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Application of Intelligent Systems in CO_2 Management: State of the Art and Future Prospects

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ABSTRACT

Machine learning (ML) integration is becoming increasingly popular in advancing the 4th industrial revolution, known as Industry 4.0. This review paper examines ML applications in CO_2 management stages: emission, capture, and conversion. ML models, including multiple linear regression (MLR), multiple nonlinear regression (MNLR), and artificial neural networks (ANN), are used in the emission phase to predict the CO_2 emissions for the countries and sectors, variables such as energy consumption, fuel usage, gross domestic product (GDP), population, and other miscellaneous socio-economic variables. In the capture stage, ML forecasts post-combustion and direct air CO_2 capture efficiencies using models such as ANN, generalized regression neural networks (GRNN), backpropagation neural networks (BPNN), and group method of data handling (GMDH), considering input variables such as catalysts, process parameters, and rheological properties. In the conversion stage, ML models, primarily ANN, multi-layer perceptron (MLP), particle swarm optimization (PSO), and genetic algorithm (GA), forecast and optimize CO_2 transformation into products such as methanol, C_2 hydrocarbons, syngas, methane, lower olefins, and biofuels, considering factors such as catalyst compositions and process conditions. This study identifies several trends, with ANN emerging as the predominant ML technique. The discoveries will benefit academia and industry in the development of CO_2 management models.

1 | Introduction

Earth's average temperature has increased by over 1°C since the Industrial Revolution, with the hottest 10 years recorded since 1998. Human activity, primarily through the release of greenhouse gases (GHGs), is responsible for the rise of GHGs. The Intergovernmental Panel on Climate Change (IPCC) acknowledges CO_2 as the main anthropogenic GHG, constituting over 70% of emissions, with residual emissions including nitrous oxide, methane, and other fluorinated gases [1]. IPCC projections suggest CO_2 concentrations could reach 570 ppm by 2100, potentially causing a 1.9°C average global temperature increase and a 3.8 m rise in sea levels. In order to address these issues, urgent actions are required to implement the Paris Climate Agreement, aiming to limit global temperature rise to well below 2°C and striving for 1.5°C [2, 3]. Due to elevated levels of CO_2, research focuses on solutions such as capturing and storing CO_2 underground or converting it into valuable

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goods [4]. Figure 1 illustrates a comprehensive Carbon Capture and Conversion (CCC) cycle.

Machine learning (ML) suggests significant potential to the CO_2 management cycle, including emission, capture, and conversion. Several studies have been reported in literature on the implementation of ML to these discrete phases, a comparative evaluation of the entire CO_2 life cycle is still lacking, which leads to a knowledge gap that is critical towards clarifying the flexibility and comparative performance of ML models on the distinct phases. This review attempts to critically evaluate the use of ML in the prediction of CO_2 emission, capture, and transformation processes. It measures the performance of the models, outlines the phase-limited trends, and outlines practical challenges, as well as research priorities. The following research questions were explored in order to reach this objective: (1) What ML models are predominant at the emission, capture, and conversion stages? (2) What are the defining data types and input-output variables of each of these stages? (3) How does the performance of ML models vary across emission prediction, capture efficiency, and conversion optimization settings? The idea is to provide a stage-wise examination of an ML application in CO_2 management, relative comparison across all stages of CO_2 management for different models used, identify operational issues, and map the future research paths. This review will contribute to the academic research and application in industrial practice by offering systematic and comparative analysis to inform the academic research and industrial practice through rigorous model comparison, data-driven knowledge, and performance analysis relevant to real-world systems.

ML is a prevalent form of AI that revolves around constructing mathematical models from training data to enable systems to self-learn and predict unknown labels [5]. Drawing inspiration from how humans learn, ML enables systems to approach complex problems by extracting patterns from data, without the need for rigid programming [6]. Over the years, ML has played a transformative role in domains such as emission forecasting, industrial process modeling, and environmental simulations, all of which are integral to various stages of CO_2 management [7].

ML is increasingly utilized across areas relevant to CO_2 mitigation, including process prediction and optimization [8, 9], predictive maintenance [10], and energy system operations [11, 12], as well as in anticipating emissions in industrial sectors. Its effectiveness is particularly evident in the petrochemical [8, 13], steel [14], and cement industries [15], where it supports emission reductions, enhances operational efficiency, and sharpens process control. These diverse applications underline ML's adaptability within the context of CO_2 management, from estimating emissions based on energy or economic parameters to modeling capture effectiveness and refining process variables in CO_2 conversion technologies. As an example, ensemble learning algorithms such as Light Gradient Boosting Machine (LightGBM) have been recently proven to be effective in predicting gas-hydrate phase equilibria in porous media [16], but hybrid machine-learning models have been competent in predicting loss circulation during drilling - a problem that resembles the uncertainty issues found in CO_2 subsurface injection [17]. In addition, machine-learning techniques have been used to model polymer injection processes in non-conventional reservoirs [18] and to analyze geomechanical processes such as stress-driven sand production [19], both of which are analogous physical and operational constraints in CO_2 storage and enhanced oil recovery (EOR) environments. The recent comparative evaluation between traditional ML and Bayesian deep learning methods for reservoir analysis further supports the significance of quantifying uncertainty in subsurface prediction, which is a key element of successful CO_2 monitoring and risk-management systems [20].

This review critically examines the applications in the field of emission forecasting, processes of carbon dioxide capture, and how CO_2 has been transformed into useful products.

2 | Overview of ML Methods

The algorithms, which are referred to as machine-learning models [21], are created to detect patterns in data and give predictions or judgments without utilizing explicitly programmed

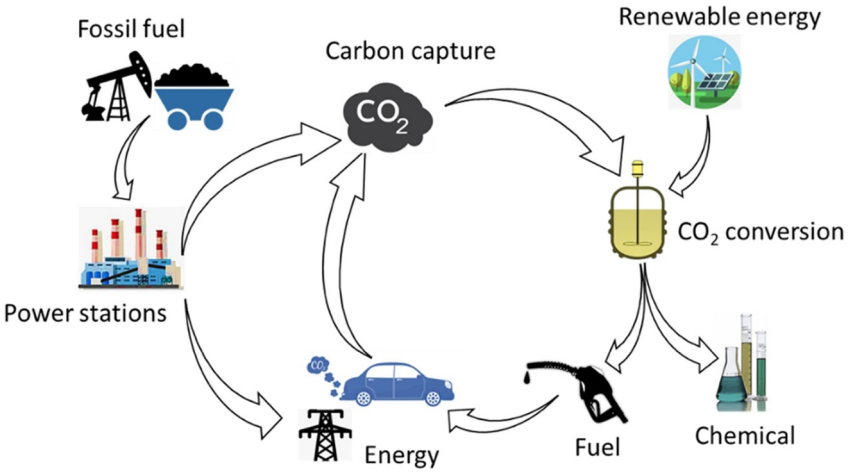


FIGURE 1 | CO_2 conversion cycle (Reprinted from Adamu et al., (2020), licensed under CC BY 4.0) [4].

rules. There is a continuum of machine-learning paradigms, such as supervised [22], unsupervised [23], and reinforcement learning models [24]. In supervised learning, models are fitted to labeled data to predict target values based on given input features using methods such as linear regression, neural networks, and decision trees. Unsupervised learning, on the other hand, attempts to find latent structure in unlabeled data and uses techniques such as PCA and k-means clustering. Reinforcement learning focuses on the learning sequentially in response to dynamic environments and improving over time by methods such as Q-learning and deep Q-networks. Autonomous cars, natural language processing, recommendation systems, and image and audio recognition are all based on machine-learning methods. The choice of models is based on the nature of the problem, the nature of the data, and the desired result. Researchers continually innovate to enhance ML capabilities. In supervised learning, models learn from labeled data, where both the input features and the correct output values are known [22]. The model learns to map input data to output labels, predicting outcomes for new inputs. Examples of supervised learning algorithms include linear regression, k-Nearest Neighbors (kNN), DTs, RF, SVMs [25], and neural networks such as feed-forward and Convolutional Neural Networks (CNN) [26]. Unsupervised learning works with unlabeled data, identifying structures and patterns. Clustering algorithms, such as K-means and hierarchical clustering, group data points with similar features, whereas dimensionality reduction methods such as PCA and t-SNE reduce the number of variables to make patterns in the data easier to see and interpret. Unsupervised methods such as autoencoders and density-based spatial clustering of applications with noise (DBSCAN), which is a clustering method that groups nearby data points and marks isolated points as noise, are useful for working with large environmental datasets that do not have labels. Autoencoders are neural network-based models that compress and then reconstruct data, helping reduce complexity and highlight key features. DBSCAN groups together data points that are close to each other and separates outliers, which helps identify unusual patterns. These techniques help find hidden trends, reduce data size, and flag anomalies. This is especially helpful in CO_2-related studies, where it is common to explore and understand the data first before building prediction models [27, 28]. Figure 2 illustrates the complete ML models under supervised, unsupervised, and reinforcement learning techniques. Methods such as Deep Q Networks (DQNs), Q-learning, and proximal policy optimization (PPO) are common. Reinforcement learning applies to gaming, autonomous systems, and robotics. In regression problems, supervised learning is often used to find a mathematical relationship that matches the model's output to actual values using simple equations. DTs, which are useful for both classification and regression, split data into smaller groups based on specific feature values. A technique for ensemble learning [29] called Random Forest (RF) [30] combines many DTs to improve prediction accuracy and reduce overfitting. Each tree is trained on a random subset of features and data. SVM is a commonly used supervised learning model for both classification and regression, which works by finding the best boundary that separates different classes of data. kNN is an easy-to-understand supervised learning method used in regression and classification, predicting labels/values of a data point based on the consensus or average of that data point of the kNNs in feature space [25]. Naive Bayes is a popular Bayesian probabilistic model for classification, which assumes that features are independent given the class label. This assumption makes it efficient for tasks

