ARTIFICIAL INTELLIGENCE FOR CLIMATE CHANGE MITIGATION ROADMAP (SECOND EDITION)

CHAPTER 9:

CARBON CAPTURE

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Carbon capture is an essential technology for climate change mitigation. Analysis by dozens of organizations, most notably the Intergovernmental Panel on Climate Change (IPCC)[1] and the International Energy Agency (IEA),[2] confirm the need for carbon capture to decarbonize key sectors (including steel, concrete, chemicals and aviation). As global greenhouse gas (GHG) emissions have continued to rise in recent years, carbon capture has received growing acceptance and been featured in international agreements, including the Dubai Consensus[3] and Sunnylands Agreement.[4]

Many governments, including those in the United States,[5,6] the European Union,[7,8] China[9] and Germany,[10] have included carbon capture as a key strategy to help achieve ambitious climate targets. National and international carbon capture programs include grants and loans for project demonstration, fiscal incentives (including tax credits and contracts for differences), infrastructure investment and robust investments in innovation. As a consequence, the number of operating and announced projects have increased significantly.[11,12]

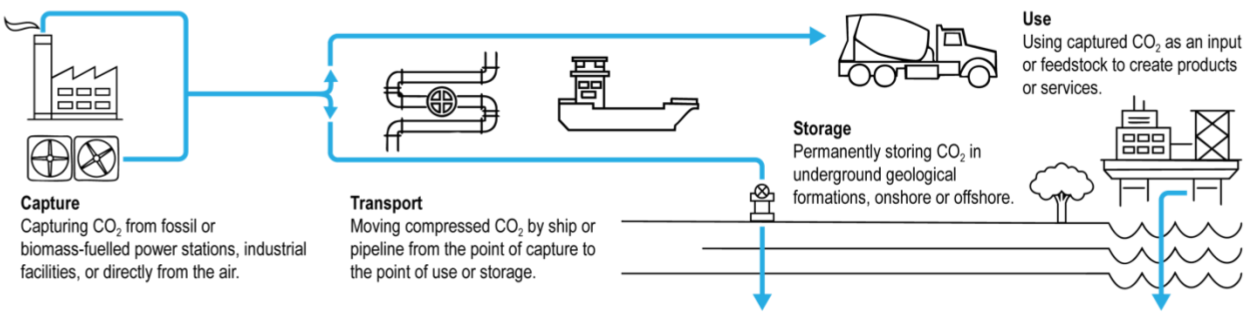

Figure 9-1. *Components of the carbon capture value chain including technology and infrastructure elements. Source: IEA, 2024*[13]

The field of carbon capture includes many forms of technology and cuts across many energy and climate sectors.[14] The core technology sets include many parts (Figure 9-1):

- separation of CO_2 from points source, the air and the ocean;
- transportation of CO_2, including pipeline construction and operation, barges, ships and trucks;
- storage of CO_2 in dedicated geological formations, including saline aquifers, depleted oil and gas fields, and basaltic formations;
- conversion of CO_2 into new building materials, chemicals and fuels and
- removal of CO_2 from the air and oceans using biomass and minerals as vectors for removal and storage to achieve climate neutrality[15]

Carbon capture systems can reduce the GHG footprint of existing fuels (e.g., bioethanol, aviation fuels), feedstocks (e.g., hydrogen) and energy sources (e.g., natural gas, biomass), as well as provide critically important climate services independent of energy production.

Despite some core technologies being quite mature,[16] integrated carbon capture systems are not widely commercialized and new technologies—including novel electrochemical means of CO_2 conversion and direct air capture operations—enter the field often. Although the costs for some applications are modest (below \$50/tonne CO_2), others are substantial (>\$100/tonne CO_2),[17] prompting decision makers to support means of reducing capital and operating expenses.

Small wonder, then, that AI could improve many aspects of this field, including technical elements (efficiency, performance, environmental benefits), commercial aspects (cost, routing) and policy concerns (equity and justice, resource allocation). The literature on AI applications in carbon capture is young, but the potential for AI to improve carbon capture appears significant, based on both primary manuscripts and reviews.[18,19]

This chapter describes some promising applications of AI in the broad field and specific subfields of carbon capture, including specific recommendations for key actors in climate and energy.

