

Artificial Intelligence in Carbon Capture and Storage Technological Advances and Future Challenges

Jingyi Wang

School of Urban Design, Wuhan University, Wuhan, China

2024302093004@whu.edu.cn

Abstract. The escalating climate crisis necessitates the rapid development of innovative carbon reduction technologies, among which Carbon Capture and Storage (CCS) is considered a pivotal solution. However, the widespread deployment of conventional CCS is hindered by challenges related to efficiency, cost, and risk management. This review explores the transformative role of Artificial Intelligence (AI), particularly machine learning and deep learning, in overcoming these challenges. By analyzing recent literature, we demonstrate AI's significant potential in optimizing CCS processes, from accelerating the discovery of novel capture materials to enhancing the safety and efficiency of storage site monitoring and enabling intelligent system management. Despite this promise, critical challenges remain, including data scarcity, the carbon footprint of AI model training, and the need for robust regulatory frameworks. This study concludes that interdisciplinary collaboration and a focus on developing dynamic, data-driven approaches are crucial for realizing the full potential of AI-CCS integration, paving the way for its effective contribution to global decarbonization goals.

Keywords: Carbon capture and storage; artificial intelligence; machine learning.

1. Introduction

In recent years, the issue of global warming and climate change, primarily driven by carbon emissions, has become increasingly severe. The World Meteorological Organization (WMO) released "The State of the Global Climate in 2024", which recorded changes in indicators such as greenhouse gas concentration, temperature, and ocean heat content, highlighting that human activities have profoundly influenced climate change, and the increasing frequency of extreme weather events poses a significant threat to the global economy and human society. A critical concern is that some of these impacts may be irreversible. Fossil fuels, including coal, oil, and natural gas, are the primary contributors to carbon dioxide emissions and play a significant role in driving global warming. Therefore, it is very important to strengthen the monitoring and governance of carbon dioxide. In this circumstance, carbon capture and storage (CCS) is an important method to control carbon dioxide and control climate change. It offers a viable pathway for reducing carbon emissions while ensuring a stable energy supply and improving energy utilization. However, with the increasing demand for carbon emission reduction, the limitations of CCS technology are highlighted. There is significant room for improvement in material selection, process monitoring, and cost reduction.

In recent years, artificial intelligence has been rapidly applied to urban governance, intelligent construction, weather forecasting and other aspects. Among them, machine learning, deep learning and other Artificial Intelligence (AI) technologies are widely used in various fields with their excellent computing and modeling prediction capabilities [1]. According to the "2025 Artificial Intelligence Index Report", as early as 2023, the US Food and Drug Administration (FDA) allowed 223 artificial intelligence devices to enter the medical market. This also demonstrates the potential of AI to empower and transform existing industries. Since there are also steps such as prediction, modeling, and decision-making in the CCS technology link, the powerful algorithm of artificial intelligence has become an important method to optimize the CCS technology process.

The purpose of this article is to summarize international articles, comprehensively analyze the interaction between CCS and AI, the reasons and application cases, and put forward the shortcomings

of the interaction between the two, so as to provide certain theoretical guidance for the intelligence, efficiency and safety of CCS technology.

2. Fundamentals of Carbon Capture and Storage

2.1. The Principle and Process of Carbon Capture and Storage Technology

According to Priya, the basic principle of CCS technology is to collect carbon dioxide existing in the air, store it in geological formations or deep ocean reservoirs, isolated from the atmosphere, and reuse the collected carbon dioxide. The CCS technology process includes three links: carbon capture, carbon transportation and carbon sequestration. Carbon capture includes direct capture, chemical capture (capture carbon dioxide after combustion), physical capture and biological capture. The carbon captured mainly comes from industrial production and domestic emissions. Carbon transportation is mainly carried by ships and pipelines. Part of the carbon is sequestered in the seabed or geology, and the other part is returned to the energy itself through chemical or biological utilization [2].

2.2. Limitations of Conventional Carbon Capture and Storage

Although CCS technology can effectively suppress carbon emissions, there are still some problems that cannot be solved or avoided by technology. For example, in the process of using combustion to capture carbon dioxide, carbon dioxide emissions are still inevitable. Even if most of the carbon dioxide in the air has been successfully sequestered in the geology or the depths of the seabed, due to the inherent limitations of storage materials, it is impossible to prevent the stored carbon dioxide from being lost and returning to the atmosphere over time. From the perspective of monitoring technology, although there are currently predictive decision-making models that assist CCS technology, due to the opacity of data, most models only focus on static data. However, in the face of more complex problems, there is a lack of models for collecting and processing dynamic data. For example, the research results of Mariëlle et al. show that most studies only focus on a single static link such as the production of membranes required in the carbon capture process, while ignoring the changes in capture capabilities caused by material consumption [3]. At the same time, in terms of economy, the high cost of CCS technology and the lack of timely adaptation of technical plans to market demands result in low economic benefits. These limitations and data challenges inherent in traditional CCS approaches highlight the urgent need for more intelligent and adaptive solutions. This is where AI comes into play, offering powerful data-driven capabilities to address these very issues.