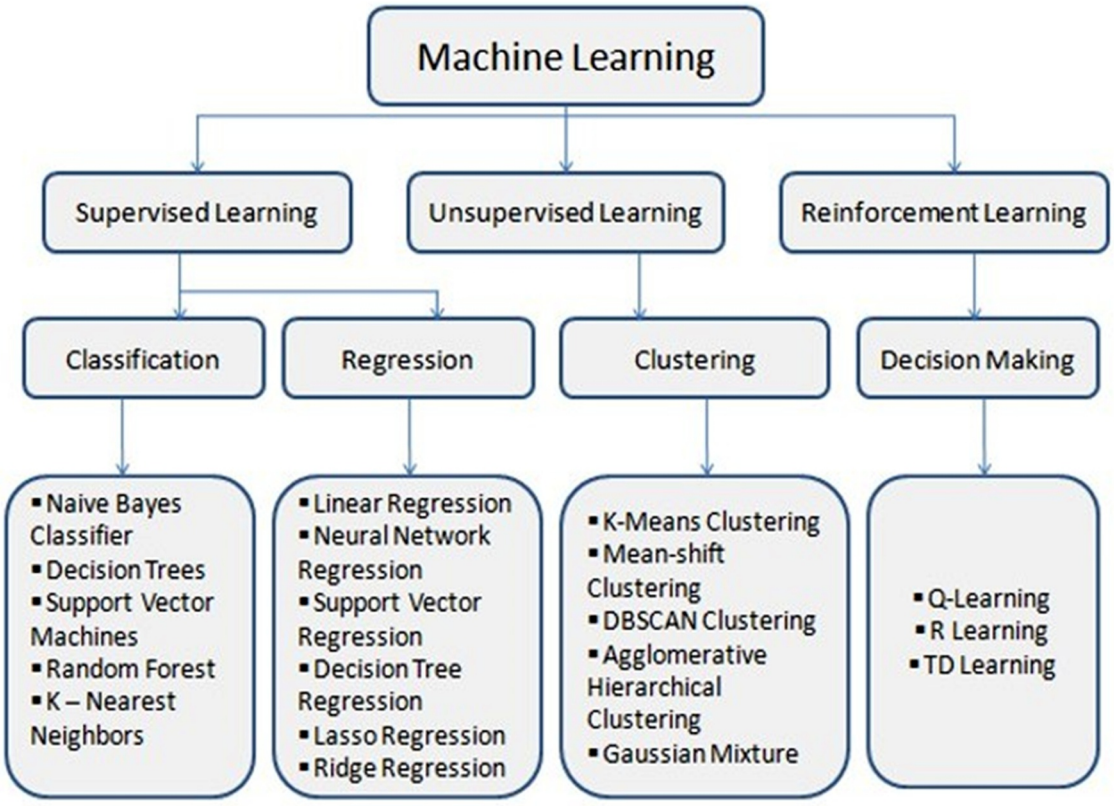


FIGURE 2 | ML models used for classification, regression, clustering, and decision making.

like text classification and spam filtering. Neural networks, inspired by the human brain's structure, are highly versatile, excelling in tasks such as speech synthesis, image recognition, and natural language processing due to their ability to learn intricate patterns from input and interconnected layers of neurons.

K-Means is an unsupervised learning method that clusters data points into K clusters based on similarity, updating centroids to minimize within-cluster variance. Unsupervised learning methods such as PCA reduce the number of variables in the data while keeping the important patterns, helping to simplify the data without losing useful information. Reinforcement learning [24] teaches agents to make decisions in dynamic environments, maximizing rewards through trial and error. GRNN (General Regression Neural Network, a type of model that works well on small datasets and is quick to train) and MLP (Multilayer Perceptron, a widely used neural network with multiple layers that learns complex patterns between input and output) are frequently used in CO_2 modeling.

3 | Methodology

The retrieval of literature involved utilizing Scopus and Google Scholar databases, focusing solely on research articles with a majority sourced from Google Scholar and supplemented by Scopus, guided by keywords in Table 1 to acquire studies on ML applications within CO_2 management stages.

The relevance of articles was determined using two rules: (1) titles encompassed at least one term from both ML and carbon categories in Table 1 and (2) titles were required to contain a term from any of the emissions, capture, or conversion in Table 1. Predefined keywords were used to classify the literature into the three subsequent stages of the CO_2 life cycle. Manual research was also conducted to make sure that all relevant articles were included. After the thorough examination, the papers were filtered out, and a set of 15 papers for the emission, 16 papers for capture, and 14 papers for the conversion phase was obtained. Figure 3 shows a percentage breakdown that illustrates the distribution of these studies in all phases of CO_2 management up to 2023. Figure 4 is a workflow diagram that represents the methodology used in this review. The literature that was systematically retrieved was then systematically arranged into the three stages of CO_2 management, namely emission, capture, and conversion. The applications of ML in these phases were relatively compared in terms of key performance indicators, thus making it possible to identify the most prevalent models of ML in managing CO_2 activities.

4 | Applications of ML Methods in CO_2 Management Stages

This section presents the use of ML methods in the key phases of CO_2 management, that is, emission, capture, and conversion, thus highlighting their respective functions, model selection criteria, and performance measures on diverse datasets. When applied to the management of CO_2, the choice of the ML models depends on the complexity of the input-output relations and the nature of the available data. As an illustration, the Gaussian radial basis function neural networks (GRFNNs) are especially effective with smaller or less structured datasets because they can learn nonlinear trends with a limited amount of training data. Conversely, ANNs and MLPs have demonstrated greater effectiveness in large-scale, high-dimensional datasets, and are regularly more effective in predictive accuracy, reduced mean squared errors, and increased generalization across CO_2 forecasting, capture modeling, and conversion yield prediction. Supervised learning methods are particularly beneficial in cases where there are labeled outputs, that is, CO_2 levels, capture efficiency, or conversion yields, thus enabling accurate predictive modeling. When labels are unavailable, unsupervised learning approaches such as clustering or PCA help uncover hidden patterns and data groupings. Regardless of the model

TABLE 1 | Keywords used in the literature survey.

Categories	Keywords used for searching in the databases
Machine learning	Data-based, DT, K-means, boosting, logistic regression, ANN, principal component analysis (PCA), multi-layered perceptron, support vector machine, linear regression, least-squares, random forest, neuro-fuzzy, data-driven, deep learning, ensemble learning, machine learning, partial least squares, moving average, naive bayes, GA, kNN, extreme learning machine
Carbon	Carbon dioxide, carbon monoxide, greenhouse gas, CO_2 as a greenhouse gas, CO_2 and global warming, CO_2, CO, GHG
Emission	Emissions data, emission sources, global emissions, industrial emissions, transportation sector emissions, emissions by energy sources, country-specific emissions, emissions trends, emissions prediction, emissions from reservoirs, forecasting emissions
Capture	Capturing technologies, capture and utilization, capture and storage, direct air, post-combustion, pre-combustion, absorption, adsorption
Conversion	Utilization, fuels, chemicals, electrochemical reduction, biological conversion, photocatalytic conversion, efficiency, bio fixation, lower olefins, microalgae fixation

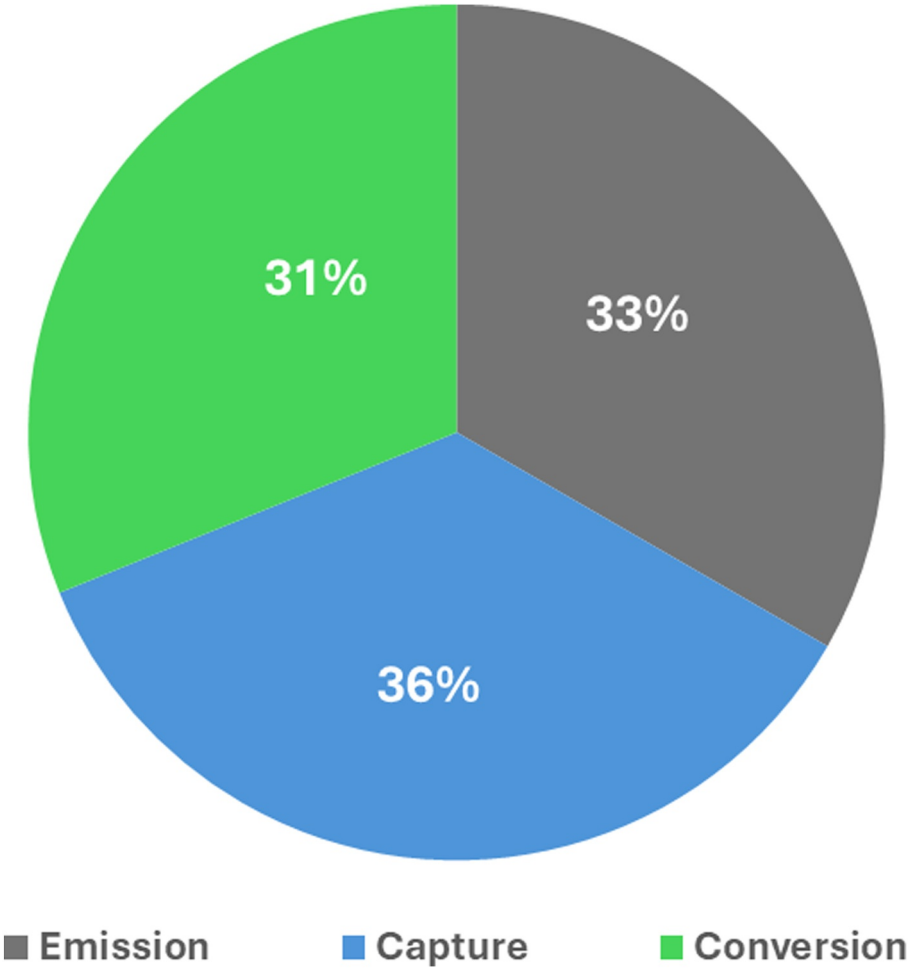


FIGURE 3 | Percentage of publications for CO_2 management stages.

