

Review article

A systematic review of machine learning approaches in carbon capture applications



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ABSTRACT

Climate change and global warming are among of the most important environmental issues and require adequate and immediate global action to preserve the planet for future generations. One of the essential technologies used to reduce CO₂ emissions and mitigate the worst effects of climate change is carbon capture technology. Many efforts have been made by scientists, industrial sectors, and policy-makers in looking for new technology to reduce greenhouse gas emissions and achieve net-zero emission goals. Research and development in creating new technology involve complex processes and require a digital system to optimize big data prediction as well as to reduce production time. A mathematical and statistical approach such as machine learning plays an important role in solving research problems, whereby this approach provides fast results in predicting big data and cost-efficient tools. In this study, a systematic review and bibliometric analysis were used to analyze the research trend, particularly on the keywords, number of publications, citations, countries, and authorship. This information is important for future research directions for researchers who venture into this area. In this study, the bibliometric analysis focuses on 2 main categories: co-authorship (countries and organizations) and keywords (author keyword). Based on the research trend, the United States (USA), China, Iran, Canada, and the United Kingdom are the leading countries contributing to this field since they have the highest publications and citations. Furthermore, the most common keywords used in the selected articles ranked according to the highest link strength. The top 6 keyword list includes machine learning, artificial neural network, CO₂ capture, CO₂ solubility, metal-organic frameworks (MOFs) and carbon capture and storage. The findings from this study can be used to open a wider spectrum for the research communities by providing global research trends, current innovations and current technology on machine learning in carbon capture application, identifying the active research areas or hot topics and future research direction to help fight climate change issue using smart advanced technology.

1. Introduction

The Fourth Industrial Revolution, also called Industrial Revolution 4.0 (IR 4.0) is an era of intelligent technology that focuses on the use of digital and automated tools in the manufacturing and production industries [1]. The evolution of technology toward more automated

processes can enhance efficiency, productivity, quality of products or systems, and reduce operation costs [2]. IR 4.0 involves digital transformation, such as the Internet of Things, artificial intelligence (AI), machine learning, deep learning, and blockchain, all of which have a great impact on the manufacturing industry [3,4]. Currently, the smart industry is moving from Industry 4.0 to Industry 5.0 [5]. Industry 5.0 is

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related to the interaction between humans and smart machines technology. An integration between Industry 4.0 and Industry 5.0 can help industry improve employee productivity, reduce production costs, and increase product quality [3,4]. Industry 5.0 will help to create highly skilled workers or labor and produce high-quality products based on research and innovation, thus, increasing customer satisfaction [5]. The evolution of Industry 5.0 is designed to focus on collaboration (integration) between human experts and smart technology (automation process). This could also enhance the skill of professional workers with digital transformation processes [5]. Generally, Research and Development (R&D) activities in industry involve complex projects and are time-consuming when introducing new products and services. The conventional method of using trial and error methods and extensive laboratory testing to predict and optimize the processes is inefficient. Therefore, digital systems are needed to optimize big data predictions help in creating new product development, and reduce production time.

Machine learning is a computational intelligence application that use data analysis involving mathematical, statistical, and software or computational methods to predict outcomes [6]. Machine learning is generally considered a subfield of AI that plays an important role in examining the big data [7]. It focuses on the use of data (as input) and various algorithms to gives computers the ability to find patterns in data (particularly big data) to use for future predictions and quality checks on optimization. Algorithms are used to make a prediction based on some input data. Error functions in the machine learning models are used to evaluate the model's prediction and accuracy [7,8]. Machine learning algorithms can be categorized into four groups such as supervised machine learning, unsupervised machine learning, semi-supervised learning and reinforcement machine learning [8,9]. A details explanation of different types of machine learning algorithms, advantages and disadvantages have been reported by Liu et al. [7] and Sarker [8].

The fundamentals of machine learning are to develop algorithms from input data and use statistical analysis to foresee an output value within an appropriate range [10]. It not only can improve the identification of trends but also understand data from multi-variety and multi-dimensionless mediums and make decisions with the least individual intervention [11]. Mathematical and statistical approaches, such as machine learning play an important role in solving research problems [12]. Machine learning can be used to predict parameters from big data, optimize and data clustering. Machine learning models are able to predict output (such as catalyst materials) using big datasets and can help to minimize prediction errors [13]. For example, the statistical models are able to find the optimal conditions (such as predicting a target property or parameter) without the need for comprehensive experimental exploration of the operating conditions. Thus, this technique can help optimize costs and improve performance [8].

Machine learning is used to design a cost-effective process, and it is easily scalable, which suitable to be used in various industrial fields [14]. For instance, some industries still rely on conventional visual inspection methods to detect defects using manual inspection by human operators. Conventional methods cannot examines deeper defects and are time-consuming. Transforming from manual visual inspection to an automated system using machine learning is beneficial to shorten production time and increase productivity. The automated system has several advantages as it saves time, cost, and energy as well as yields higher performance than traditional inspection systems [15].

The word "smart" is an acronym for "Self-Monitoring Analysis and Reporting Technology" and is used as a monitoring system for computer hardware [16]. Nowadays, the word "smart" is becoming popular and being used to describe digital technology that saves energy, and time, reduces costs, and protects the environment [17]. The use of smart technologies creates incredible opportunities in many applications that benefit productivity and energy-saving, especially in the manufacturing and production industries. The concepts of smart digital technology such as AI and machine learning are becoming a trend among researchers and are widely used in all aspects, including carbon capture applications. For

instance, Yan et al. [11] have discussed in-depth the potential of machine learning applications for carbon capture, utilization, and storage technologies. They reported that machine learning is a powerful tool for optimizing and predicting outcomes and give high prediction accuracy. Machine learning can be used to predict carbon dioxide (CO₂) solubilities in various solvents and CO₂ adsorption capacities in adsorbent materials. Meanwhile, a comprehensive overview of the basics of machine learning related to advanced energy materials was reported by Liu et al. [7] by showing the prominence of machine learning in the carbon capture sector. Mazari et al. [12] used various machine learning models to predict the physical and thermodynamic properties of ionic liquids in carbon capture applications. Vo et al. [18] developed efficient integrated process model for hydrogen recovery and CO₂ capture from hydrogen plants. They combined dynamic-model-based artificial neural network (ANN) for an integrated process. They compared the cost performance and the prediction error of the ANN prediction with experimental results. The results revealed that the predicted results by ANN are close to the experimental results with high prediction accuracy. In other words, the ANN models fit very well with experimental results. The ANN model provided smaller prediction errors (less than 2% error) compared to experimental results and was subsequently used to minimize the production cost of the CO₂ capture process. Recently, Oh et al. [19] developed a statistical model using a deep neural network (type of machine learning) to predict the CO₂ solubility of amine in a power plant. Machine learning indicated high predictive accuracy and a cost-effective method [19]. Added to the small success probabilities, high operation cost, and time-consuming nature of the conventional approaches, machine learning is deemed essential for current CO₂ capture technologies [7]. Besides being used in manufacturing and production, machine learning can also help researchers to predict the process on a small-scale (laboratory scale) and improve the product with less time compared to experimental studies [20].

