrosion of the equipment (Åhlén 2023).

  Strategies to cut energy requirements and costs include (a) developing more efficient liquid-based solvents (e.g., those with faster reaction times, reduced liquid to be heated and cooled [without increasing viscosity], and the ability to absorb more CO_2 and produce less heat during reactions); (b) improving the absorber packing design and materials; (c) better managing the released exotherms; and (d) prolonging the life of the solvent. If more CO_2 could be trapped per liter of liquid solvent, the equipment could be downsized, reducing upfront capital costs (Global CCS 2022).

  Ionic liquids (IL) may offer a more affordable alternative to amines for carbon capture from flue gas. These tailor-made salts, made up of ions with a low melting point (< 100 °C), are less volatile and corrosive than amines and can provide efficient CO_2 solubility. Researchers have shown that ILs may be tuned to capture CO_2 efficiently under a wide variety of stream compositions and conditions. Research is needed to address concerns about the environmental sustainability of non-biodegradable ILs (Elmobarak 2023).

  Some solvents (including amines and ILs) can dissolve CO_2 without a chemical reaction, releasing fewer exotherms and requiring less heat to release the CO_2 in the stripper. The key disadvantage is that physical solvents also tend to dissolve other gases (e.g., nitrogen and methane) at low levels, so this approach is generally used for streams that are 15% CO_2 or more (Global CCS 2022).

- ***Sorbents.*** Solid adsorbents reportedly offer better adsorption capacity/selectivity and lower regeneration energy requirements than solvents, which may help lower costs (Khraisheh 2020). Key factors in adsorption are the pore size of the adsorbent and the temperature and partial pressure during the process (Buckingham 2022). Choosing a suitable sorbent for a post-combustion PSC system is complicated by the varied extents to which available sorbents meet the performance and economic criteria of specific systems. These criteria most commonly include CO_2 adsorption capacity, CO_2 selectivity, tolerance of water and impurities in the flue gas, adsorption kinetics, sorbent synthesis and costs, ease of regeneration, stability across repeated adsorption-desorption cycles, and mechanical/thermal stability (Raganati 2021). Solid CO_2 adsorbents capture CO_2 using physisosorption, chemosorption, or carbonation (Buckingham 2022).

  Some adsorbents leverage the size exclusion or “molecular sieving” properties of zeolites, activated carbons, and metal organic frameworks (MOFs) to select CO_2 from other flue gas components (Buckingham 2022). Unfortunately, materials used in this manner tend to have low selectivity for CO_2 due to the weak interactions involved (Ozkan 2022).

  Zeolites are naturally occurring adsorbents with a microporous crystalline structure. They show promise for post-combustion capture as they offer high adsorption capacities (high porosity) and fast adsorption kinetics under mild operating temperatures (less than 30° C), and they exhibit stability across adsorption-desorption cycles. Other advantages include their structural diversity and excellent recyclability (Raganati 2021). A disadvantage of zeolites is that their CO_2 capture capacity declines rapidly in the presence of water, which competes with CO_2 for adsorption, and at higher temperatures—becoming negligible above 200 °C (Wang et al., 2011). As a result, higher temperatures are required for regeneration—increasing energy usage.

Activated carbons can be regenerated easily, remain stable over many cycles, and are widely used because of their affordability (compared to other adsorbents). Disadvantages of activated carbons are that they tend to have a lower adsorption capacity than zeolites under low CO_2 density or pressure and their adsorption capacity is diminished when moisture or impurities are present in the flue gas (Raganati 2021).

Metal organic frameworks (MOFs) are synthesized by combining metal ions or clusters and organic molecules (ligands) into a network. These highly adaptable crystalline structures have prompted the development of more than 90,000 MOFs with diverse pore sizes, geometries, and functionalities for various applications. ML is actively used to predict specific materials properties based on input descriptors (e.g., pore geometry and functional groups chemistry) and for the discovery of new MOF structures (Moosavi 2020). Disadvantages of MOFs include their challenging manufacturing process and tendency to absorb moisture during carbon capture at high temperatures in power plants (Buckingham 2022).

- ***Membranes.*** In membrane separation, gas with a high CO_2 content is introduced through a tube on one side of a long membrane (often wound on a cylindrical tube). The membrane allows some components of the CO_2 to pass through and exit through a separate outlet, while the rest of the gas exits at the end of the tube. One benefit of membrane systems is that they can be easily scaled up or down for different purposes. Unlike liquid absorption systems, which need to be redesigned for each new facility, the size of a membrane facility can be increased by adding more membrane cartridges. The modularity and selectivity of membranes make them an attractive option for a range of PSC applications with different CO_2 partial pressures (Ozkan 2022). The disadvantages of membrane systems are that they are prone to fouling (dirt and contaminants build up), and the level of CO_2 purity after passing through a single membrane is generally quite low—necessitating a series of membrane modules (Anderson 2020). The need for high pressure gradients across the membranes is also a challenge to large-scale deployment (Chang 2022).
- ***Cryogenic separation*.** Cryogenic processes can produce high-purity CO_2 that can be readily transported and used without additional processing. Supplying the cryogenic chill can be expensive (both capital expenditure (CAPEX) and OPEX) unless a low-cost cold energy source is available (Chang 2022).
- ***Hybrid technologies*** combine different kinds of material (e.g., sorbent-membrane) into a single system to increase efficiency. ***Novel concepts*** embrace innovative solutions for CO_2 capture, such as electrochemical processes, porous liquid sorbents, or additive manufacturing of materials to enhance thermodynamic operations and reduce equipment footprint (NETL 2021).

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