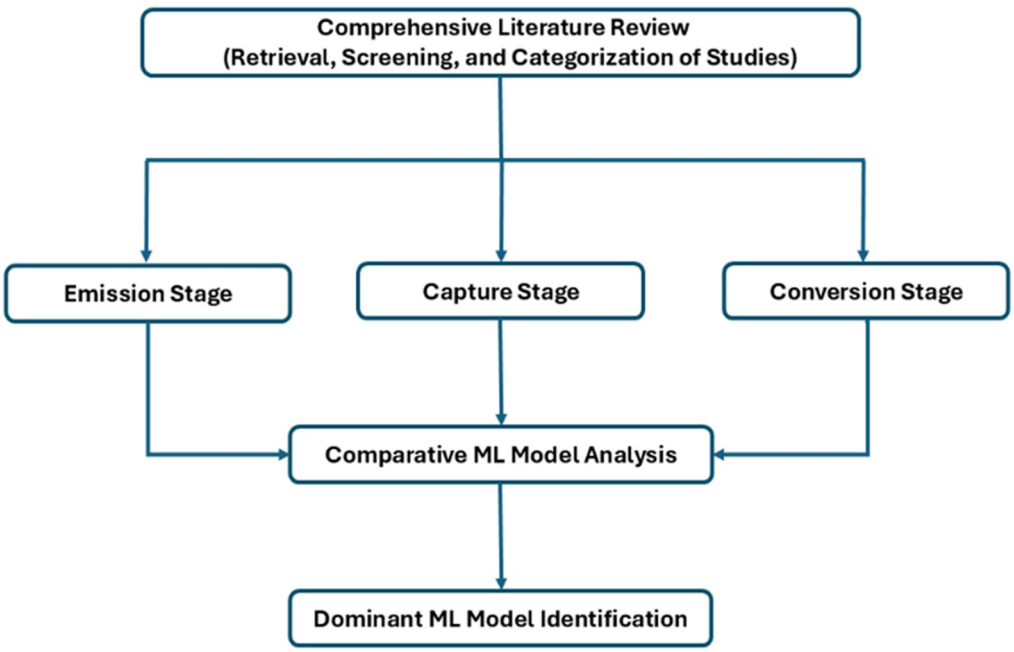


FIGURE 4 | Workflow diagram illustrating the methodology.

used, preprocessing steps such as normalization, dimensionality reduction, and feature selection are essential to improve accuracy, interpretability, and generalizability of the results.

4.1 | CO_2 Emission

Climate change, primarily driven by GHG emissions such as CO_2, poses significant environmental and health challenges, causing direct health issues such as breathlessness and indirect issues such as acid rain and global warming, with intensified flooding and landslides highlighting the urgent need for change [2, 46]. Figure 5 gives the complete breakdown of CO_2 emission sources.

Numerous studies have been conducted on the application of ML in the emissions phase of CO_2 management. Some of the reported literature on CO_2 emissions is reported below.

Ahmadi et al. [31], Ahmadi et al. [32], Baareh et al. [33], Komeili et al. [34], Ghalandari et al. [35], Jalaee et al. [36], Sheta et al. [37], and Rezaei et al. [38] examined the impact of consumption of oil, coal, natural gas, renewable energy, and GDP on the emissions of CO_2. Ahmadi et al. [31] applied the GMDH-ANN method to predict CO_2 emissions in Iran, Kuwait, Saudi Arabia, Qatar, and the UAE, achieving an R^2 value of 0.9988 and an AAE of 2.3%. Ahmadi et al. [32] found that the GMDH-ANN model outperformed linear correlation in forecasting carbon emissions for several Central Asian countries with an R^2 of 0.9999 and an AARD of 0.61%. Baareh et al. [33] used a BP-trained ANN model for CO_2 emissions prediction, achieving MD of 125.61, ED of 606.65, and MMRE of 0.016. Komeili et al. [34] used ANNs with NRBF and Tansig transfer functions to forecast CO_2 levels in Southeast Asia, with NRBF achieving an R^2 of 0.9997 and an MSE of 5.77. Ghalandari et al. [35] found that the ANN-MLP model trained with the LM algorithm outperformed the GMDH model for studying CO_2 emissions in Italy, the UK, Germany, and France with an R^2 of 0.9999 and AARD of 0.33%. Jalaee et al. [36] introduced a hybrid model of COANN, which achieved an R^2 of 0.9990 and RMSE of 0.0194, thus indicating accurate and strong estimation of global CO_2 emissions when British Petroleum Company Plc and BP Amoco Plc data were used. Neural Network Auto-Regressive with eXogenous Input model (NNARX) and Evolutionary Product Unit Neural Network (EPUNN) ANN models were designed by S. Sheta et al. [37] to predict CO_2 emissions globally using global energy consumption, and the EPUNN model has an RMS of 100.95, VAF of 99.33, ED of 267.10, and MAE of 79.17. Rezaei et al. [38] have used a GMDH-ANN model to predict CO_2 emissions in Norway, Sweden, Denmark, and Finland with an R^2 of 0.998 and an ARE of less than 1%, indicating good predictive power. Appiah et al. [39] developed a model of ANN through the Levenberg Marquardt algorithm to forecast the emissions by the BRICS countries, including knowledge about their energy usage and the economic framework, and obtained the values of $R = 0.99976$ and MSE = 0.0003345. Acheampong et al. [40] used a BP-trained ANN to predict the intensity of carbon emissions in Australia, Brazil, China, India, and the U. S., with the results showing the value of the R^2 of 0.80, 0.91, 0.95, 0.99, and 0.87, respectively. Li et al. [41] used the IPSO-BP model to forecast the carbon emissions of cement-industry in China between 2016 and 2050, which outperformed a traditional BP neural network with the following $R^2 = 0.99947$ and MSE = 0.0292. Chen et al. [42] found that GRNN was better than MNLR and MLR in predicting CO_2 emissions of freshwater reservoirs with an RMSE of 418.48, an MAE of 295.34, an R^2 of 0.61, and an NSE of 0.60. Khajavi et al. [43] used a hybrid model that is a combination of RF, Support Vector Regression (SVR), and RSM to model the association between road transport and CO^2 emission in 30 large cities in China and achieved an R^2 of 0.9641, an RMSE of 2374, and a MAE of 1169.597. Mutascu et al. [44] used an ANN trained on LM to predict U.S. CO_2 emissions and found that the ANN gave an R^2 of 0.9248 and RMSE of 0.070275, which was better than the simulations made by the VAR. Sajid et al. [45] looked into the carbon emissions in China and the sources of these emissions. The authors found that linear regression was more effective than ANN with an R^2 of 0.9999 and an MSE of 0.0020. Table 2 is a comparative summary of the literature where machine-learning and AI methods were used to predict CO_2 emission, including the input variables, the modeling methods, and the accuracy.

4.2 | CO_2 Capture

Carbon capture and storage (CCS) is a strategy that shows encouraging outcomes in addressing global warming and

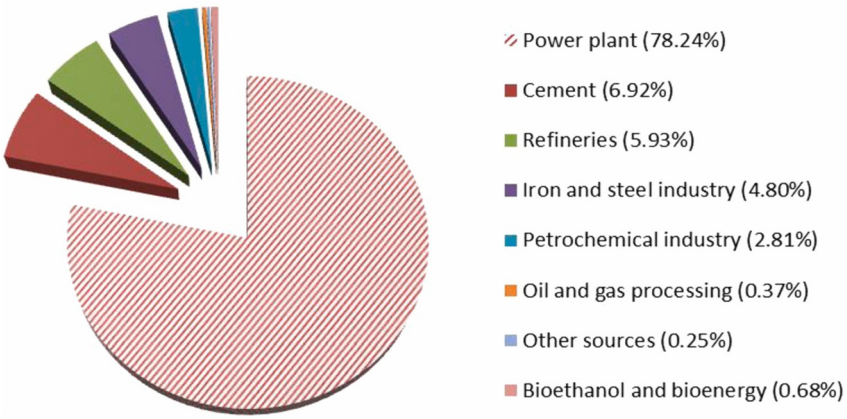


FIGURE 5 | Breakdown of the dominant CO_2 emission sources (Reprinted from Song et al., (2019) with permission from Elsevier. *Source:* IEA (Open Access/CC BY 4.0) [2, 47].

TABLE 2 | Summary of published data on AI and ML models for CO_2 emission prediction.

Authors (first author et al.)	Emission location	Input variable	Output variable	ML/AI methods	Best model performance
Ahmadi et al. [31]	Five Middle Eastern countries (Iran, Kuwait, Qatar, Saudi Arabia, and the UAE)	Consumption of oil, natural gas, coal, GDP of the countries, and renewable energy (mtoe)	CO_2 emissions	GMDH-ANN	**GMDH-ANN:** $R^2 = 0.9988$, Average absolute error = 2.3%
Ahmadi et al. [32]	Turkmenistan, Uzbekistan, Kazakhstan, and Azerbaijan.	Consumption of oil, consumption of natural gas, consumption of coal, GDP, and consumption of renewable energy	CO_2 emissions	Linear correlation, GMDH-ANN	**GMDH-ANN:** $R^2 = 0.9999$, AARD = 0.61%
Baareh et al. [33]	N/A	Global oil, natural gas, coal, and primary energy consumption	CO_2 emissions	ANN	**ANN:** MD = 125.6063, ED = 606.6500, MMRE = 0.0160
Komeili Birjandi et al. [34]	Southeast Asia. Malaysia, Indonesia, Singapore, Vietnam.	Oil, natural gas, coal, GDP, renewable (including hydro power)	CO_2 emissions	MLP-ANN	**MLP-ANN (NRBF):** $R^2 = 0.9997$, MSE = 5.77
Ghalandari et al. [35]	Germany, UK, France, Italy.	Consumption of oil, consumption of natural gas, consumption of coal, GDP, consumption of renewable energy, and nuclear energy consumption	CO_2 emissions	GMDH-ANN, ANN-MLP	**ANN MLP:** $R^2 = 0.9999$, AARD = 0.33%
Jalaee et al. [36]	World's carbon dioxide emission	Consumption of global oil, consumption of natural gas, consumption of coal, and primary energy	CO_2 emissions	COANN	**COANN:** $R^2 = 0.9990$, RMSE = 0.0194
Sheta et al. [37]	Global carbon dioxide emission	Consumption of global oil, consumption of natural gas, consumption of coal, and primary energy	CO_2 emissions	MLP (NNARX), EPUNN	**EPUNN:** RMS = 100.95, VAF = 99.330%, ED = 267.10, MAE = 79.17
Rezaei et al. [38]	Four Nordic countries (Norway, Finland, Sweden, and Denmark)	Oil, natural gas, coal, and the consumption of renewable energy	CO_2 emissions	GMDH-ANN	**GMDH-ANN**: $R^2 = 0.998$, ARE (%) < 1
Appiah et al. [39]	World development indicators. FAOSTAT.	Livestock production, trade exports, trade imports, crop production, economic growth, consumption of renewable energy, and consumption of nonrenewable energy	CO_2 emissions	LM-ANN	**LM-ANN:** $R = 0.99976$, MSE = 0.0003345

(Continues)

TABLE 2 | (Continued)