1.1. Significance of the Study

In carbon capture technology, the application of machine learning has slowly occupied both large-scale (industries) and small-scale (R&D and laboratory-scale) including the deployment of solvent-based post-combustion capture [21], ionic liquids [22], adsorbents [23], and membranes [24–26]. Machine learning has been employed to evaluate the solvents in regards to their physical and chemical properties during the design and selection stage. It is applied to predict CO₂ solubilities in the solvents as well as to simplify the procedure [22,27,28]. The process of simulation, modelling, controlling, and optimizing of the CO₂ capture processes are also accomplished using machine learning [21,29,30]. Moreover, it aids in enhancing the multiphase flowmeters' accuracy in the CO₂ pipelines and monitoring the CO₂ storage process [31,32]. All these innovations come to minimize the time and cost of CO₂ capture operations. Taking into consideration the above potentials, it is critical to understand the current status, development route, and future perspectives of machine learning in CO₂ capture technologies. Based on the observations from the literature, most of the studies use machine learning in the CO₂ absorption process to predict thermodynamic properties. Limited studies have been carried out to systematically predict CO₂ adsorption capacity based on their textural properties (surface area, pore volume), elemental composition properties (carbon, hydrogen, nitrogen and oxygen content) and CO₂ adsorption parameters (temperature, flow rate and pressure). In addition, screening of materials, optimization process and comprehensively validating machine learning models and data in CO₂ capture applications is needed.

There are several review articles published on machine learning in CO₂ capture and storage application. For instance, Yan et al. [11] reviewed the applications of machine learning in CO₂ capture. They discussed the potential of machine learning in pre-combustion (chemical-looping), oxy-fuel combustion, post-combustion (absorption and adsorption), CO₂ transportation, storage and utilization (focuses on

electrochemical reduction). They have also identified areas where more research is needed such as pre-combustion process and CO₂ utilization in a large-scale application. Rahimi et al. [20] reviewed machine learning in CO₂ capture, but their work focuses on post-combustion processes, such as the CO₂ absorption and CO₂ adsorption process. They discussed how machine learning tools can help to predict the thermodynamic properties of absorbents (solvents), and predicted a cost-effective process in solid adsorption, particularly for metal-organic frameworks (MOFs). They have outlined future recommendations for implementing machine learning in CO₂ capture especially on membrane process. Gupta and Li [33] reviewed the benefit of a machine learning tool in CO₂ capture, storage, and utilization applications such as post-combustion, pre-combustion and oxy-fuel combustion processes, in real applications. They discussed several studies on machine learning models to predict CO₂ capacity using different types of databases such as hypothetical MOFs and Nano porous materials genome. They have also stated some recommendations for future research to develop a cost-effective method using machine learning. Christiano et al. [34] reviewed CO₂ capture and utilization that focuses on electrochemical conversion, process of injecting CO₂ into existing oil fields using CO₂-enhanced oil recovery, and method for recovering additional oil using supercritical CO₂. They have outlined the importance of life cycle assessment in CO₂ capture and utilization using machine learning.

Many studies have been conducted in the past to predict the CO₂ capture performance using machine learning models. However, no study reported on global research trends, analyze the impact of citation reports, the importance of keywords on a specific topic, or on research collaboration. The citation and keyword analysis help researchers to get a preliminary idea about the current research trend on a specific topic and whether their current research has an impact in a particular field. This detailed information can be determined by bibliometric analysis.

In addition, none of the studies has systematically gathered and reviewed all the publications related to machine learning for CO₂ capture. The researchers are unable to find the most prominent areas, purposes, values (publication trend), and research gaps in machine learning for CO₂ capture. To meet this, the objective of this study is to provide an insight of the current trend, hot topic and technology development indication, which will be beneficial in discovering the viewpoint for the subsequent research directions and future prospects. Henceforth, data extracting analysis based on bibliometric study were performed to discover the research progress and trends in machine learning for CO₂ capture processes, whereby the breakthrough of research gaps on this topic is achieved through a systematic review.

1.2. Practical implications

This study will be helpful for researchers to understand the research trend and enhance their knowledge for their future studies. Furthermore, bibliometric analysis is beneficial to obtain the potential opportunity for research collaboration, for preparing research grant application and to identify current development on machine learning in CO₂ capture. From that, they will get ideas to produce effective research grants. Also, data from the bibliometric analysis can help researchers to identify problems and collaborate with policymakers to develop policy solutions.

2. Overview of bibliometric analysis and systematic review

Bibliometric analysis is the quantitative evaluation of scientific publications through statistical techniques [35]. It provides an understanding of past and present literature by mapping the historical progress and current trends within a particular time [36]. Other than it can envisage the impact of field areas and discovering emerging developments [37]. The analysis can also illustrate the objectives, characteristics and dynamic research areas of the given field [38]. Thus, this offers a bright insight into future research focuses. It is based on a set of

metrics, for instance, co-occurrence, citation, co-citation, and bibliographic coupling. Every metric is evaluated in different forms based on the research indicators, such as the countries, organizations, and authors, in addition to their interrelationships [39]. From the analysis, the recognition of the most active countries, institutions, and authors combined with uncovering the collaboration between those criteria can be achieved [40]. With these merits, the bibliometric has earned immense popularity and many experts have applied this bibliometric analysis method in carbon capture applications. Major growth in publications from 2015 onwards was identified when Wong et al. [41] conducted a bibliometric analysis for CO₂ utilization from 1995 to 2019. Moreover, the research gaps between CO₂ capture and utilization focusing on the planning method were reported by Tapia et al. [42]. Under the same discipline (CO₂ capture and utilization), Wan et al. [43] examined the number of publications between 1999 and 2009 on CO₂ reduction trends by microalgae. Similar research using microalgae for direct air CO₂ capture was then investigated by Maghzian et al. [44] in recent years. The findings from both works presented with an increased number of publications and patents were registered by the companies in terms of commercialization and economization. It indicated a promising outlook for CO₂ capture among scholars, and additional studies are necessary for this field due to research gaps found in multiple areas [44]. Omoregbe et al. [45] evaluated research trend in carbon capture using a bibliometric analysis based on publications from 1998 to 2018. This literature disclosed the ability of bibliometric analysis to find the publications' growth, research trends, and most active areas. This analysis can be completed with computer assistance and mapping software (such as VOSviewer, CiteSpace, CitNetExplorer, BibExcel, and HistCite) [46].

Herein, the visualization of the similarities viewer (VOSviewer) tool is chosen for a bibliometric analysis due to its easy operation and multifunction [47,48]. The analysis can be accomplished by assessing all available articles for over 20 years. The tool can analyze huge quantities of data related to the field and allow greater reviews accompanied by wider scope, informative, and less prejudiced bibliometric maps. As the outcomes of this bibliometric analysis are projected to direct the scientists to discover the most active areas of machine learning for CO₂ capture, the research gaps and focuses on niche areas of this topic can be revealed using a systematic review.