A. Capture Technology

Separating CO_2 from industrial waste streams, ambient air or the oceans requires chemical, physical or electrical processes, such as electrical-swing adsorption, humidity-swing adsorption and phase-change systems. These processes use chemical agents (e.g., liquid solvents and solid sorbents), functional components (e.g., contactors and membranes), well-functioning reactors and integration with other systems. For each of these steps, AI can play a role and already has begun to do so.

i. Materials discovery and functionalization

AI can assist in discovering new materials with properties that enable profound improvements in energy use, efficiency, strength and other key properties.[20,21] (See Chapter 6 of this Roadmap.) Carbon capture is particularly well suited for these approaches,[22] in part because of the key role materials (including liquid solvents, solid sorbents and membranes) play in CO_2 separation. AI speeds up the discovery of new materials[23,24] that can improve performance, including in the CO_2 loading of chemical systems, heat capacity,[25] energy consumption in CO_2 regeneration and longevity. In particular, metal-organic frameworks (MOFs) have proven well-suited to discovery through AI tools, which can collapse the range of possible materials into promising options in terms of structure, composition and design.[26]

However, having a library of suitable materials will not lead to deployment if the materials are not made or functionalized. AI has proven helpful in prioritizing which materials to fabricate and test based on their estimated performance, but benefits of these materials cannot be realized until they are built into filters, monoliths and other gas-contact media. AI has already proposed ways to improve functionalization (e.g., ways to structure solid sorbents to improve loading and performance).[27] Studies that demonstrate how AI can enhance manufacturing and functioning of other materials (e.g., carbon nanotubes[28]) show promise for carbon capture materials, as well. Given the very large range of approaches to manufacturing and functionalizing carbon capture materials, AI could help identify processes and pathways with high performance and chance of success.

ii. Novel capture system

AI can also accelerate development of novel processes for capture, regeneration and CO_2 conversion. Many novel processes are still designed through trial and error, including novel fluidized bed reactors, use of ionic liquids and dual-function processes that perform both CO_2 capture and conversion to chemicals like methanol. AI has proven useful in accelerating system design and testing—for example by helping identify and improve a novel regeneration process (electrochemically mediated amine regeneration).[29] Exploration of these process engineering and design options is only at the earliest stages.

iii. Capture system operation, optimization and integration

AI tools have already been applied to manufacturing and industrial production processes to good effect. (See Chapter 5 of this Roadmap.) Carbon capture systems can benefit from similar applications. This includes the use of digital twins of existing or planned facilities to assess and implement tools for efficiency gains. One study found that, by improving clean electricity delivery from the grid, AI tools could help carbon capture systems improve capture rates by >16% and reduce energy use by >35%.[30] Additional approaches include efficiency improvements through heat integration and reactor design optimization. Another study used AI to better optimize temperature, pressure and composition to enhance CO_2 solubility to increase uptake and reduce energy costs.[31] These tools have the potential to dramatically improve system performance, reducing capital cost, operating expense and energy consumption (Figure 9-2).