Authors (first author et al.)	Emission location	Input variable	Output variable	ML/AI methods	Best model performance
Acheampong et al. [40]	Australia, Brazil, China, India, USA.	Technology (R&D), financial development, and consumption of energy, economic growth, industrialization, Urbanization, foreign direct investment, trade openness, population	CO_2 emission intensity	ANN	**ANN:** **For Australia:** R^2 = 0.80110, MSE = 0.01020 **For Brazil:** R^2 = 0.91390, MSE = 0.00420 **For China:** R^2 = 0.95210, MSE = 0.00330 **For India:** R^2 = 0.99440, MSE = 0.00042 **For the USA:** R^2 = 0.87210, MSE = 0.00530
Li et al. [41]	China's cement industry	Production of cement, consumption of heat, coal consumption, and China's cement industry power consumption	Forecasting the peak situation in China's cement industry's carbon emissions	BP-NN, IPSO-BP	**IPSO-BP:** R^2 = 0.99947, MSE = 0.0292
Chen et al. [42]	Freshwater reservoirs	Latitude, mean depth, potential net primary productivity, and age	CO_2 flux emissions	MLR, MNLR, BPNN, GRNN	**GRNN:** R^2 = 0.61, RMSE = 418.48, MAE = 295.34, NSE = 0.60
Khajavi et al. [43]	Road transport induced CO_2 emissions in China	Fixed capital stocks in transport, storage, and post, energy consumption of inland transport, possession of registered civil vehicles, employment in transport, urban units-traffic-storage-and post, the density of highways, railways in operation and inland waterways, electricity consumption in the transport sector, value-added of the transport sector-storage-and post, total passenger and freight turnover of highways-railways-and waterways	Emissions of CO_2 from the combustion of fossil fuels in inland transport vehicles	RF, SVR, RSM.	**RF-SMA:** R^2 = 0.9641, RMSE = 2374

(Continues)

TABLE 2 | (Continued)

Authors (first author et al.)	Emission location	Input variable	Output variable	ML/AI methods	Best model performance
Mutascu et al. [44]	CO_2 emissions in the USA	Consumption of solar energy, consumption of wood energy, consumption of wind energy, net trade, consumption of waste energy, and consumption of biofuel. GDP, consumption of geothermal energy, total biomass energy consumption, and hydroelectric power consumption	CO_2 emissions of natural gas, CO_2 emissions of aviation gasoline, CO_2 emissions of distillate fuel oil, hydrocarbon gas liquids and CO_2 emissions, total emissions CO_2, CO_2 emissions of jet fuel, CO_2 emissions of kerosene, lubricants, CO_2 emissions, motor gasoline, excluding ethanol CO_2 emissions, petroleum coke CO_2 emissions, coal CO_2 emissions. CO_2 emissions of residual fuel oil, other petroleum products, CO_2 emissions, petroleum, excluding biofuels, CO_2 emissions	ANN	**ANN:** $R^2 = 0.9248$, RMSE = 0.070275
Sajid et al. [45]	Chinese carbon emissions	GDP, agglomeration, urbanization, savings, renewable, intensity, energy, fossils, population, FDI	Chinese carbon emissions (referred to as PBA)	Linear regression, ANN	**Linear regression:** $R^2 = 0.9999$, MSE = 0.0020

climate change. CCS is widely recognized as a crucial technology for decreasing atmospheric CO_2 emissions from power plants and other major industrial sites. These emissions are a primary source of GHGs that contribute significantly to global climate change [48, 49].

There exist two primary categories of CO_2 capture methods: post-combustion, focused on directly extracting CO_2 from flue gas streams, and pre-combustion, aimed at advancing low carbon-intensive combustion systems such as integrated gasification combined cycle (IGCC) and oxyfuel combustion. Oxyfuel combustion involves the utilization of pure oxygen to diminish the carbon footprint in power generation [50]. CO_2 capture technology has different pathways. Within the past few decades, industry and academia have explored multiple capture routes, which are illustrated in Figure 6.

Various studies on the application of ML in the capture stage of CO_2 management have been documented. The following literature specifically focuses on CO_2-capturing solvents. Zhou et al. [51], Sipocz et al. [52], Khalilzadeh et al. [53], Mirarab et al. [54], Chan et al. [55], and Fu et al. [56] studied amine-based CO_2 capture. Zhou et al. [51] studied the amine-based post-combustion CO_2 capture method using ANN-SA and Adaptive Neuro-Fuzzy Inference System (ANFIS) models, identifying key parameters affecting CO_2 production and process efficiency, with ANFIS outperforming ANN-SA by achieving higher prediction accuracy of 95.0% for Reboiler Heat Duty, 96.0% for CO_2 Production Rate, 92.3% for Lean Loading, and 95.8% for CO_2 Absorption Efficiency. Sipocz et al. [52] trained an ANN using Amine-based simulator CO2SIM absorption plant data to capture and model the non-linear relationship between CO_2 capture process parameters. The ANN achieved a high prediction accuracy with average errors of 0.02% for CO_2 capture, 0.06% for rich load, and 0.20% for reboiler duty. Khalilzadeh et al. [53] developed an ANN to model CO_2 loading capacities in amino acid salt solutions with amine additives across a broad range of temperatures and pressures, showing high predictive performance with R^2 = 0.9951, ARD = 4.04%, MSE = 0.0053, and MBE = −0.00003768 across diverse conditions and types of salt. Mirarab et al. [54] forecasted CO_2 solubility in the ionic liquid propyl amine methyl imidazole alanine [pamim][Ala] using an ANN and found the MLP network outperformed the RBF network with R^2 = 0.999, SD = 0.002, R = 1.00, and MSE = 0.00000753. Chan et al. [55] applied a piecewise linear ANN (PWL-ANN) alongside an ANN to analyze key process parameters in a carbon capture system using amine-based solvents. Although both models performed well, ANN achieved higher prediction accuracy for all outputs: CO_2 Production Rate with R^2 = 0.9366 and MSE = 0.00122, Reboiler Heat Duty with R^2 = 0.8400 and MSE = 31800000, Lean Loading with R^2 = 0.7593 and MSE = 0.00319, and CO_2 Absorption Efficiency with R^2 = 0.9269 and MSE = 0.00214. Fu et al. [56] developed a BPNN to predict CO_2 capture efficiency using monoethanolamine (MEA) in a large-scale coal-fired power plant. The model demonstrated strong predictive performance, with R^2 values of 0.97722, 0.99801, and 0.98258 for output variables such as MEA circulation, CO_2 capture, and steam consumption, respectively.

MOFs, known for their large surface areas and high porosities, interact with nonpolar linear CO_2 through coordinative bonds at unsaturated metal sites [57]. This interaction results in the adsorption of CO_2 on the MOF surface. Deng et al. [58] used 4 ML algorithms (BPNN, DT, RF, SVM) trained with LM to investigate direct CO_2 capture, with RF achieving the best prediction results with an R-value of 0.981. DESs with reline as an absorbent are effective for CO_2 separation due to their high solubility, negligible losses, and high-purity CO_2 product due to poor N_2 and O_2

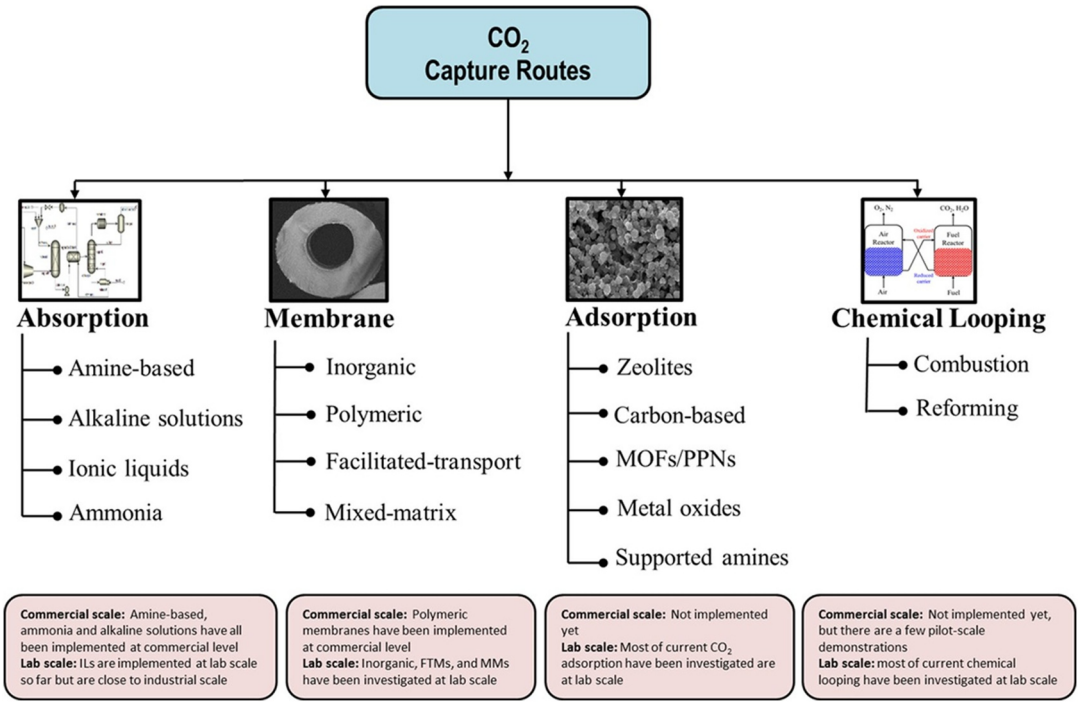


FIGURE 6 | Various carbon-capture technologies and the corresponding materials currently under investigation (Reprinted from Al-Mamoori et al., (2017) with permission from Wiley) [49].