2.3. The Necessity and Advantages of Artificial Intelligence Introduction

According to the above, CCS technology urgently needs a powerful data analysis technology to assist it. And the algorithms and data processing capabilities of artificial intelligence are well-suited to address these gaps. For example, technologies such as machine learning and deep learning train large models of CCS technology through the analysis of massive amounts of data. This model helps environmental engineers and even investors make the next decision efficiently.

3. The AI Framework for Carbon Capture and Storage Enhancement

3.1. Machine Learning in Carbon Capture and Storage

Machine learning (ML), a subset of artificial intelligence, enables computers to learn automatically from data and make predictions or decisions using algorithms and statistical models. Machine learning is divided into supervised learning (SL), semi-supervised learning (SSL), and unsupervised learning. This algorithm includes the following steps-Dataset acquisition, data processing optimization, determine target variable, dataset partitioning, build model through algorithm, algorithm parameter tuning training, result generation and evaluation [4].

Research by Nikolett et al. has found that machine learning is primarily applied to the monitoring and optimization of CCS technology. The underlying logic of this approach is to learn from previous mistakes and shortcomings, thereby increasing the accuracy of the algorithms while reducing costs in the carbon capture process [5].

3.2. Deep Learning in Carbon Capture and Storage

Deep learning (DL), an advanced subset of machine learning, utilizes deep neural networks with multiple layers to automatically extract hierarchical features from raw data. By mimicking the structure of the human brain, DL models excel at identifying complex patterns in unstructured data such as images, sounds, and text, making them suitable for tackling nonlinear and high-dimensional problems in CCS.

Ahmed et al. employed a Temporal Fusion Transformer (TFT) model to overcome the limitations of traditional simulation methods for optimizing CO₂ storage. Their study utilized data from six U.S. oil fields representing diverse geological formations to model CO₂ injection responses and predict storage efficiency under Water-Alternating-Gas (WAG) scenarios. The TFT model achieved a high coefficient of determination (R^2) of 0.87 in processing time-series data, demonstrating exceptional accuracy. This deep learning-based approach successfully enhanced the prediction of CO₂ storage rates and utilization efficiency [4].

3.3. Potential Applications of Other AI Technologies

Beyond ML and DL, other AI technologies like reinforcement learning (RL) and digital twins show significant potential for advancing CCS.

Take digital twin technology as an example. Digital twins are a new concept in the context of the "Metaverse" in recent years. Its principle is to apply models, sensors and other data to complete the mapping process in virtual space, so as to reflect the corresponding full life cycle process of physical equipment. In Wang et al.'s research on smart agriculture CCS, they designed a self-learning and self-deployment system, and then built a virtual system based on digital twin technology that is highly consistent with the real CCS link, and then iteratively optimized this digital twin model [6]. Through this optimization process, it is possible to predict the situation parameters and preset conditions according to highly accurate conditions. Therefore, digital twin technology can help decision makers make better decisions by improving more accurate numbers and a more accurate model analysis process to enhance the feasibility and efficiency of CCS.

4. Application Analysis of AI in Carbon Capture and Storage

4.1. Revolutionizing the Capture Phase

The carbon capture stage involves multiple variables (e.g., gas flow rate, temperature, pressure, adsorbent characteristics) and complex physicochemical reactions, often leading to challenges in efficiency and high energy consumption. AI technologies are particularly valuable for optimizing this complex process.

ML models can rapidly screen and optimize potential carbon capture materials, such as Metal-Organic Frameworks (MOFs). For example, Surojit and Li used a dataset of 1,166 network structures to build a model that analyzed material characteristics like pore volume, surface area, and porosity. This model successfully identified the top-performing 1,000 MOFs from a pool of several thousand candidates [7].

In another study, Zhang et al. developed a computational platform integrating Monte Carlo tree search (MCTS) and recurrent neural networks (RNNs) to design MOFs with high adsorption capacity, ease of synthesis, and stability under humid conditions. The platform identified key structural descriptors for optimal performance. Consequently, the researchers designed and screened six MOF structures

with a CO₂ adsorption capacity exceeding 2 mmol/g, outperforming 96.9% of materials in existing databases and significantly accelerating the discovery of efficient adsorbents [8].