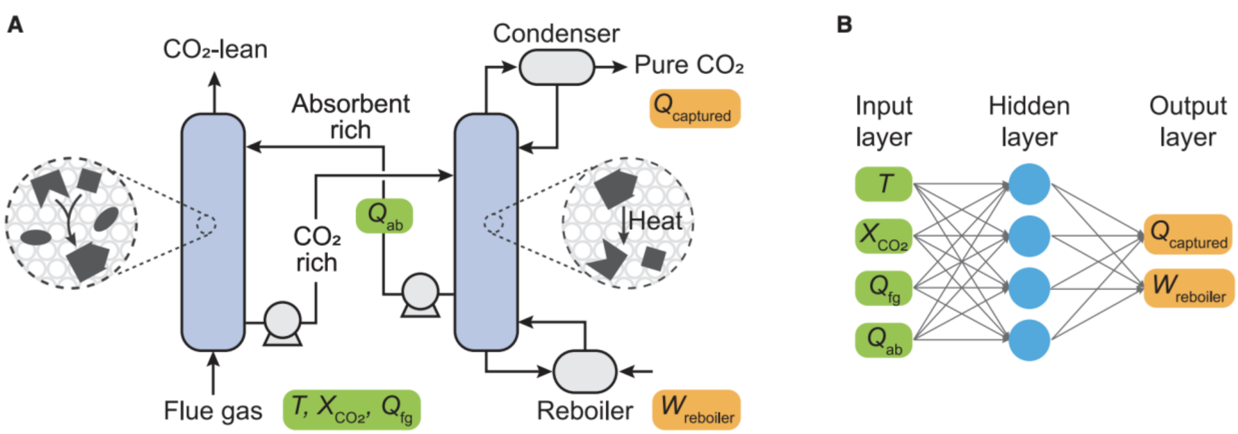

Figure 9-2. *An example of an implementation of machine learning (ML) for a CO_2-capture process. (A) Simplified flow diagram of an absorbent-based CO_2-capture process. (B) Illustration of an artificial neural network serving as an ML algorithm to correlate the reboiler-specific duty ($W_{reboiler}$) and CO_2-capture rate ($Q_{captured}$) as model outputs to the key operational parameters, including the flue gas temperature (T), CO_2 fraction (X_{CO2}) and flow rate (Q_{fg}), and the absorbent flow rate (Q_{ab}) as inputs. Source: Rahimi et al, 2021.*[27]

B. Transportation and Storage

i. Transportation

Once captured, CO_2 is moved to storage sites using a mix of approaches, including pipelines, ships and barges, and trucks. AI tools have already begun to help governments, private industry and communities develop plans for CO_2 transport that maximize CO_2 volume while minimizing cost and risks.[32,33] One study in China—a country with many large point-sources and very few CO_2 pipelines—

estimated total cost and network size for pipelines could be reduced by 12.5% using AI tools,[34] reducing embodied carbon emissions in fabrication and construction, as well as capital cost.

ii. Geological storage

Manipulating fluids in deep geological formations involves uncertainty, inference, interpretation of monitoring tools and making choices that require trade-offs. For geological storage of CO_2, critical uncertainties can involve the presence or absence of storage porosity (pore volume), the permeability of storage formations, the ability of overlying units to trap CO_2, and connectivity between units, across rock bodies and faults. In some cases, local data (field scale) and regional data (decades of exploration and production) are abundant and can help shape key choices. In other cases, geological data are scarce and operators face greater uncertainties.

AI can help in both cases. Where data are relatively abundant, workers have used AI to assess critical components of CO_2 storage systems, including geological storage efficiency,[35] trapping and overall site performance,[36,37] and monitoring[38] (Figure 9-3). In locations with lower data quality or volume, studies have used synthetic data volumes to train AI.[39] Although initial results have been impressive, the lack of large data volumes risks generating hallucinations in greenfield sites or frontier basins, requiring greater human intervention and validation. Finally, AI can serve to identify prospective new sites for CO_2 storage—an approach piloted by Microsoft[40] and others, where data availability may be either abundant or scarce.