solubility [59]. Sun et al. [60] used ANN to study a PCC process achieving R^2 values of 0.9996, 0.9987, and 0.9903 for total energy consumption, CO_2 purity, and CO_2 recovery rate, respectively. MPDL-based solvents show promise for the PCC process. Blending MPDL-based solvents with reactive amines such as MEA, AMP, and PZ enhances CO_2 absorption kinetics [61]. Nimmanterdwong et al. [62] used an ANN to forecast transport characteristics of MPDL-based solvents (MPDL, MPDL-MEA, MPDL-AMP, MPDL-PZ) for CO_2 absorption, utilizing learning algorithms LM, BR, and SCG in models with varying hidden neurons. The BR-ANN model with 6 hidden neurons performed exceptionally well, achieving an R^2 of 0.99996 and an MSE of 0.0000346. NaOH captures CO_2 efficiently through fast carbonation reactions, converting NaOH to sodium carbonate (Na_2CO_3) or sodium bicarbonate ($NaHCO_3$). Higher NaOH amounts increase the CO_2 removal rate [63]. Naeem et al. [63] used an MLPNN trained with the LM and BR algorithm to predict the CO_2 concentration's C_{out}/C_{in} ratio in a fluidized bed reactor for CO_2 capture, achieving an R^2 of 0.9838, AARD (%) of 1.9217, and an MSE of 0.000735. Kianpour et al. [64] explored CO_2 extraction using dry NaOH sorbent with an ANN model trained by the LM to optimize capture process parameters, achieving high prediction accuracy of ARE = 0.1144, and MSE = 0.0081, and then validated these results through supplementary experiments. Chemical adsorption allows carbon molecular sieves (CMS) to effectively capture CO_2 at ambient temperatures through carbonation reactions, and adjusting CMS amounts and pressure enhances CO_2 removal. Ghaemi et al. [65] used RSM and ANNs to study CO_2 absorption and reduction, comparing MLP, RBF, and RSM models with correlation coefficients of 0.99784, 0.9497, and 0.8958, respectively. MLP closely matches experimental and give a mean squared error of 6.246 × 10^−4 and an R^2 of 0.99784. Supercritical carbon dioxide can be trapped and sequestered in saline aquifers by solubility trapping, through which the brine is injected with supercritical CO_2 to fix the gas in long-term storage and help in mitigating climate change. Menad et al. [66] investigated CO_2 solubility in saline aquifers using two neural network models (Radial Basis Function Neural Network (RBFNN) and MLP) optimized with GA, PSO, ABC, and LM algorithms, with RBFNN-ABC achieving an impressive R^2 of 0.9896 and RMSE of 0.0572 in predicting CO_2 solubility in brine. Ionic liquids (ILs) demonstrate excellent CO_2 capture potential due to low volatility, high solubility, and thermal stability, with temperature and pressure manipulation optimizing solubility. Baghban et al. [67] evaluated the prediction abilities of models such as LSSVM, ANFIS, MLP-ANN, and RBF-ANN for determining CO_2 solubility in various ionic liquids, with the LSSVM model showing excellent predictive accuracy (R^2 = 0.9942, MRE = 15.40%, MSE = 0.000352, RMSE = 0.01887, STD = 0.246451). Activated carbon's porous structure and extensive surface area allow for effective CO_2 absorption through physical interactions and bonding, with its high CO_2 storage capacity increasing with pressure and decreasing with temperature. Rostami et al. [68] developed an MLFNN to predict CO_2 adsorption on activated carbon, achieving R^2 = 0.999947, ARD (%) = 0.871243, AARD (%) = 2.871263, and RMSE = 0.001411. Jadoon et al. [69] developed an AI framework for monitoring SCU and a cryogenic unit in the cement manufacturing facility, generating 550 data samples using MATLAB, Excel, and Aspen Plus models by adjusting process conditions. The ensemble models showed high correlation coefficients of 0.9888 for CO_2, 0.9663 for SO_2, and 0.9970 for NO estimation, indicating the model's accuracy in predicting process composition. Table 3 outlines various ML and AI models used in CO_2 capture studies, detailing key input parameters, techniques applied, and reported performance.

4.3 | CO_2 Conversion

The conversion of CO_2 into fuels and chemicals presents a promising strategy for managing atmospheric concentration and recycling GHGs. However, the industrial implementation of this approach faces limitations due to the insufficient selectivity and activity of existing catalysts. To overcome this challenge, ML applications and theoretical modeling are employed to reveal chemical reaction mechanisms and devise new catalysts for efficient CO_2 conversion. This approach successfully circumvents repetitive and time-consuming trial-and-error experimental processes, making it a robust and effective methodology [70, 71]. Figure 7 represents various pathways for CO_2 utilization.

Several studies on ML applications in the conversion stage of CO_2 management have been reported. Some of the literature that is categorized on the basis of products produced is reported below.

i. Methanol Production:

Khademi et al. [72] used an ANN to investigate a conventional model with two jacketed reactors connected in series for methanol. The ANN gives good predictions for Conventional Methanol Production with Reactor Outlet: MSE = 0.0042, AARD = 0.0035, and Unit outlet: MSE = 0.0042, AARD = 0.0040, and Modified Methanol Production with Reactor outlet: MSE = 0.009, AARD = 0.0024, and Unit outlet: MSE = 0.008, AARD = 0.0024. Chuquin-Vasco et al. [73] used an ANN with $Cu/ZnO/Al_2O_3$ catalyst to predict methanol flux, finding the LM-trained ANN had the best performance with an RMSE of 0.0085 and an R of 0.9442.

Vanjari et al. [74] conducted a comparative analysis of different ML models to investigate the direct catalytic CO_2 hydrogenation process for methanol production. The GBRT and ANN models demonstrated superior performance compared with other ML models, achieving R^2 = 0.95, RMSE = 6.06, and R^2 = 0.95, RMSE = 6.05 for methanol selectivity, and R^2 = 0.95, RMSE = 2.06 and R^2 = 0.94, RMSE = 2.29 for CO_2 conversion, respectively.

ii. Synthesis Gas (Syngas) Production:

Istadi et al. [75] combined an ANN with GA to model the Catalytic-dielectric barrier discharge process for syngas production through methane and CO_2 conversion. The ANN-GA gives good prediction for all process parameters with CH_4 conversion: R^2 = 0.997 and $\%E$ = 8.29, C_2^+ selectivity: R^2 = 0.998 and $\%E$ = 20.39, H_2 selectivity: R^2 = 0.991 and $\%E$ = 14.86, C_2^+ yield: R^2 = 0.997 and $\%E$ = 21.59 and H_2/CO ratio: R^2 = 1 and $\%E$ = 12.53. Hossain et al. [76] used ANN models to simulate hydrogen-rich syngas production via methane dry reforming over $Ni/CaFe_2O_4$ catalysts in a stainless steel reactor with a

TABLE 3 | Summary of published data on AI/ML approaches for CO_2 capture prediction.

Authors (first Author. et al.)	Capture location	Catalyst/ absorbent/ adsorbent	Input variable	Output variable	ML/AI methods	Best model performance
Zhou et al. [51]	Post-combustion CO_2 capture process	Amine-based	Pressure of inlet steam of reboiler, concentration of amine, efficiency of absorption, flue gas CO_2 concentration into absorber, circulation rate of amine solvent, flow rate of outlet steam of reboiler	CO_2 absorption efficiency, reboiler heat duty, production rate of CO_2, lean loading	ANN-SA, ANFIS	**Accuracy from ANFIS:** CO_2 absorption efficiency = 95.8%, reboiler heat duty = 95.0%, CO_2 production rate = 96.0%, lean loading = 92.3%
Sipocz et al. [52]	N/A	Amine based	Temperature Inlet flue gas, mass flow, Inlet flue gas, mass frac, CO_2 Inlet flue gas, removal efficiency, solvent lean load, solvent circulation rate.	Rich load, mass flow CO_2 captured, specific reboiler duty	ANN	**ANN:** **Rich load:** Average error = 0.06% **Mass flow of CO_2 captured:** Average error = 0.02% **Specific reboiler duty:** Average error = 0.20%
Khalilzadeh et al. [53]	N/A	Amino acid salt solutions	CO_2 partial pressure, apparent molecular weight, Solute's mass concentration, solution density, temperature	Solubility (loading capacity of CO_2 in amino acid salt solutions)	ANN	**ANN:** R^2 = 0.9951, MSE = 0.0053, MBE = 0.00003768, ARD (%) = 4.0396
Mirarab et al. [54]	N/A	Propyl amine methyl imidazole alanine ionic liquid	Ionic liquid content, water content, pressure, and temperature.	CO_2 capture rate	BPMLP, RBF, ANN	**BPMLP:** R^2 = 0.999, R = 1.00, MSE = 0.00000753, SD = 0.002

(Continues)

TABLE 3 | (Continued)

Authors (first Author. et al.)	Capture location	Catalyst/ absorbent/ adsorbent	Input variable	Output variable	ML/AI methods	Best model performance
Chan et al. [55]	Datasets of the CO_2 capture plant taken from clean energy technology research institute. (CETRI)	Amine based	Mass flow of CO_2 in the flue gas, steam flows through reboiler, amine concentration, CO_2 concentration in the flue gas, pressure of steam through reboiler, flow rate of off-gas, pressure of reboiler, and circulation rate of amine.	CO_2 absorption efficiency, production rate of CO_2, heat duty of reboiler, lean loading	ANN PWL-ANN	**ANN:** **CO_2 absorption efficiency:** $R^2 = 0.9269$, MSE = 0.00214 **CO_2 production rate:** $R^2 = 0.9366$, MSE = 0.00122 **Reboiler heat duty:** $R^2 = 0.8400$, MSE = 31800000 **Lean loading:** $R^2 = 0.7593$, MSE = 0.00319
Fu et al. [56]	Eastern China's coal-fired power plant expansion project.	Monoethanolamine (MEA) aqueous	Flow of total flue gas, liquid-gas ratio, circulation amount of MEA, heat required for the regeneration per unit of MEA (Q/L), steam consumption in the regeneration tower, lean liquid average molecular weight (m_{lean})	CO_2 capture amount, gas and liquid temperature	BPNN	**BPNN:** **MEA circulation in CO_2 capture:** $R^2 = 0.97722$, MSRE = 0.001945 **Total flue gas flow in CO_2 capture:** $R^2 = 0.99801$ **Steam consumption in CO_2 capture:** $R^2 = 0.98258$, MSRE = 0.001987
Deng et al. [58]	CO_2 captured from the air	MOF	Pore-limiting diameter (PLD), volumetric surface area (VSA), largest cavity diameter (LCD), heat of adsorption, porosity, density	Adsorption selectivity	RF, BPNN, DT, SVM	**RF:** $R = 0.981$

(Continues)

TABLE 3 | (Continued)