A systematic review is a qualitative technique employed for the informational subject assessment of documented data to identify themes, patterns, and concepts [49]. Unlike bibliometric analysis, which requires at least 200 articles to be reviewed [50], a systematic review employs the traditional techniques that involve a narrow scope of analysis, and therefore, tends to incorporate a smaller quantity of articles for review [51]. For example, only between tens (for example, 50) and low hundreds (for example, 100–300) of articles are implicated in the review. It is commonly conducted more systematically by identifying the research questions at the initial phase [52]. Therefore, by combining the bibliometric analysis and systematic review, this paper can entirely empower interested groups, such as the public and researchers to search the most active areas, current interests, research gaps, and future directions on machine learning for CO₂ capture technologies.

3. Research methodology

3.1. Data collection: databases, keywords, and selection criteria

Fig. 1 shows the framework of the research analysis in this work. This paper is divided into two major sections of analysis namely systematic review and bibliometric analysis with the selected topic of machine learning for CO₂ capture. For the systematic review section, the following research questions were formulated and must be addressed in order to obtain the research gaps and future directions of machine learning for CO₂ capture:

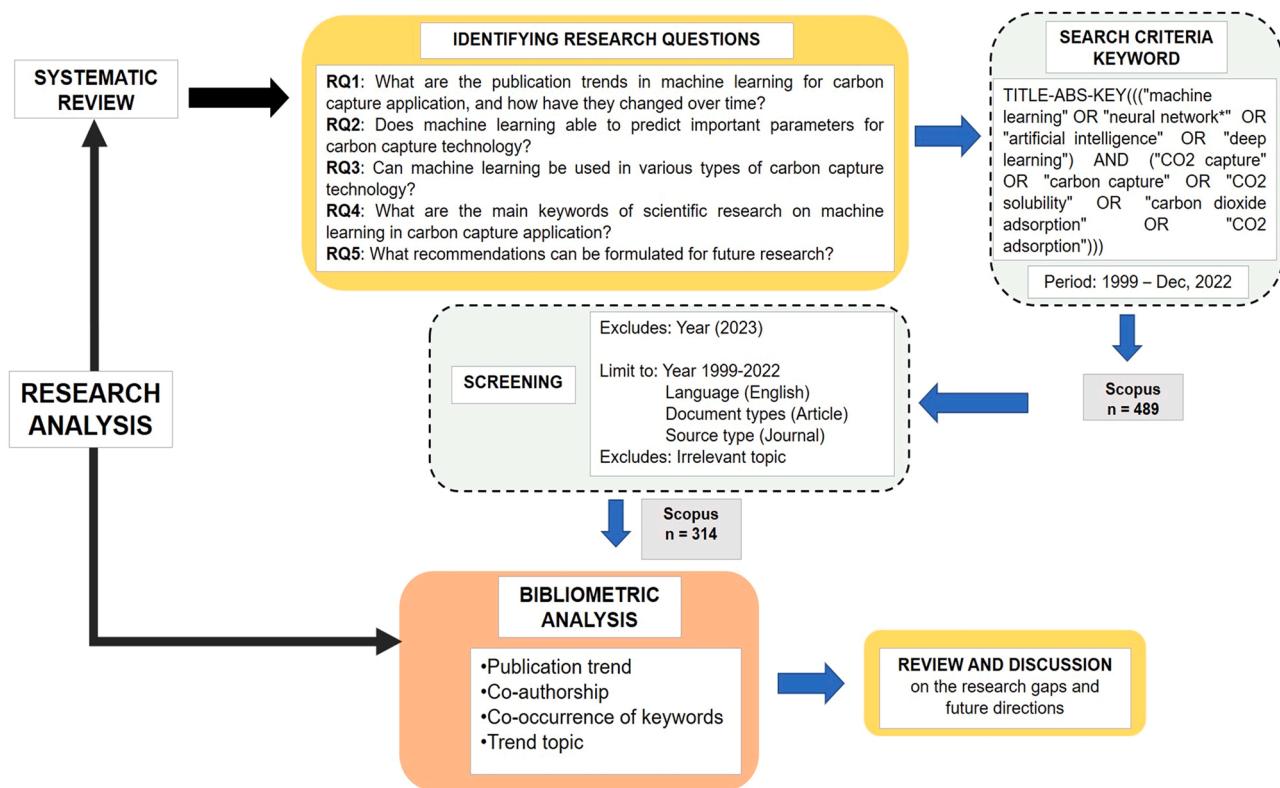


Fig. 1. : Research analysis framework for systematic review and bibliometric analysis on the machine learning for carbon capture applications.

- (i) Research question 1 (RQ1): What are the publication trends in machine learning for carbon capture application, and how have they changed over time?
- (ii) Research question 2 (RQ2): Does machine learning able to predict important parameters for carbon capture technology?
- (iii) Research question 3 (RQ3): Can machine learning be used in various types of carbon capture technology?
- (iv) Research question 4 (RQ4): What are the main keywords of scientific research on machine learning in carbon capture application?
- (v) Research question 5 (RQ5): What recommendations can be formulated for future research?

To answer the proposed research problem or research questions, a combination of the systematic review and bibliometrics were used to analyze the research trends in the field of carbon capture technology (particularly in machine learning applications) (**Table 1**). For RQ1 and RQ3, this study uses search strings to compile articles before analyzing the research trend via VOSviewer software (bibliometric method). For RQ4 and RQ5, the Bibliometrix R-Package using Biblioshiny App (for non-coders) was used to analyze the research trend on a specific topic, mapping publications, citations or authors, predict research trends, and the recommendation of future research directions.

In general, the subsequent main steps for the systematic review included identification, screening, and eligibility [53]. Identification is a procedure to explore any synonym, related terms, and variation for the main keywords of the study [52]. In comparison to the research questions, the search string was articulated with different categories of keywords specifically related to: (i) machine learning tools and (ii) carbon capture technologies to identify suitable documents.

TITLE-ABS-KEY was used in the Scopus database to represent the documents' titles, abstracts, and keywords. This method allows us to discover all publications that are pertinent to our research questions and goals [54]. Several keywords (single and combination keywords) related

Table 1
Summary of research questions and potential solution.