4.2. Securing Transport and Storage

A critical step in the CCS process is the geological storage of carbon dioxide. M. Ali et al. leveraged AI to innovate and accelerate the prediction of CO₂ solubility trapping, a key mechanism in saline aquifers [9]. They developed an Artificial Neural Network (ANN) model using a large synthetic aquifer dataset. The model was built and trained using Python and TensorFlow, with its performance evaluated based on the coefficient of determination (R^2) and root mean square error (RMSE). The ANN model successfully predicted the timing and efficiency of the solubility trapping mechanism. This demonstrates that the ANN model is a valuable tool for predicting storage effectiveness, especially in scenarios where traditional simulations are infeasible.

4.3. Intelligent System Integration

At the strategic level, AI technologies, particularly machine learning, provide robust decision-support capabilities for the integrated management of CCS projects. These capabilities include intelligent monitoring and maintenance, data fusion and analysis, multi-objective optimization, and the development of intelligent management systems, all of which enhance the timeliness and reliability of decisions.

For instance, Rene et al. employed advanced genetic algorithms to analyze the costs, efficiency, and impacts of residential energy consumption. Based on a network framework, their research facilitated the design of an optimal CCS infrastructure layout, demonstrating AI's utility in strategic planning [10]. At the operational management level, Zhang and colleagues developed an AI-driven decision support system for CCS projects. This system leverages real-time data and AI simulations to evaluate various operational scenarios, thereby assisting managers in making informed decisions promptly. The implementation of such a system significantly improves the management efficiency and operational accuracy of CCS technology [11].

5. Challenges and Constraints

5.1. Data and Generalization Constraints

Although existing research confirms AI's potential to enhance CCS technology, its application faces limitations rooted in data and algorithms. Machine learning models fundamentally rely on large volumes of high-quality data for training. A significant challenge is the generalizability of these models. While algorithms like Neural Networks (NN), Multilayer Perceptrons (MLP), and ANN have proven effective for specific CCS problems, they often remain tailored to particular (static) datasets and struggle to adapt to new, unforeseen scenarios or dynamic conditions.

For example, models trained on historical data from a specific capture facility may not perform accurately when applied to a new site with different geological characteristics or operational parameters. Consequently, enhancing model accuracy and reliability necessitates further research focused on expanding data diversity, strengthening dynamic monitoring capabilities, and developing more adaptable algorithms.

5.2. Carbon Emissions in Artificial Intelligence Model Training

The core of machine learning involves training models on extensive datasets to enable accurate predictions and decision-making. While pivotal for technological advancement, this process carries a significant carbon footprint. According to research by Surojit et al., training a single large machine learning model can emit approximately 300,000 kilograms of carbon dioxide-equivalent to the energy consumption of 125 flights from Beijing to New York [7]. Such substantial emissions raise ecological

concerns, creating a paradox where a technology aimed at mitigating climate change may itself contribute to the problem [12].

This issue is exacerbated by the approaches to data collection. A dataset with limited numerical range can restrict model diversity and flexibility, leading to poor performance in real-world applications. Conversely, pursuing high accuracy through comprehensive data collection inevitably demands greater computational resources, further increasing carbon emissions. This highlights a critical trade-off between model performance and environmental impact. Addressing this challenge requires a multi-faceted approach, including algorithmic optimization, improvements in computational efficiency, and the use of renewable energy sources for powering data centers. Future research must prioritize balancing model accuracy with environmental sustainability.

5.3. Ethical and Regulatory Hurdles

The integration of AI and CCS, while promising, introduces a set of ethical, legal, and social challenges that must be addressed to ensure responsible deployment. The absence of robust quantitative standards, regulatory frameworks, and transparent oversight could lead to technical failures and erode public trust.

Technically, the lack of standardized metrics makes it difficult to consistently monitor and evaluate the safety and efficacy of CCS projects. Parameters such as CO₂ capture efficiency, storage integrity, and long-term environmental impact assessment require clear and universally accepted criteria. The International Energy Agency (IEA) estimates that the world must capture and store about 700 million tons of CO₂ annually by 2030 to meet climate goals [13]. Without proper regulation, this rapid scaling could lead to the proliferation of inadequately vetted projects, where commercial interests might override safety considerations, posing significant ecological risks.

Policy instruments like "carbon pricing," adopted in countries such as Canada and Sweden, demonstrate how legal frameworks can incentivize green technology adoption, including CCS, by internalizing the cost of emissions. However, effective governance of the AI-CCS nexus requires more than economic incentives. It demands collaborative efforts between academia, industry, and policymakers to establish clear legal guidelines, promote public education, and ensure project transparency. Only through such comprehensive measures can CCS technology, empowered by AI, be implemented safely and gain broad social acceptance.