Authors (first Author. et al.)	Capture location	Catalyst/ absorbent/ adsorbent	Input variable	Output variable	ML/AI methods	Best model performance
Sun et al. [60]	Post-combustion CO_2 capture (PCC) process	Deep eutectic solvents (DES), reline	Flow ratio (CO_2/absorbent mole amount), desorption pressure, absorption pressure	Total energy consumption, CO_2 purity, CO_2 recovery rate	ANN	**ANN: Total energy consumption:** $R^2 = 0.9996$ **CO_2 purity:** $R^2 = 0.9987$ **CO_2 recovery rate:** $R^2 = 0.9903$
Nimmanterdwong et al. [62]	Post-combustion carbon capture	N-methyl-4-piperidinol -based solvents	MPDL mole fraction, MEA mole fraction, AMP mole fraction, PZ mole fraction, temperature	Density of CO_2, viscosity of CO_2, physical CO_2 diffusivity	ANN	**BR-ANN:** $R^2 = 0.99996$, MSE = 0.0000346
Naeem et al. [63]	Fluidized bed reactor	Sodium hydroxide solid sorbent	Time, CO_2 volume percentage, temperature, air flow rate	C_{out}/C_{in}	ANN	**ANN:** $R^2 = 0.9838$, MSE = 0.000735, AARD (%) = 1.9217
Kianpour et al. [64]	Atmosphere	Dry NaOH sorbents	Air humidity, NaOH loading, temperature	CO_2 removal rate	ANN	**ANN:** MSE (%) = 0.0081, ARE (%) = 0.1144
Ghaemi et al. [65]	N/A	Carbon molecular sieves	Temperature, pressure, time	Adsorption % of CO_2, adsorption capacity of CO_2	MLP (ANN), RBF, RSM	**MLP(ANN):** $R^2 = 0.99784$, MSE = 0.0006246
Menad et al. [66]	Atmosphere	Saline aquifers	Pressure, temperature, and molality of NaCl	CO_2 solubility	MLP-LM, RBFNN-GA, RBFNN-PSO, RBFNN-ABC	**RBFNN-ABC:** $R^2 = 0.9896$, RMSE = 0.0572
Baghban et al. [67]	N/A	Ionic liquids	Critical temperature (T_c), critical pressure (P_c), pressure (P), operational temperature (T), Acentric factor (ω)	CO_2 mole fraction	LSSVM, MLP-ANN, ANFIS, RBF-ANN	**LSSVM:** $R^2 = 0.9942$, RMSE = 0.01887, MSE = 0.000352, MRE (%) = 15.40, STD = 0.246451
Rostami et al. [68]	N/A	Activated carbon	CO_2 partial pressure, CO_2 temperature	CO_2 adsorption density	MLFNN	**MLFNN:** $R^2 = 0.999947$, RMSE = 0.001411, ARD (%) = 0.871243, AARD (%) = 2.871263

(Continues)

TABLE 3 | (Continued)

Authors (first Author. et al.)	Capture location	Catalyst/ absorbent/ adsorbent	Input variable	Output variable	ML/AI methods	Best model performance
Jadoon et al. [69]	Cement plant	N/A	Temperature of flue gas, flow rate of flue gas, pressure of flue gas. S6-IN flowrate, S6-IN temperature, S6-IN pressure, S9-IN flowrate, S9-IN temperature, S9-IN pressure, Tank-1 temperature, Tank-2 temperature	Mass fractions of CO_2, mass fractions of SO_2, mass fractions of NO	Least squares boosting (LSBoost) ensemble	**LSBoost ensemble:** **Mass fractions of CO_2:** $R^2 = 0.9888$, RMSE = 0.0065 **Mass fractions of SO_2:** $R^2 = 0.9978$, RMSE = 0.0000995 **Mass fractions of NO:** $R^2 = 0.9970$, RMSE = 0.00000103

continuous-flow fixed-bed. Results reveal that the ANN-RBF model was outperformed by the ANN-MLP model with R^2 values of 0.9726, 0.8597, 0.9638, and 0.9394 for H_2 yield, CO yield, CH_4 conversion, and CO_2 conversion, respectively. Ayodele et al. [77] studied methane dry reforming in a fixed-bed reactor with a cobalt catalyst, using an ANN trained with forward propagation to predict CH_4 and CO_2 conversions, and H2 and CO generation rates, achieving predictions with R^2 of 1. Ayodele et al. [78] used MLP and NARX neural network models to assess Ni-catalyst reforming of CO_2 and CH_4, with BR-NARX excelling at MSE of 3.24×10^{-9} and R^2 of 0.998 for thermocatalytic conversion predictions.

iii. C_2 and C_2^+ Hydrocarbon Production:

Ayodele et al. [79] used an RBF-ANN model to forecast thermocatalytic CO_2 oxidative coupling of methane to C_2 hydrocarbons, with excellent results: R^2 of 0.990, SSE of 0.224, and predicted selectivity and yield of C_2 hydrocarbons with R^2 values of 0.989 and 0.998, respectively. Istadi et al. [75] employed a hybrid ANN-GA model to study catalytic-dielectric barrier discharge for C_2^+ hydrocarbon formation from CO_2 and methane. The model provided good predictions with CH_4 conversion: $R^2 = 0.997$ and $\%E = 8.29$, C_2^+ selectivity: $R^2 = 0.998$ and $\%E = 20.39$, H_2 selectivity: $R^2 = 0.991$ and $\%E = 14.86$, C_2^+ yield: $R = 0.997$ and $\%E = 21.59$ and H_2/CO ratio: $R^2 = 1$ and $\%E = 12.53$. Istadi et al. [80] developed a hybrid ANN-GA model to study the effect of process parameters on the noncatalytic dielectric barrier discharge (DBD) method for the production of C_2^+ hydrocarbons from CO_2 and CH_4. The model gives good predictions with MSE = 0.0034 and $R = 0.9938, 0.9955, 0.9877, 0.9978$ for CH_4 conversion, C_2^+ selectivity, H_2 selectivity, and C_2^+ yield, respectively.

iv. Biomass Productivity:

Hossain et al. [81] compare BRT, ANN, and SVR models for boosting biomass productivity with air and CO_2, finding SVR outperforms others with $R^2 = 0.779$, MAE = 0.013 for biomass, and $R^2 = 0.911$, MAE = 0.0128 for CO_2 fixation (RCO_2). Kushwaha et al. [82] introduced a novel hybrid prediction model combining ANFIS and GA for forecasting microalgae CO_2 fixation, outperforming ANFIS with RMSE, R^2, and AARD values of 0.00056, 0.98457, and 0.032156, respectively.

v. Lower Olefins (LO) Production

Chandana et al. [83] developed an ML framework using ANN models (BR and LM algorithms) to forecast catalyst activity in the hydrogenation of CO_2 into lighter olefins, where ANN-BR outperformed other ML models in prediction and closely matched experimental data with R values of 0.90 and 0.8, RMSE values of 8.43 and 16.73, and AAD values of 5.8 and 9.5 for test data, respectively.

vi. Methane Production

Wiheeb et al. [84] developed an ANN to study CO_2 conversion in a falling film reactor. This study shows that the ANN model gives a very close estimation of CO_2 conversion. The average error predicted by the ANN was 0.6%, which is within the

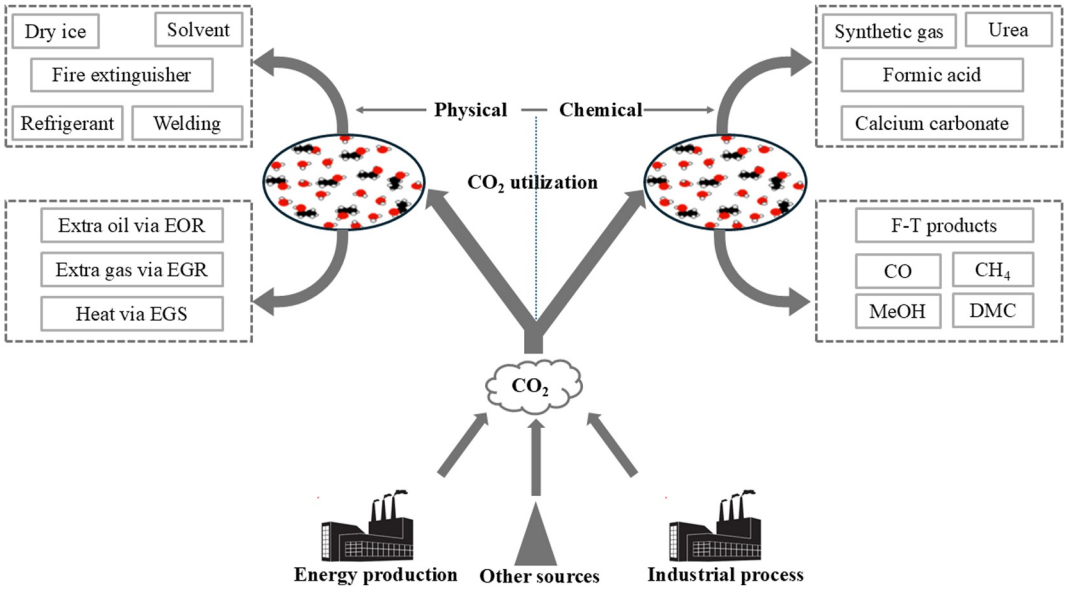


FIGURE 7 | Various pathways for CO_2 utilization (Adapted from Rafiee et al., (2018) with permission from Elsevier) [71].

acceptable level. Alsaffar et al. [85] studied the impact of process parameters on hydrogen production via catalytic methane dry reforming, constructing 10 different ANN models varying hidden neurons from 1 to 10, and found the optimal performance in the model with a 4-9-2 topology, having R^2 of 0.960 and 0.947 for CH_4 conversion and hydrogen yield, respectively.

Table 4 presents a selection of ML/AI-based approaches applied in CO_2 conversion studies, highlighting input features, algorithm types, and predictive performance.

4.4 | Summary of Applications of ML Techniques in CO_2 Management Stages

ML techniques play a crucial role in all three CO_2 management stages: emission, capture, and conversion.

In the CO_2 emission stage, researchers rely on ML models to accurately estimate CO_2 emissions, considering factors such as energy resource consumption, fuel usage, GDP, population, and sector-specific characteristics. In this stage, models such as ANN, MLR, and MNLR are commonly applied due to their ability to handle complex, nonlinear relationships. ML-based estimations provide critical insights into emissions trends across regions and industries, enabling more informed decisions by policymakers and environmental agencies. These models help assess the impact of economic and industrial variables on the global carbon footprint, contributing to effective climate action strategies.