Research Questions	Answer
Research question 1 (RQ1): What are the publication trends in machine learning for carbon capture application, and how have they changed over time?	RQ1: Refer to Fig. 2 on growth of publications from the Scopus database (1999–2022) and Section 4 for detail explanation on the publication trend.
Research question 2 (RQ2): Does machine learning able to predict important parameters for carbon capture technology?	RQ2: To predict properties (such as thermodynamic properties) on carbon capture technology, keyword search strings have been used to search related topic. Then, top 3 most cited articles were compiled and presented in Tables 2 and 4 .
Research question 3 (RQ3): Can machine learning be used in various types of carbon capture technology?	RQ3: Keyword search string has been used to find the suitable article related to machine learning in carbon capture applications. The data has been compiled and presented in Tables 2 and 5 .
Research question 4 (RQ4): What are the main keywords of scientific research on machine learning in carbon capture application?	RQ4: The Bibliometrix R-package using Biblioshiny App (for non-coders) has been used to analyze the research trend on a specific topic.
Research question 5 (RQ5): What recommendations can be formulated for future research?	RQ5: Future recommendations has been outlined. Please refer to Section 4 . Future recommendation).

to machine learning in carbon capture applications have been searched. The results have been compiled in terms of the number of publications and presented in [Table S1](#) (see supporting documents). Based on the list of keywords ([Table S1](#)), the total publication related to machine learning in carbon capture applications were around 300 documents. Therefore, from the outcome of this bibliometric analysis, scientists or researchers can obtain information on the most active areas on machine learning in carbon applications and research gaps (through publication by year and citation report). Here is the example of keywords that was used to

analyze the trend of publication.

The articles were extracted from the Scopus database from 1999 to 2022 with search strings of TITLE-ABS-KEY (((“machine learning” OR “neural network*” OR “artificial intelligence” OR “deep learning”) AND (“CO₂ capture” OR “carbon capture” OR “CO₂ solubility” OR “carbon dioxide adsorption” OR “CO₂ adsorption”))). The synonyms are unified to each group associated with a Boolean “OR” and categories are connected using a Boolean “AND” [55]. It resulted in 489 articles from Scopus database. During the screening phase, the selected documents were only restricted to the English language and journal article. The irrelevant topic and latest publication in 2023 were excluded, and this process refined the publications into 314 documents (Fig. 1). This step was carried out by reading the article’s titles and abstracts, followed by the full text of the article’s assessment. Moreover, the 314 articles taken from the Scopus database is used to make systematic review and bibliometric analysis. The sample size of the articles was sufficient for the bibliometric analysis. The 314 articles were collected and compiled between the year 1999 to December, 2022 (updated until February, 28 2023).

3.2. Data analysis

In this study, two types of bibliometric analyses were conducted, namely performance analysis and science mapping. Performance analysis explores the quantitative data of publications and contributions of researchers (for example, the total of documents (publications) and number of citations in the field) annually [56]. The 314 articles from the Scopus database were compiled in a Microsoft Excel spreadsheet to perform a descriptive analysis of the publication trends per year. Science mapping is a method of measuring the impacts and total link strengths of number of documents, and citations [57]. For example, article’s co-occurrence weight and total strength of the co-authorship links with other researchers. It includes collaboration networks of countries, organizations, and authors that were performed using VOSviewer, according to the 314 articles from Scopus. The findings of bibliometric mapping were improved through the semantic network analysis in which the co-occurrence of keywords analysis was done to map their research clusters in the present scholarly reports. Furthermore, the Bibliometrix R-Package using Biblioshiny App (for non-coders) was used to analyze the research trend through trend topics and a three-field plot

[58]. To analyze and visualize the data on co-occurrence (keywords), VOSviewer (Version 1.6.19) was used [47]. Furthermore, the keywords were cleaned to eliminate similar and duplicate results and grouped the keyword using OpenRefine tool (Version 3.7.1) [59,60]. This tool is useful to group similar keyword together.

4. Results and discussion

4.1. Growth of publications (Research question 1: RQ1-RQ3)

The quest for net-zero CO₂ emission has appeared as an evolving issue for more than 20 years. A total of 314 articles in machine learning for CO₂ capture from the Scopus database were reported between 1999 and 2022. There were also unproductive years of publications in this field, for example, in the years 2000–2007, 2009 and 2012, due to the absence of publications related to machine learning for carbon capture applications. Fig. 2 and Table 2 shows the growth of publications and a summary of research trends from 1999 to 2022. The least quantity of publications (n = 1) was documented in the years 1999, 2008, and 2010 (Fig. 2). The publication trend on this topic is a crucial parameter to know where the interests of the researchers are directed every year. A rapid increase in publications has been reported since 2015. Based on Fig. 2, publication trend on topic machine learning in carbon capture applications have increased drastically from 55 no. of documents (publication) in 2021–94 no. of documents (publication) in 2022. This is evident that this topic has become a hot topic and has many areas to be explored.

The initial paper was published in 1999 after the political events associated with climate change since 1997 (Table 3). From the Kyoto Protocol, the mandatory goals for developed countries were to lessen emissions of CO₂ and other greenhouse gases, including methane (CH₄), nitrous oxide (N₂O), hydrofluorocarbons (HFCs), perfluorocarbons (PFCs), sulphur hexafluoride (SF₆) and nitrogen trifluoride (NF₃). From this strategy, the first article reported on the computational method to remove greenhouse gases such as CO₂ and N₂O was published in 1999 using an artificial neural network tool to predict gas solubility in amine solutions [61]. After 8 years, another paper correlated to the same research area was established. The neural networks and mathematical regression remained the focus on the prediction of CO₂ solubility in the absorbents, specifically in ionic liquids [62]. Its usage as the CO₂

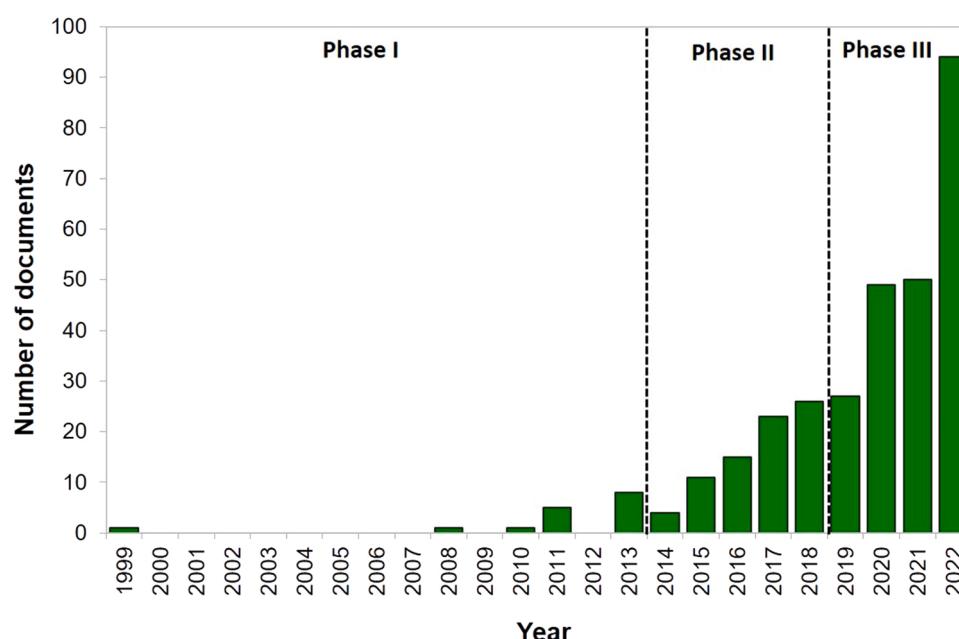


Fig. 2. : Growth of publications from Scopus database.