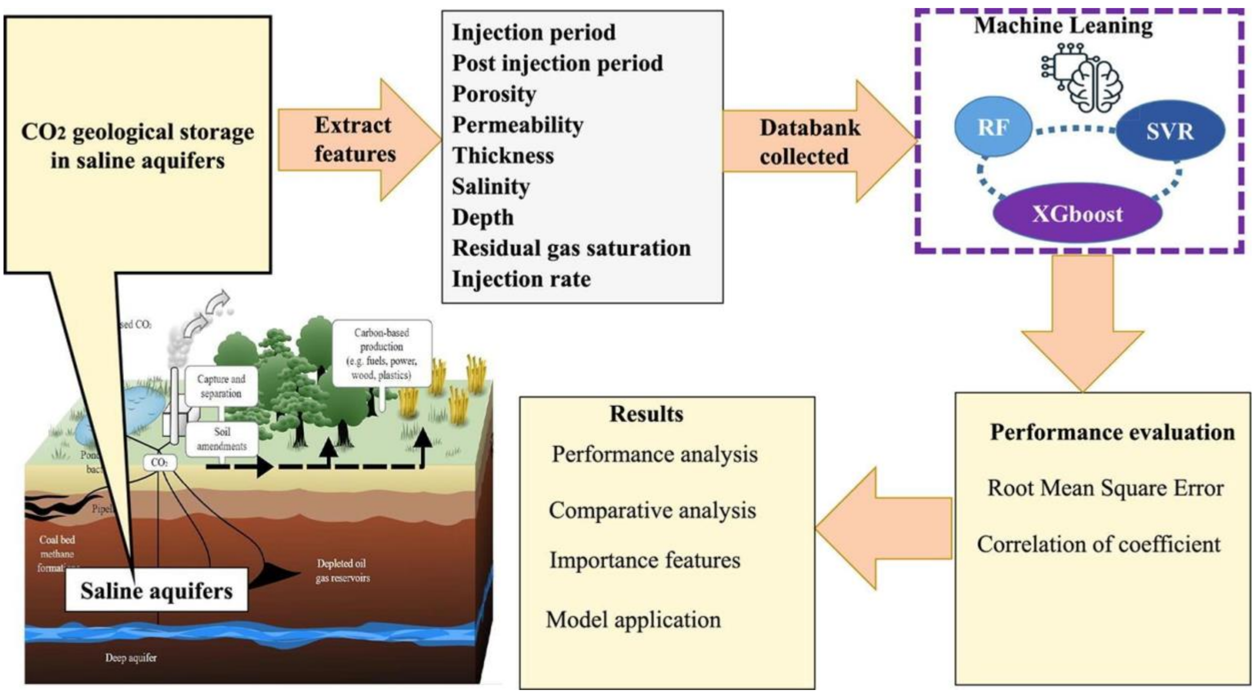

Figure 9-3. *A representative process flow for using machine learning (ML) systems to predict and manage performance of subsurface CO_2 storage systems. From Thanh et al., 2022.37*

AI approaches are likely to prove useful and accurate for traditional energy companies with large, complex in-house data sets. Already, industry has begun to pursue research and operational collaborations using AI tools. For example, Total Energies has partnered with Cerebras[41] and IBM[42] to identify and de-risk high-quality CO_2 storage sites. Similarly, Halliburton has developed an AI based analytical system to understand subsurface risks,[43] which could be used to predict the performance of geological CO_2 storage systems. In some cases, these specific tools began as means to optimize oil and gas production and have been converted or modified for geological CO_2 storage (e.g., optimizing CO_2-enhanced oil recovery (EOR) for oil production or for geological storage with AI).[44,45] These serve as an example of how AI only delivers climate benefits when asked to deliver them.

C. CO_2 Conversion to Products

Like CO_2 separation, CO_2 recycling and conversion processes involve chemical agents and materials, functional components (e.g., contactors), and fit-for-purpose reactors. AI can play similar roles in these endeavors as it plays in capture technologies, including material discovery, reactor optimization and system integration. Opportunities are many and broad,[46] involving direct chemical synthesis, biological intermediaries, novel reactors and materials, and mineralization (Figure 9-4).