In the CO_2 capture stage, ML plays a vital role in estimating capture efficiencies in both post-combustion and direct air capture systems by modeling complex interactions among catalysts, process variables, and rheological properties. Commonly used ML models in this stage include ANN, BPNN, GRNN, and GMDH, which are effective in handling nonlinear relationships and multivariable dependencies. Rheological properties such as viscosity, density, and flow behavior index are critical, as they influence mass transfer rates, pressure drop, and solvent regeneration efficiency. These properties are typically measured using rheometers and viscometers and are integrated as high-impact input features in ML models. Their importance is often assessed by using feature selection techniques such as correlation analysis or recursive feature elimination. Incorporating such features significantly improves predictive accuracy and allows for more realistic simulation of capture processes. By leveraging ML, the goal is to reduce greenhouse gas emissions and enable cost-effective, scalable, and sustainable CO_2 capture solutions.

During the CO_2 conversion stage, ML is used to predict and optimize the transformation of CO_2 into value-added products such as methanol, syngas, methane, lower olefins (LO), biofuels, and C_2/C_2+ hydrocarbons. Widely used models include ANN, MLP, and optimization techniques such as GA and PSO, which help identify ideal catalysts, feedstock combinations, and operating conditions. ML methods support the development of sustainable and economically feasible CO_2 utilization routes while minimizing emissions. In this context, optimizing CO_2 conversion pathways offers both environmental and economic advantages. Environmentally, converting CO_2 into useful fuels and chemicals reduces reliance on fossil-based resources and supports carbon neutrality goals. Economically, it creates opportunities to generate revenue from captured CO_2, improving the overall feasibility of carbon utilization strategies. ML contributes to this potential by enhancing reaction efficiency, identifying effective catalysts, and reducing energy demands, helping to lower operational costs while maximizing output performance.

Overall, ML enables more data-driven and scalable CO_2 management by aligning prediction accuracy with the specific needs of each stage. This includes enhancing emission forecasting with hybrid LSTM models (long short-term memory networks designed to learn from sequential time-based data) [86], improving capture system modeling through deep learning and

TABLE 4 | Summary of published data on AI/ML approaches for CO_2 conversion.

Authors	Conversion method	Reactant	Product	Catalyst/absorbent	Input variable	Output variable	ML/AI methods	Best model performance
Khademi et al. [72]	Conventional model with two jacketed reactors connected in series	Methane, hydrogen, water.	Methanol.	Cu/Al_2O_3 and Zn/Al_2O_3	Pressure, temperature	Reactor outlet, unit outlet	ANN	Conventional methanol production: Reactor outlet: MSE = 0.0042, AARD = 0.0035 Unit outlet: MSE = 0.0042, AARD = 0.0040 Modified methanol production: Reactor outlet: MSE = 0.009, AARD = 0.0024 Unit outlet: MSE = 0.008, AARD = 0.0024
Chuquin Vasco et al. [73]	CO_2 hydrogenation	CO_2, hydrogen.	Methanol	$Cu/ZnO/Al_2O_3$	Reactor temperature, reactor pressure, mass flow of hydrogen, mass flow of CO_2	Flow of methanol	ANN	ANN-LM: R = 0.9442, RMSE = 0.0085

(Continues)

TABLE 4 | (Continued)

Authors	Conversion method	Reactant	Product	Catalyst/absorbent	Input variable	Output variable	ML/AI methods	Best model performance
Vanjari et al. [74]	Direct catalytic CO_2 hydrogenation	CO_2, hydrogen.	Methanol	Different catalysts with different compositions, their preparation conditions, and operating conditions mentioned in the input variable	Support type, calcination temperature (^oC), reaction pressure (atm), active metal 1 composition (wt%), H_2/CO_2 mole ratio, promoters 2 composition (wt%), calcination time(h), active metal 1, reaction temperature, metal: Support, promoter 3, preparation method, promoter 2, GHSV (h^{-1}), promoters 3 composition (wt%), promoters 1 composition (wt%), promoters 1, active metal 2, active metal 2 composition (%)	Catalyst activity (CO_2 conversion & methanol selectivity)	MLP LASSO RIDGE SVR GP GBRT RT ANN-LM ANN-BR	GBRT: CO_2 conversion: $R^2 = 0.95$, RMSE = 2.06 Methanol selectivity: $R^2 = 0.95$, RMSE = 6.06 ANN-BR: CO_2 conversion: $R^2 = 0.94$, RMSE = 2.29 Methanol selectivity: $R^2 = 0.9$, RMSE = 6.05
Istadi et al. [75]	Catalytic-dielectric barrier discharge	CO_2, methane	Synthesis gas, C_2^+ hydrocarbons	12.8CaO–6.4 MnO/CeO_2	Reactor wall temperature, effects of CH_4/CO_2 feed ratio, discharge voltage, total feed flow rate	C_2^+ yield, H_2/CO ratio, conversion of CH_4, selectivity of C_2^+, selectivity of H_2	ANN	**C_2^+ yield:** $R^2 = 0.997$, $\%E = 21.59$ H_2/CO ratio $R^2 = 1$, $\%E = 12.53$ **CH_4 conversion:** $R^2 = 0.997$, $\%E = 8.29$ **C_2^+ selectivity:** $R^2 = 0.998$, $\%E = 20.39$ **H^2 selectivity:** $R^2 = 0.991$, $\%E = 14.86$

(Continues)

TABLE 4 | (Continued)

Authors	Conversion method	Reactant	Product	Catalyst/absorbent	Input variable	Output variable	ML/AI methods	Best model performance
Hossain et al. [76]	Methane dry reforming	CO2, methane.	Syngas production	$Ni/CaFe_2O_4$	Reaction temperature, catalyst metal loadings, feed ratio	CO_2 conversion, CH_4 conversion, yield of H_2, yield of CO	ANN	**ANN-MLP:** **CO_2 conversion:** $R^2 = 0.9394$, $R = 0.9692$ **CH_4 conversion:** $R^2 = 0.9638$, $R = 0.9818$ **H_2 yield**: $R^2 = 0.9726$, $R = 0.9862$ **CO yield:** $R^2 = 0.8597$, $R = 0.9272$
Ayodele et al. [77]	Methane dry reforming	CO_2, methane.	Syngas production	Cobalt catalyst	Partial pressure of CO_2, partial pressure of CH_4, CH_4/CO_2 ratio, reaction temperature	Rate of production of H_2, rate of production of CO, conversion of CO_2, conversion of CH_4	ANN	**ANN: Conversion of CH_4**: $R^2 = 1.00$, MAPE = 3.18, MPE = 1.54, MAE = 1.76 **Conversion of CO_2**: $R^2 = 1.00$, MAPE = 3.46, MPE = 1.88, MAE = 2.46 **Syngas ratio:** $R^2 = 1.00$, MAPE = 9.66, MPE = 4.18, MAE = 0.08
Ayodele et al. [78]	GHGs reforming	CO_2, methane.	Synthesis gas	Ni based	Calcination temperature (°C), reduction temperature (°C), Ni loading (wt%), reaction temperature, time on stream(h)	Conversion of CH_4 (%), conversion of CO_2 (%)	MLP, NARX	**BR-NARX:** $R^2 = 0.998$, MSE = 0.00000000324

(Continues)

TABLE 4 | (Continued)

Authors	Conversion method	Reactant	Product	Catalyst/absorbent	Input variable	Output variable	ML/AI methods	Best model performance
Ayodele et al. [79]	Thermo-catalytic CO_2 oxidative	CO_2, methane.	C_2 hydrocarbons	CaO-MnO/CeO_2	Amount of MnO in catalyst (%), amount of CaO in catalyst (%), reaction temperature, CO_2/CH_4 ratio	C_2 hydrocarbons selectivity, C_2 hydrocarbons yield.	RBF-ANN	**RBF-ANN:** $R^2 = 0.990$, SSE = 0.224 **C_2 hydrocarbons selectivity:** $R^2 = 0.989$ **C_2 hydrocarbons yield:** $R^2 = 0.998$
Istadi et al. [80]	Noncatalytic dielectric barrier discharge	CO_2, methane.	C_2^+ hydrocarbons	N/A	Feed ratio of CH_4/CO_2, discharge voltage, and flow rate of total feed	C_2^+ yield, H_2 selectivity, CH_4 conversion, C_2^+ selectivity	ANN	**ANN:** MSE = 0.0034 **C_2^+ yield:** $R = 0.9978$ **H_2 selectivity:** $R = 0.9877$ **CH_4 conversion:** $R = 0.9938$ **C_2^+ selectivity:** $R = 0.9955$
Hossain et al. [81]	Bio fixation	Air, CO_2.	Biomass productivity (BP), CO_2 bio fixation (R_{CO2}).	N/A	Light-dark cycles, temperature, nitrogen-phosphorus ratios	Biomass productivity (BP), CO_2 bio fixation (R_{CO2})	BRT, ANN, SVR	**SVR:** **BP:** $R^2 = 0.779$, RMSE = 0.0296, MAE = 0.0136, FB = 0.0061, MARE = 1.2587 **R_{CO2}:** $R^2 = 0.911$, RMSE = 0.0189, MAE = 0.0128, FB = 0.0088, MARE = 0.4131

(Continues)

TABLE 4 | (Continued)

Authors	Conversion method	Reactant	Product	Catalyst/absorbent	Input variable	Output variable	ML/AI methods	Best model performance
Kushwaha et al. [82]	Carbon dioxide fixation by microalgae	CO_2, microalgae.	Biofuels etc	N/A	Temperature, pH. CO_2%, amount of *N* (mg/L), amount of *P* (mg/L)	CO_2 fixation rate	ANFIS, GA-ANFIS	GA-ANFIS: $R^2 = 0.98457$, RMSE = 0.00056, AARD = 0.032156
Chandana et al. [83]	Direct hydrogenation of CO_2 to lighter olefins over promoter-added multi-functional catalysts.	CO_2, hydrogen.	Lower olefins (LO)	Different catalysts with different compositions and their preparation and operating conditions are mentioned in the input variable.	Calcination temperature (^oC), calcination time (h), H_2/CO_2 mole ratio, reaction temperature (^oC), reaction pressure (in atm), gas hourly space velocity (GHSV) ($MLg^{-1}h^{-1}$), promoter 1, promoter 1 composition (wt%), promoter 2, promoter 2 composition (wt%), active metal 1, active metal 1 composition (wt%), active metal 2, active metal 2 composition (wt%), active metal 3, active metal 3 composition (wt%), support type, preparation method	Catalyst activity (i.e. CO_2 conversion (%) & LO selectivity (%)) as output parameter	ANN-BR, ANN LM, MLR RR, SVR GPR, PFRT GBRT	ANN-BR: **CO_2 conversion (%):** $R = 0.90$, RMSE = 8.43, AAD = 5.8 LO selectivity (%): $R = 0.8$, RMSE = 16.73, AAD = 9.5
Wiheeb et al. [84]	N/A	N/A	N/A	N/A	Liquor monoethanolamine (QMEA) volumetric flow rate, temperature (T) of liquid, molar concentration of monoethanolamine (CMEA), mole fraction of CO_2 in gaseous mixture (Y)	CO_2 conversion (%)	ANN	ANN: Average error = 0.6%

(Continues)

TABLE 4 | (Continued)

Authors	Conversion method	Reactant	Product	Catalyst/absorbent	Input variable	Output variable	ML/AI methods	Best model performance
Alsaffar et al. [85]	Catalytic methane reforming	N/A	N/A	N/A	Oxygen (O_2) concentration in the feed, GHSV, reaction temperature, CH_4/CO_2 ratio	CH_4 conversion, hydrogen yield	ANN	ANN: SSE = 0.076 CH_4 conversion: R^2 = 0.960 Hydrogen yield: R^2 = 0.947

process monitoring [87], and optimizing conversion conditions using catalyst design frameworks [88]. Selecting appropriate models based on task complexity and data availability remains essential to improving overall system efficiency.