6. Conclusion

6.1. Conclusion

This study provides a comprehensive exploration of the application of artificial intelligence (AI), particularly machine learning (ML) and deep learning (DL), in optimizing Carbon Capture and Storage (CCS) technology. Through a systematic analysis of existing literature, the study concludes that AI holds significant potential for enhancing the efficiency, safety, and intelligence of the entire CCS chain—from material design and process optimization to system-level decision support. Specifically, AI methodologies (e.g., neural networks, genetic algorithms, digital twins) offer innovative solutions to inherent bottlenecks in conventional CCS—such as high energy consumption, elevated costs, and monitoring difficulties—by enabling efficient processing of complex data, optimization of operational parameters, and prediction of system behavior and risks. This research not only offers theoretical support and practical insights for professionals working towards carbon neutrality but, more importantly, addresses a notable gap in the cross-disciplinary literature integrating AI with carbon management technologies, thereby fostering interdisciplinary dialogue.

6.2. Outlook

This study provides a systematic review of the application framework and potential of AI in CCS, offering a valuable theoretical reference and integration of case studies for this interdisciplinary field.

However, the research has limitations, primarily as a literature-based analysis lacking empirical data support and specific algorithm validation. Future work should focus on the following areas for optimization. First, efforts should be directed toward building high-quality, standardized, specialized databases for CCS to provide a reliable foundation for AI model training. Second, it is crucial to develop lightweight AI algorithms capable of processing dynamic, real-time data to balance model accuracy against computational carbon emissions. Lastly, there is an urgent need to foster interdisciplinary collaboration among data scientists, chemical engineers, and geologists. By establishing joint research frameworks, the gap between model predictions and field applications can be bridged, ultimately advancing AI-CCS technology from theoretical optimization toward safe, efficient, and large-scale commercial deployment.

References

- [1] Cao Lulu. Application of artificial intelligence on the CO₂ capture: a review. *Journal of Thermal Analysis and Calorimetry*, 2021, 145 (4): 1751-1768.
- [2] A.K. Priya, Balaji Devarajan, Avinash Alagumalai, et al. Artificial intelligence enabled carbon capture: A review. *Science of The Total Environment*, 2023, 886: 163913.
- [3] Mariëlle Corsten, Andrea Ramírez, Li Shen, et al. Environmental impact assessment of CCS chains- Lessons learned and limitations from LCA literature. *International Journal of Greenhouse Gas Control*, 2013, 13: 59-71.
- [4] Ahmed Wagia Alla, Mohamed Alghazal, Turki Alzahrani. Modern Deep Learning Framework Using Temporal Fusion Transformer to Optimize Sequestration Efficiency and Oil Production in CCUS Projects. *Middle East Oil, Gas and Geosciences Show (MEOS GEO)*, 2025.
- [5] Nikolett Sipöcz, Finn Andrew Tobiesen, Mohsen Assadi. The use of artificial neural network models for CO₂ capture plants. *Applied Energy*, 2011, 88 (7): 2368-2376.
- [6] Wang Zhe, Zhu Xinhua, Sang Yiwei, et al. Research on Key Technologies of CCUS Supply Chain Digital Twin System for Smart Agriculture. *Energy Proceedings*, 2023, 33.
- [7] Surojit Gupta, Li Lan. The potential of machine learning for enhancing CO₂ sequestration, storage, transportation, and utilization-based processes: a brief perspective. *Artificial Intelligence and Machine Learning in Energy Storage and Conversion Materials*, 2022, 74 (2): 414-428.
- [8] Zhang, L., Chen, H. AI-driven decision support system for optimizing CO₂ capture processes. *Environmental Science & Technology*, 56 (3): 1456-1464.
- [9] M. Ali, Z. Hamdi, H. Elochukwu, et al. Acceleration of CO₂ Solubility Trapping Mechanism for Enhanced Storage Capacity Utilizing Artificial Intelligence. *SPE Norway Subsurface Conference*, 2024.
- [10] Rene Markovič, Marko Gosak, Vladimir Grubelnik, et al. Data-driven classification of residential energy consumption patterns by means of functional connectivity networks. *Applied Energy*, 2019, 242: 506-515.
- [11] Christophe McGlade, Paul Ekins. The geographical distribution of fossil fuels unused when limiting global warming to 2°C. *Nature*, 2015, 517 (7533): 187-190.
- [12] Payal Dhar. The carbon impact of artificial intelligence. *Nat Mach Intell* 2, 2020, 2 (8): 423-425.
- [13] IEA, Direct Air Capture 2022. Paris: International Energy Agency, 2022.