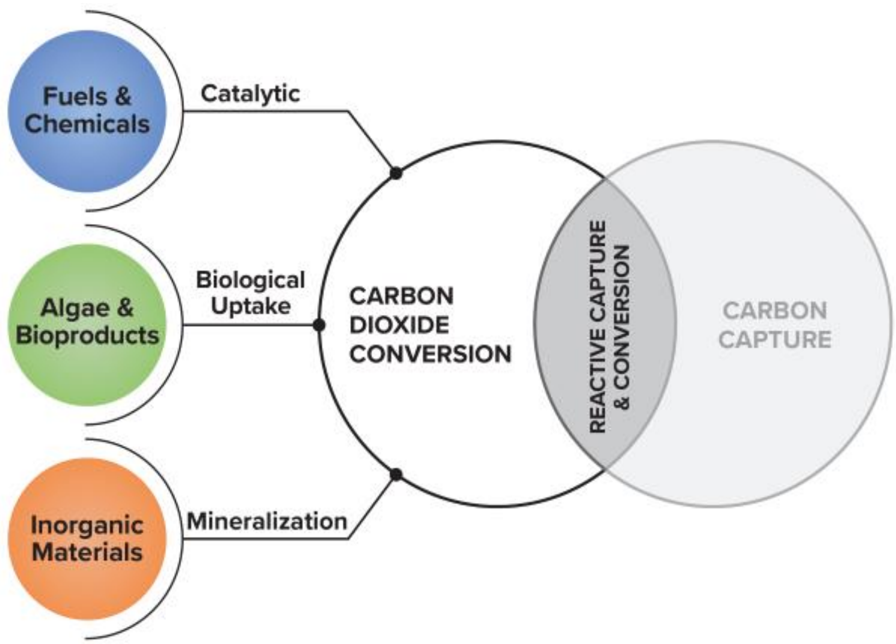

Figure 9-4. *Potential applications of AI for CO_2 conversion and recycling, including subdisciplines of high interest. From NETL.47*

- Chemical reduction of CO_2: Many CO_2 recycling pathways begin by converting CO_2 (carbon dioxide) to CO (carbon monoxide) or other simple organic compounds, such as methanol (CH_3OH). AI has already discovered special materials and processes that chemically reduce CO_2 through electrocatalysis,[48] photocatalysis,[49] enhanced biological processes[50] and multi-phase thermal catalysis.[51]

- **Novel chemical synthesis:** AI has begun to recognize novel approaches to making compounds out of CO_2. This includes turning CO_2 into starches, proteins and complex hydrocarbons.[22,52,53] One intriguing use of AI involved identifying "dual-purpose" materials that combine capture and conversion in one chemical step.[54,55]
- **Characterizing waste and input streams:** Industrial and municipal waste streams are often complicated mixes of many materials, compounds and substances. In some cases, these waste streams have substantial fractions of reactive compounds that could be well-suited to mineralization or other CO_2 utilization pathways.[56] AI can simplify and streamline these wastes for improved use.[57]

D. Other Carbon Capture, Utilization and Storage (CCUS)-related AI Applications

A cross-cutting technical concern with deploying carbon capture, utilization and storage (CCUS) involves accurately characterizing and understanding the full life-cycle assessment. Since new CCUS facilities commonly require energy, materials, land, construction and water, it is important to both understand the likely life-cycle implications, including both construction and operational phases, as well as to identify potential pathways to improve life-cycle. In the case of some CO_2 utilization pathways, this can be particularly complicated, as they include multiple supply chains and complex displacement pathways. AI can help provide life-cycle analysis, including initial life-cycle estimates, assessments of improvement opportunities and quantification, and trade-offs in design and operation of facilities between cost, carbon intensity and key environmental attributes (e.g., water consumption).[58]

AI could also help address non-technical issues associated with deploying CCUS. For example, existing facilities may need to update air or water permits when retrofitting for carbon capture or use. This process can be cumbersome, with long timelines and high expense. Similarly, permits for CO_2 storage wells require substantial data and analysis and are often backlogged. AI, including both large language models (LLMs) and digital twinning, could help facilitate both drafting and reviewing of permits, reducing time and costs. AI could help prepare the necessary written documents to receive tax credits for carbon storage or utilization under programs such as those in the US Inflation Reduction Act.[59]

Finally, AI can help ensure that local stakeholders do not suffer environmental burdens or health risks associated with CO_2 pipelines or siting other carbon capture facilities. Specifically, AI can help assess and provide environmental baselines[60] and monitor changes in the environment[61] from construction or pollution. AI can help consider the trade-offs in CO_2 transportation options, including cost, risks and environmental burdens. Initial work at the US National Energy Technology Lab (NETL) and the US Environmental Protection Agency (EPA) suggest potential AI applications and tools to help planners, regulators, investors and community stakeholders develop projects of all kinds in ways that are equitable and just.