A comparative assessment indicates that ANN models often outperform traditional approaches such as MLR and MNLR, particularly in highly nonlinear scenarios. Additionally, optimization techniques such as GA and PSO can improve model accuracy by refining hyperparameters (adjustable parameters, such as learning rate, number of neurons, or training duration, that determine how the model learns and generalizes from data) and identifying optimal process settings, especially during CO_2 conversion. To balance model accuracy and interpretability, future research could implement strategies such as combining transparent models (e.g., DTs) with complex models (e.g., deep neural networks) using model stacking or applying surrogate models to approximate and explain deep learning behavior. Interpretable frameworks can also be integrated to provide insight into high-performing predictions, supporting a practical trade-off between performance, explainability, and computational cost.

5 | Challenges, Future Prospects, and Recommendations

CO_2 management presents key challenges such as accurately estimating emissions, developing efficient capture technologies, and improving catalyst selectivity for better conversion. These are compounded by data limitations, existing process constraints, and the need for economic feasibility.

ML techniques face limitations such as bias and interpretability issues. These limitations can significantly affect the deployment of ML models across the CO_2 management cycle. For example, biases in training data, such as limited regional or sector coverage, can reduce model generalizability and lead to inaccurate predictions of CO_2 emissions, capture efficiency, or conversion performance. These issues often arise in underrepresented settings like small industrial plants, developing regions, or nonstandard reactor systems. Although ANNs have shown strong predictive performance, they also present certain limitations. These include their "black box" nature, which makes them difficult to interpret, as well as the risk of overfitting when trained on small or noisy datasets. Additionally, ANNs often require large amounts of data and computational resources to perform effectively, which may not always be feasible in industrial CO_2 management scenarios. These factors must be carefully considered when selecting models for practical deployment.

In the capture and conversion stages, where safety, efficiency, and regulation are critical, the inability to explain model outputs can reduce stakeholder trust and hinder operational adoption. This is especially important in industrial CO_2 systems, where decision-making must be transparent and verifiable. To address data limitations, future efforts should focus on generating more diverse, high-resolution datasets through experimental trials, sensor-based monitoring, and industry collaborations. Data

augmentation techniques and synthetic data generation can help expand limited datasets, whereas federated learning frameworks may enable knowledge sharing across facilities without compromising data privacy. These strategies can collectively improve model robustness, fairness, and real-world adaptability.

To mitigate these challenges, several strategies can be implemented. Addressing data bias involves diversifying training datasets across regions, feedstocks, and process conditions, as well as employing bias-reducing ML techniques and resampling techniques. For interpretability, simpler and more transparent models, such as DT or linear models, can be used where appropriate. In cases where more complex models are necessary, these can be supported with step-by-step logic or visual explanations to help users understand the decision process. Additionally, combining domain knowledge with data-driven models, such as integrating expert-guided rules or physics-based modeling, can enhance both model accuracy and transparency. These approaches improve reliability and make ML tools more suitable for real-world CO_2 applications.

Despite these advances, real-world validation introduces further obstacles. These include limited access to computational infrastructure in industrial environments, unstable or varying process conditions that affect model robustness, and inconsistent or non-standardized datasets across facilities, which hinder generalization and benchmarking. High computational costs and memory demands may limit the feasibility of deploying deep learning models in industrial settings, particularly where resources are constrained or real-time processing is required. Scalability also becomes a challenge when models trained on synthetic or lab-scale data are applied to full-scale operations characterized by dynamic and noisy environments, as performance may not transfer well due to differences in system size, operating conditions, and data variability. Additionally, the limited availability of high-quality operational datasets can hinder robust training, benchmarking, and adaptation of ML solutions. Addressing these challenges will require streamlined model architectures, cross-platform testing, and broader access to representative CO_2 datasets.

Beyond technical and validation barriers, a broader implementation must also consider economic, policy, and social factors. High implementation costs may limit adoption in smaller or resource-constrained industries, whereas regulatory uncertainty and social factors such as limited technical training, resistance to automation, and concerns about data privacy can reduce stakeholder engagement and delay the deployment of AI-driven solutions. This calls for collaboration between data scientists, engineers, policymakers, and social scientists to ensure solutions are both effective and practical.

Extensive integration of ML techniques will be essential for effective CO_2 management, as demonstrated by recent advancements including hybrid ML-physical models that enhance the accuracy of CO_2 sequestration predictions [89, 90], reinforcement learning approaches that significantly reduce energy consumption in amine-based capture systems [91], and physics-informed neural networks that improve the simulation of storage and injection processes in geological reservoirs [92]. In the emission stage, advanced ML models such as boosting and bagging will improve emission predictions using diverse data sources. Real-time monitoring and AI-based agents will enhance emission reduction efforts. In the capture stage, automated discovery of new capture materials will benefit from reinforcement learning and generative approaches. ML can also enhance our understanding of molecular interactions, leading to better solvents and capture methods. In the conversion stage, meta-learning and hybrid ML-simulation models will optimize reactor conditions, enhancing CO_2 conversion. Recommendations include further research into ML models for more precise emission estimation, optimizing CO_2 capture systems, and improving knowledge of catalytic conversion mechanisms for sustainable CO_2 utilization.

6 | Conclusion and Recommendations

The present review highlights the central role of ML in the further progress of the intelligent systems development of CO_2 management, including emission prediction, capturing carbon, and transforming it into value-added products. Replacing empirical, trial-and-error methods with data-driven modeling (empirically testing emission forecasting models, tuning process parameters in capture systems, or screening catalysts and reaction conditions in conversion processes without computational guidance) can lead to a new paradigm in the performance and decision-making process at all levels of the carbon management lifecycle with inputs of ML. The most widely used models of all three stages of CO_2 management have been neural networks due to their ability to model nonlinear relationships, high-dimensional data, and learn intricate input-output relationships with very little human intervention. Their versatility and predictive power can be highlighted by the fact that they have always performed well in the field of emission forecasting, solvent and process optimization, and catalyst screening. Moreover, optimization algorithms such as GA and PSO have also been used to augment model effectiveness by hyperparameter fine-tuning and accuracy improvement. Although the implementation of ML in CO_2 management is promising, there are still several critical challenges. These are a lack of quality data, challenges in using complex models, and a lack of solutions that can be scaled to real-life applications. To overcome these challenges, hybrid models that use ML and domain-specific physical simulations, the development of transparent architectures, and the availability of standardized and high-quality datasets to be validated will be needed. The novelty of this review is that it combines cross-stage analysis of ML applications in CO_2 management, including emissions, capture, and conversion, with a comparative assessment of model performance of different techniques. In contrast to the previous literature, which is limited to a single stage or a particular model, this review provides a cohesive viewpoint that connects the algorithm selection and the input-output dynamics with the relevance to the domain. The future research should focus on real-time learning systems, explainable AI (referring to techniques that make the internal logic and decision-making of AI models understandable to human users), and reinforcement learning-based methods to expedite the identification of new materials and optimization of the process settings. Additionally, successful AI implementation in the management of CO_2 requires proactive cooperation

between AI scientists, engineers, and industry experts to guarantee the feasible implementation and mass use. With the further development of intelligent systems, their application in CO_2 management opens an interesting opportunity to promote sustainable industrialization, reduce greenhouse gas emissions, and significantly contribute to the global climate goals.

Nomenclature

%E	percentage error
AARD	average absolute relative deviations
ABC	artificial bee colony
AI	artificial intelligence
ANFIS	adaptive neuro-fuzzy inference system
ANN	artificial neural networks
ARE	absolute relative error
BPNN	backpropagation neural networks
BR	Bayesian regularization
BRT	boosted regression trees
CCC	carbon capture and conversion
CNN	convolutional neural networks
DT	decision tree
ED	euclidean distance
EPUNN	evolutionary product unit neural network
GA	genetic algorithm
GBRT	gradient boosted regression trees
GHGs	greenhouse gases
GMDH	group method of data handling
GRNN	generalized regression neural networks
IPCC	Intergovernmental Panel on Climate Change
kNN	k-nearest neighbors
LightGBM	light gradient boosting machine
LM	Levenberg-Marquardt
LSBoost	least squares boosting
MAE	Mean absolute error
MAPE	mean absolute percentage error
MD	Manhattan distance
ML	machine learning
MLFNN	multi-layer feed-forward neural network
MLP	multi-layer perceptron
MMRE	mean magnitude of relative error
MPE	mean percentage error
MSE	mean squared error
MSRE	mean squared relative error
NNARX	neural network auto-regressive with exogenous input model
NRBF	normalized radial basis function
NSE	Nash–Sutcliffe efficiency
PCA	principal component analysis
PSO	particle swarm optimization
PWL-ANN	Piecewise LInear ANN
R^2	coefficient of determination
R	Pearson correlation
RBFNN	Radial Basis Function Neural Network
RF	Random Forest
RMSE	root mean squared error
SCG	scaled conjugate gradient
SSE	sum of squared errors
STD	standard deviation
SVM	support vector machine
SVR	support vector regression

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Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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