Table 2

Summary of research trend from 1999 to 2022.

PHASE I (1999-2013)	PHASE II (2014-2018)	PHASE III (2019-2022)
Summary of research trend (topic): CO₂ absorption:	Summary of research trend (topic): CO₂ absorption [67,68]	Summary of research trend (topic): CO₂ absorption:
i) Prediction of thermodynamic properties of amine-based solvent (lab-scale) [64]	i) Thermodynamic properties and equilibrium solubility for CO ₂ absorbents (amine-based solutions).	i) Prediction of thermophysical properties in potassium and sodium-based amino acid salt solutions [71]
ii) Investigation on the relationship of significant parameters with CO ₂ production rate, identification of the leakage rate, batch simulation and prediction of CO ₂ loadings.	ii) Investigation on the effects of parameters towards CO ₂ absorption and multi-optimization	ii) Prediction of thermophysical properties in blended solutions (ionic liquids and amines) [72]
iii) Amine-based post-combustion CO ₂ capture (Pilot scale in Canada) [65]	Summary of research trend (topic): CO₂ adsorption:	iii) Screening different aqueous blends of ionic liquids, amines and ethanol [73]
iv) Oxyfuel combustion (Pilot scale in Germany) [66]	i) Prediction of CO ₂ adsorption on activated carbon [69]	iv) Screening of tertiary amines [74]
	ii) Screening and prediction of equilibrium isotherm characteristics using vacuum swing adsorption [70]	Summary of research trend (topic): CO₂ adsorption:
		i) Prediction of CO ₂ adsorption capacity using metal-organic frameworks (MOFs) as adsorbent [75]
		ii) Prediction of heat capacity of nanoporous materials [76]
		Summary of research trend (topic): membrane
		i) Prediction of MOF-based mixed matrix membranes for CO ₂ capture [77]
		Summary of research trend (topic): CO₂ storage [28,78]
		i) Estimation of carbon capture process
		ii) Prediction and modelling of carbon capture process
		iii) Prediction of CO ₂ storage site integrity

Table 3

Political events from 1997 to 2017 adopted from [79].

Year	Key Events and Policy
1997	COP 3 adopts Kyoto Protocol
2001	The US Government retreat from the Kyoto Protocol
2005	Kyoto Protocol enters into force and EU emission Trading was launched
2006	The Government of China started aiming to cut carbon intensity through its five-year plan
2007	IPCC published the 4th Assessment Report
2009	COP 15 urges to limit global warming to 2 °C above the pre-industrial level
2010	Green Climate Fund was established
2012	COP 18 in Doha extended the Kyoto Protocol and NAMA facility was established
2013	COP 13 in Warsaw proposed the UNFCCC to formulate INDC
2014	IPCC issued the 5th Assessment Report
2015	COP 21 resulted in the Paris Agreement to pursue net-zero GHG emission
2017	The US Government announced the withdrawal from the Paris Agreement

absorbent is intended to conquer amines limitations that include a corrosive nature, demand for high energy for CO₂ regeneration, and additional costs during the operation due to their volatility and thermally degradation over time [63].

The growth of publications from 2010 to 2013 was unstable (inconsistent trend). The maximum publications were observed in 2013 and no publication was reported in 2012. At phase 1, there were lack of studies reported on machine learning in carbon capture applications. At this stage (Phase I), amines still received the greatest attention among scholars for CO₂ absorption [80,81] (Table 3). Moreover, the application of the statistical approach and numerous types of machine learning (such as artificial neural networks (ANN), neuro-fuzzy modelling, and inferential modelling technique) for CO₂ capture has been extended to the pilot plant-scale measurements by 2010 [66,80,82,83]. The researchers concentrated on examining the parameters' impact on CO₂ absorption [83-86], identifying the leakage rate [66], predicting the CO₂ solubility in absorbents and production rate of CO₂ [87-89], monitoring and controlling the CO₂ capture (for example absorption efficiency) [84] and storage (for example corrosion rate) [90], and optimization [64,81] at both small (laboratory-scale) and large-scale applications. Although the publications were only limited to the CO₂ absorption technology in Phase I, the trend began to grow gradually between 2014 and 2018 (Phase II) with a wider research scope. This increment was stimulated by higher CO₂ emissions in Phase II compared to Phase I. As such, increased global industrialization caused the CO₂ discharge among developing countries to rise by 43.2% from 2000 to 2013 [91]. This trend was also constituted after several notable political events, particularly the Paris Agreement in 2015. The Paris Agreement demands restricting global warming to well below 2 °C (ideally to 1.5 °C) compared to the preindustrial levels [92]. It is expected that global releases to summit immediately with a quick drop from 45% of CO₂ concentrations in 2010 by 2030 and fall off rapidly in the following years to accomplish net zero emission by 2050 [92].

As a result, the researchers widened their concerns on machine learning for CO₂ capture with 4–26 articles per year at this level (Phase II). Many studies have focused on ionic liquids to predict of thermodynamic properties, and the equilibrium solubility of CO₂ in a broad range of absorbents. Ionic liquids are regarded as an auspicious alternative agent for CO₂ capture because they possess structure tunability, high thermal stability, and minimal vapor pressure [11]. Amino acids such as potassium lysinate [93,94] and sodium glycinate [95], and inorganic solvents namely trisodium phosphate solutions have also drawn substantial interest in the CO₂ absorption process [96]. During this period, CO₂ adsorption and CO₂ storage areas have emerged with numerous types of adsorbents and CO₂ storage processes. As such, metal organic frameworks (MOFs) [97–99] and zeolites [100,101] adsorbents were predicted for the adsorption of CO₂. For the CO₂ storage system, many experts have published research articles on CO₂ solubility in crude oil plants [102–106] and monitoring the CO₂ corrosion rate in pipelines of CO₂ storage.