E. Barriers

In addition to the many barriers confronting CCUS, increasing adoption and use of AI in CCUS presents specific challenges. The first and most critical issues, as is often the case, are data-related, including *access*, *quality* and *volume*. *Data access* involves the availability of specific compounds (catalysts, sorbents, solvents), reactors and facilities that might benefit from AI applications, which are likely to be limited due to intellectual property constraints, operational security and other commercial concerns. *Data quality* issues are related, including ensuring accurate metadata population and tracking and avoiding duplication of results and analyses, which require time, attention and specific coding to resolve. *Data volume* issues will most likely involve insufficient data, especially given the relatively small number of operating CCUS companies and facilities. While these could be overcome over time, these issues will likely prove challenging in the near- to mid-term.

The second set of challenges are workforce-related. CCUS broadly faces workforce shortfalls,[62,63] which are likely to be compounded by lack of training or familiarity with AI tools, methodologies and potential application. Although some corners of the CCUS enterprise are relatively familiar with AI tools and approaches (e.g., molecular discovery, digital mirroring), many groups in the ecosystem and value chain are unlikely to have the facility and sensibility to seek or employ AI-based tools today, whether for permitting or for reactor design.

F. Risks

Some of the barriers described above may manifest specific risks of AI use. For example, the lack of data for some applications could lead to generation of pseudo-data, which can increase the chance of hallucinations or simple errors. Similarly, the lack of trained workforce could introduce bias and fail to recognize specious results (e.g., in financial or regulatory affairs).

Some risks, independent of other barriers, could prove substantial. Since almost all CCUS projects and developments are taking place in countries within the Organization for Economic Co-operation and Development (OECD), geographic bias is an enormous risk, ranging from estimated costs to permitting ability or climate justice concerns. This could prove particularly true for subsurface studies and planning, where lack of subsurface data in key geographies or applications (e.g., *in situ* mineralization) could limit the ability of AI tools to generate useful and accurate results. Since geology varies greatly from region to region, misapplying Ai results could prove devastating to project success, which in turn might risk the CCUS enterprise.

Such risks could be mitigated at relatively low costs through a combination of management, training and review, but they would most likely require additional human and financial resources, which could prove hard to find.

G. Recommendations

1. *National governments and private companies should expand current research, development and demonstration (RD&D) programs in carbon capture to include AI methodologies, with commensurate increased funding.*
   a. *Specific use-inspired research topics would include material discovery (especially sorbents and solvents for carbon capture), functionalization of materials, and novel reactor design (including catalysts for CO_2-to-products). They should consider prioritizing efforts beyond simple material discovery and focus on more applied and operational aspects of CO_2 capture. Near-Medium term*
   b. *Applied research topics could include optimizing systems (including heat integration, use of digital twins, minimization of heat and electricity demands) and designing key infrastructure pathways (including location, size and operation for CO_2 transportation and storage design), operation and MMRV (measurement, monitoring, reporting and verification)). Near and medium term, with near term emphasis.*
   c. *Government granting entities must hire and/or train personnel that are sufficiently trained and knowledgeable to be able to review AI-related proposals well. Near and medium term.*
2. *Asset owners, utility owners and operators, industrial manufacturers and key state-owned enterprises should use AI tools and methodologies to accelerate assessment of CCUS pathways for existing and planned assets. This should include cost-benefit determinations in comparison with other decarbonization options, with the goal of establishing a ranking of opportunities. Near term.*
3. *National governments should use AI, including LLMs and other generative AI platforms, to streamline permitting processes for carbon capture in all forms. This includes permitting wells for CO_2 injection and processing pipeline rights of way, power electronic designs, and processing revisions to air permits for facility retrofits. Near term.*
4. *National governments and private companies should use AI to improve resource characterization for carbon capture, with emphasis on characterizing geological storage resources. AI-enabled resource characterization should extend beyond bulk storage terms and volume estimates to include understanding of injectivity, permeability fields and risks posed by pre-existing wells. Where possible, national and state governments and some private companies should make data available for training, either through voluntary sharing and federation or mandates. Near term.*
5. *Professional societies, academic experts and carbon accounting bodies should launch training programs on the potential for AI in carbon capture. This could include use of AI for life-cycle assessments of carbon capture systems, as well as the RD&D topics stated above. Near and medium term.*

6. *National governments, private companies and academic researchers should immediately commence with identifying key data requirements for enabling AI in carbon capture. Once identified, these three groups should work to gather, federate and share these data while providing fair, judicious access. Near term.*

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