The publications sharply increased as of 2019, and 2020 was the first productive year as the number of publications was more than 49 articles in that year. A remarkably growing quantity of documents was observed in the following year. Aside from the achievements in climate change mitigation ratified by the Policy makers, the scientists' interest in machine learning for CO₂ capture technologies might be the impetus for the publication's improvement [20]. Many recent studies have focused on the Fourth Industrial Revolution especially on the use of mathematical and computational methods such as machine learning to predict outcomes or products. Therefore, publications on machine learning for carbon capture technology increased progressively in Phase II and III. From 2019–2022, the machine learning application for CO₂ capture grew from 27 in 2019–94 articles in 2022. During this phase, more publications were made on CO₂ adsorption with new adsorbents such as various types of activated carbons [107] and CO₂ storage technology at a large-scale application. This was seen in the estimation of commercial

scale injection capacity and storage of CO₂ in the Jacksonburg-Stringtown oil field, West Virginia, USA [108]. Another study was reported on carbon capture and storage using integrated workflow in 3D geological model construction for evaluation of CO₂ storage capacity of a fractured basement reservoir in Cuu Long Basin, Vietnam [109]. To summarize, the primary reason for an improvement of publications related to machine learning for CO₂ capture from 1999 to 2022 could be global events, economic growth, rapid population growth, urbanization, and industrialization. These findings confirmed that this topic is suitable to be investigated quantitatively and qualitatively. Every phase and year have different dynamic research patterns, nevertheless, the publications could not be the only indicator to evaluate the overall performance of the research field. Based on the publication trend, top 3 most cited articles were reported on thermodynamic model prediction, modelling and optimization and CO₂ storage (Table 4). Bibliometrics analysis can help researchers to observe hot topics in research, track the past research, and predict future trends.

Citations may be observed as a measure of the usefulness of the topic, impact and influence of a publication. Furthermore, the citations could reveal the quality and originality of the reported articles. The influence of the articles in snatching the researchers' attention showed the importance of the active areas through citations. For instance, the most cited articles from the paper compilation are summarized in Table 5. It

shows that the publication by Fernandez et al. [97] was the most cited document, with 192 citations. The work on the prediction of MOFs structures using machine learning in CO₂ capture applications certainly displayed a strong interest as it was also advocated by Anderson et al. [116]. It utilized five additional machine learning algorithms to predict absolute metrics for all MOFs and had 103 citations in recent years. Besides that, there is a growing interest in ionic liquids and amines until 2018 and 2020. The highest citations for ionic liquids were observed in 2017 with 92 citations [117]. Meanwhile, amines-based absorbents had 66 citations in 2017 [111].

To have a better understanding of the emerging research areas and to learn which areas are most significant in terms of publications and citations that are linked to machine learning for the CO₂ capture topic, the social network and semantic analyses are discussed in detail in the next section. Social network analysis evaluates the collaboration trend and the responsibility of prominent participants (countries, organizations, and authors) in the collaboration networks [120]. It will be valuable to establish future research collaboration and discover the gaps in research works among the experts in particular countries or organizations. Meanwhile, in the semantic analysis, the co-occurrence of keywords expresses how the authors' research interests interconnect and overlap through their research clusters, for example research objectives, methodologies, and limitations. The bibliometric analysis in this study only

Table 4

List of top 3 most cited articles on thermodynamic model prediction, modelling and optimization and CO₂ storage (updated until February, 28 2023).

Objective of study	Total citations	Machine learning algorithm models	Results	Year	References
Post-combustion (Thermodynamic model prediction)					
To predict CO ₂ solubility in ionic liquids. Screening various types of ionic liquids at different temperature and pressure ranges.	77	Artificial neural network (ANN) and support vector machine (SVM). Data points: 10,116	Both models showed good fitting and prediction effects on the CO ₂ solubilities. However, the better fit was achieved for the ANN model. The results show that LSSVM model can predict loading capacity with high accuracy compared to other machine learning models.	2020	Song et al.[110]
To predict CO ₂ loading capacity in various solvents at different temperature, pressure, mass composition of solution, and average molecular weight of solution.	66	Multi-layer Perceptron Artificial Neural Network (MLP-ANN), Radial Basis Function Artificial Neural Network (RBF-ANN), Least Square Support Vector Machine (LSSVM), and Adaptive Network-based Fuzzy Inference System (ANFIS).	The results show that LSSVM model can predict loading capacity with high accuracy compared to other machine learning models.	2017	Baghban et al.[111]
To evaluate the effect of surface functionalization on the CO ₂ performance of graphene oxide-amine nanofluids.	31	Least-squares support vector machines (LSSVM), adaptive neuro-fuzzy inference systems (ANFIS), generalized regression (GR), radial basis function (RBF), cascade feedforward (CFF), and multilayer perceptron (MLP) neural networks	The high prediction is obtained using CFF neural network due to low mean squared and root mean squared errors.	2021	Zhou et al.[112]
Modelling and optimization					
To screen various types of amines using response surface methodology (RSM) and ANN on CO ₂ capture cost. To compare the results of RSM and ANN models.	35	ANN Data points (range): 270–840	The CO ₂ capture cost obtained from RSM algorithm close to those obtained by ANN algorithm.	2013	Nuchitprasittichai et al.[64]
To screen various types of adsorbents using RSM (central composite design) and ANN for CO ₂ capture by VSA	53	ANN model Data points: 74	ANN model can predict high performance of CO ₂ purity (95%) and recovery (90%) on several adsorbents in VSA process	2016	Khurana et al.[70]
To predict of MOF performance in vacuum swing adsorption using genetic algorithm in machine learning	71	Genetic algorithm Data points: 1632	Only 482 MOFs materials achieve high CO ₂ purity (95%) and recovery (90%). Machine learning model has high prediction accuracy up to 91%.	2020	Burns et al.[113]
Carbon capture and storage					
To predict storage efficiency using artificial neural network	68	ANN algorithm model Data points: 1450	The results reveal that ANN model has good predictive ability on storage efficiency with low error (less than 1.2%)	2017	Kim et al.[114]
To predict oil recovery and CO ₂ storage using ANN in the Permian basin (USA).	43	ANN algorithm model	The results reveal that ANN model can predict the oil recovery and CO ₂ storage high accuracy in the real field.	2020	Vo Thanh et al. [115]
To detect anomalies in monitoring well pressure data streams for carbon capture and storage	36	Convolutional neural network (CNN), long short-term memory (LSTM) neural network and combined CNN and LSTM (ConvLSTM)	Results reveal that the ConvLSTM perform better results with high accuracy than other models.	2019	Zhong et al.[116]

Table 5

List of top 10 most cited articles over 20 years (1999–2022) (updated until February, 28 2023).

No	Title	Journal	Year	Citations	Keywords	Key influencing factors	Type of machine learning	Outcome/Remarks	Ref.
1.	Rapid and Accurate Machine Learning Recognition of High Performing Metal Organic Frameworks for CO ₂ Capture	The Journal of Physical Chemistry Letters	2014	192	Quantitative structure property relationship, Machine learning, Metal organic frameworks, Chemical structure, Mathematical methods	To predict high-performing or low-performing of MOF structure	Support vector machines learning (SVM) model.	Using the machine learning models as part of a screening protocol would result in high prediction output.	[97]
2.	Role of Pore Chemistry and Topology in the CO ₂ Capture Capabilities of MOFs: From Molecular Simulation to Machine Learning	Chemistry of materials	2018	103	Functionalization, Metal organic frameworks, Functional groups, Mathematical methods, Selectivity	Pore chemistry and topology on various CO ₂ capture metrics	Six different machine learning algorithms were used such as multiple linear regression (MLR), SVM, conditional inference decision trees (DT), random forests (RF), neural networks (NN), and gradient boosting machines (GBM).	Decision trees were used to predict the adsorbent material (MOFs) properties and compared with other machine learning models.	[116]
3.	Rigorous modelling of CO ₂ equilibrium absorption in ionic liquids	International Journal of Greenhouse Gas Control	2017	92	CO ₂ capture, CO ₂ absorption, Ionic liquids (IL), Solubility, Model, Prediction	CO ₂ solubility in 67 different of ionic liquids	Least Square Support Vector Machine (LSSVM), Adaptive Neuro-Fuzzy Inference System (ANFIS), Multi-Layer Perceptron Artificial Neural Network (MLP-ANN), and Radial Basis Function Artificial Neural Network (RBF-ANN)	The results showed that the LSSVM model was gave high accuracy compared to other models.	[117]
4.	The use of Artificial Neural Network models for CO ₂ capture plants	Applied Energy	2011	85	ANN; Chemical absorption; Levenberg-Marquardt; Scaled Conjugate Gradient	To develop and validate ANN model for CO ₂ capture plant	ANN	The results indicated that the ANN models are very powerful tool for fast simulation of complex research problem with produce a high prediction accuracy.	[80]
5.	Prediction of CO ₂ solubility in ionic liquids using machine learning methods	Chemical Engineering Science	2020	77	CO ₂ solubility, Ionic liquids, Machine learning, Group contribution, Artificial neural network, Support vector machine	CO ₂ solubility in ionic liquids at different temperatures and pressures	ANN and -SVM-	The results indicate that ANN models give high prediction accuracy on the CO ₂ solubilities in ILs than the SVM-based model.	[110]
6.	Prediction of MOF Performance in Vacuum Swing Adsorption Systems for Post-combustion CO ₂ Capture Based on Integrated Molecular Simulations, Process Optimizations, and Machine Learning Models	Environmental Science & Technology	2020	71	Separation science, Isotherms, Adsorption, Metal organic frameworks, Materials	CO ₂ performance and productivity of different types of Metal-organic framework (MOF) materials	ANN and Gradient-boosted decision tree model	Machine learning models were used to predict 30 materials in vacuum-swing adsorption (VSA) process with full process simulation. The overall prediction accuracy of 91% was achieved.	[113]
7.	Prediction of storage efficiency on CO ₂ sequestration in deep saline aquifers using artificial neural network	Applied Energy	2017	68	Carbon capture and storage, Deep saline aquifer, Artificial neural network	To predict storage efficiency using artificial neural network	ANN	The results show that ANN model has high accuracy to predict storage efficiency with produce low error (less than 1.2%).	[114]

(continued on next page)

Table 5 (continued)

No	Title	Journal	Year	Citations	Keywords	Key influencing factors	Type of machine learning	Outcome/Remarks	Ref.
8.	Modeling of CO ₂ capture ability of [Bmim][BF4] ionic liquid using connectionist smart paradigms	Environmental Technology and Innovation	2021	66	CO ₂ capture, Ionic liquids [Bmim][BF4], Intelligent modelling, Comparison study, Cascade feed-forward neural network	CO ₂ solubility in ionic liquids	AI techniques, including four ANN, cascade feed-forward neural network, SVM, ANFIS	The results indicate that the cascade feed-forward neural network achieved high accuracy to predict solubility of CO ₂ in ionic liquids.	[118]
9.	Prediction of CO ₂ loading capacities of aqueous solutions of absorbents using different computational schemes	International Journal of Greenhouse Gas Control	2017	66	Carbon dioxide, loading capacity, CO ₂ capture, Modeling, Solubility	CO ₂ loading capacities of aqueous solutions	MLP-ANN, Radial Basis Function Artificial Neural Network (RBF-ANN), LSSVM, and ANFIS	The results show that LSSVM model has high accuracy to predict CO ₂ solubility in aqueous solution.	[111]
10.	Machine learning exploration of the critical factors for CO ₂ adsorption capacity on porous carbon materials at different pressures	Journal of cleaner production	2020	55	CO ₂ sequestration, Carbon adsorbents, Sustainable waste management, Low-carbon development, Biomass utilization	To predict the CO ₂ adsorption capacity and physicochemical properties of porous carbon material	Random forest (RF) model	The results indicate that RF model has high accuracy to predict physical and chemical properties of porous carbon materials (high prediction: R ² > 0.9).	[119]

focuses on the co-authorship, keywords, and citations.

4.2. Current progress and research trends of the literature (bibliometric analysis)

4.2.1. Co-authorship pattern

4.2.1.1. Countries analysis. Most of the published articles were from six countries, namely the China, Iran, United States, the United Kingdom, France and South Korea and they have a significant contribution in terms of scientific production. China, Iran and the United States are the main countries that contributed to the research topic of machine learning for CO₂ capture. The country analysis indicates the research interests and the areas that every country supports. Commonly, the pattern is directly proportional to the reserves and shortages presence in each country. From 1999–2022, researchers from various countries (>50 countries) have contributed to the knowledge of machine learning for CO₂ capture. As shown in Fig. 3(a), China, Iran and United States were the most productive country due to more than 60 publications. This is ascribed to its goal of reducing 6% of CO₂ emissions by 2012 (Bulletin, 2002). The efforts started with the first modelling study for large-scale amine-based post-combustion CO₂ capture that was operated at the International Test Centre of CO₂ Capture (ITC) located in Regina, Saskatchewan, Canada [121]. However, after its withdrawal from the Kyoto Protocol in 2011 because of an unfair balanced of economic growth and inability to meet the terms of reducing CO₂ production [122], Canada was not in the first rank of highest publications, but Canada was among the top 6 countries producing research on machine learning for carbon capture applications. The highest publications reported by China and United States were due to the fast-growing of research activity. This is anticipated due to the development of CO₂ capture technologies in these countries with several commercially operational facilities and facilities that were under progress including pilot and demonstration facilities under the research and development phase. Economic growth and industrial progress also have a significant role in this interest since these countries have all the advanced equipment to conduct the research works efficiently. As the world's first and second-largest economies, their governments attempted to accomplish

environmental sustainability through a string of policies and actions [120].

The United States strategized long-term policies for the development of AI and machine learning technologies to prioritize their usage in optimizing decision-making and operations on scientific research, thereby increasing their productivity and contributions to machine learning for CO₂ capture [123]. The involvement of the European countries might be credited to the reality that Europe has been at the forefront of the progress towards “net-zero CO₂ emission” even earlier than the United Nations Framework Convention on Climate Change that was implemented on 9 May 1992, and the Kyoto Protocol on 11 December 1997 [123]. At the same time, China’s dedication to the mitigate climate change issue and many of article reported from China contribute to the investigations concerning the lessening of CO₂ emissions.

As seen in Fig. 3(b), both countries have sufficient foundations of research funding provided by their governments. The National Nature Science Foundation of China and the U.S. Department of Energy were the biggest funding agencies that supported research works. The research at the development stage (small-scale production) needs sufficient funding to generate a good product, and the product obtained can then be used in large-scale production. Therefore, government support and research collaboration between national and international organizations are the most important factor in achieving this goal. Furthermore, bibliometric analysis is beneficial to obtain the potential opportunity for research collaboration, for preparing research grant application, to find active researcher that works in this field and to identify current development on machine learning in CO₂ capture.

From Fig. 4, the collaboration strengths between those countries were separated into 5 clusters, which were represented by the following colors: red (Cluster 1), green (Cluster 2), blue (Cluster 3), yellow (Cluster 4), and purple (Cluster 5). The size of each circle indicates the number of articles published by the country and Iran, China, the United States, and Canada have the highest citation record. The lines connecting the circles showed the research collaboration among countries, and the thickness implies the strength of the link, for example a strong co-authorship collaboration [124]. The distance between circles (distance of the connecting lines) showed the research collaboration activity among

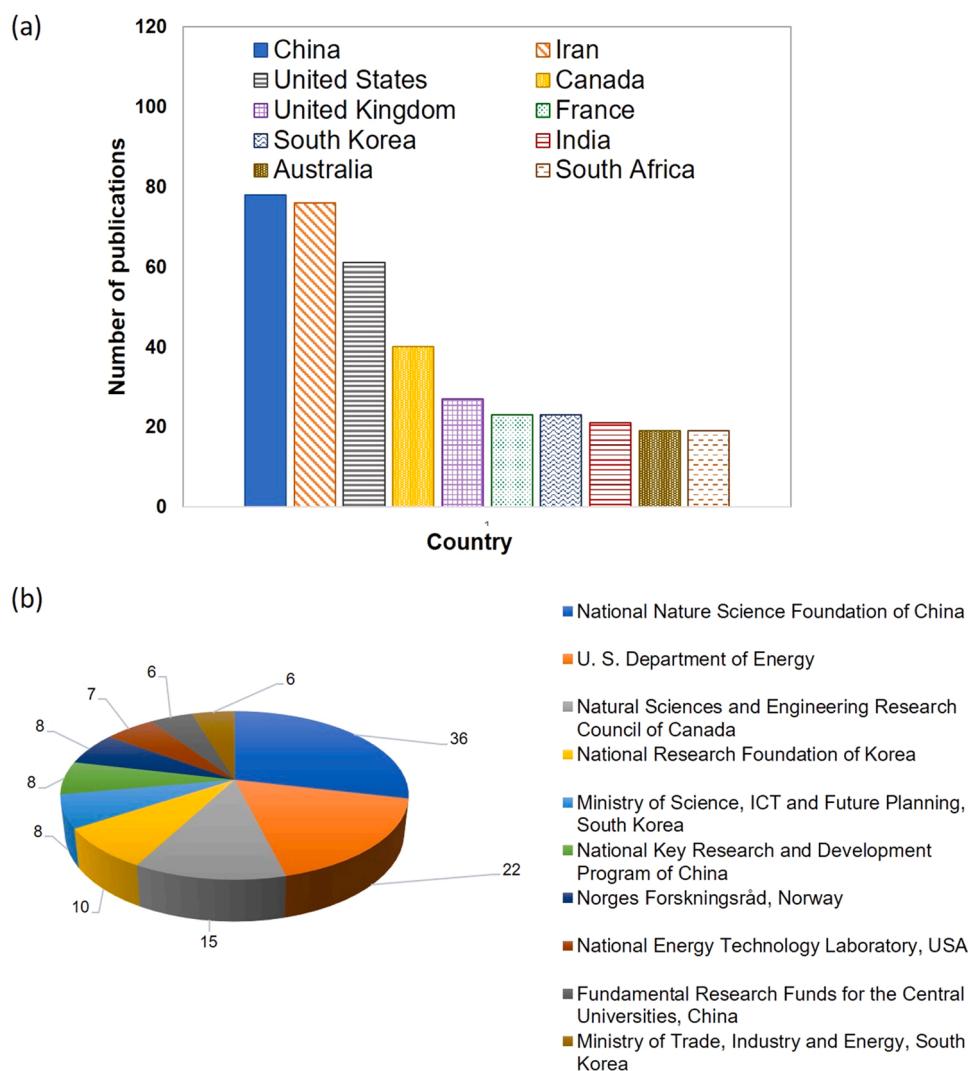


Fig. 3. : a) Top 10 countries with highly published articles from 1999–2022, and **b)** Top 10 funding agencies that supported research works in machine learning for CO₂ capture between 1999 and 2022.

countries, similar research areas or interests and how frequent authors work together to write article for publication [47]. In Cluster 3, Iran had the biggest collaboration strength with other countries (87 of total link strength). Meanwhile, China has 73 total link strength, the United States has 54 total link strength, and Canada has 50 total link strength, with the deepest link with other countries respective to Clusters 1, 3, and 4. In Clusters 2 and 5, the strongest relationships with other countries are shown by Saudi Arabia (20 total link strength) and South Korea (15 total link strength). The collaborations made by these countries suggest that they are attempting climate change using machine learning CO₂ capture not only with the developed countries but also with other developing countries.

4.2.2. Semantic network analysis: co-occurrence of keywords

Keywords are the crucial parts of an article in which they highlight the important contents of the literature. Keywords also help to improve the visibility of the articles in search engines and indexers. Table 6 shows the top 20 most frequent keywords used by the authors over 20 years in publications related to machine learning in carbon capture applications. The hot topics or keywords used in the selected articles ranked according to the highest link strength. The top 10 list includes CO₂ capture, machine learning, carbon capture, artificial intelligence, carbon dioxide, artificial neural network, deep learning, CO₂, and CO₂

solubility. From here, we can see that different keywords used for CO₂ capture technologies would give a different number of appearances in the search engines. Keywords of CO₂ capture had a higher frequency of simultaneous occurrences (40) and total link strength (69) compared to carbon dioxide, CO₂, and carbon capture. Besides that, the right usage of keywords is also vital for articles' visibility. This is because similar keywords such as ionic liquids and ionic liquid can give different impacts whereby the frequency of occurrences for ionic liquids was higher than ionic liquid.

Aside from that, the clustering network for the co-occurrence of authors' keywords is presented in Fig. 5. In this type of map, the keywords used by the authors are illustrated in accordance with different colors. The colors indicate different clusters, and the cluster categories was based on the keywords clustering analysis and total link strength. Every keyword was characterized as a node and the size of the node revealed the frequency of occurrences. In other words, the bigger the node, the more the keywords were used in the analyzed research articles. The link between the two nodes (keywords) was symbolized by a curved line, whereby a wider line indicates a greater relationship (link strength). For instance, the connections of each keyword of all machine learning models (for example artificial intelligence, neural network and deep learning) to the machine learning keyword were strongly connected. Based on VOSviewer analysis, the keywords were categorized

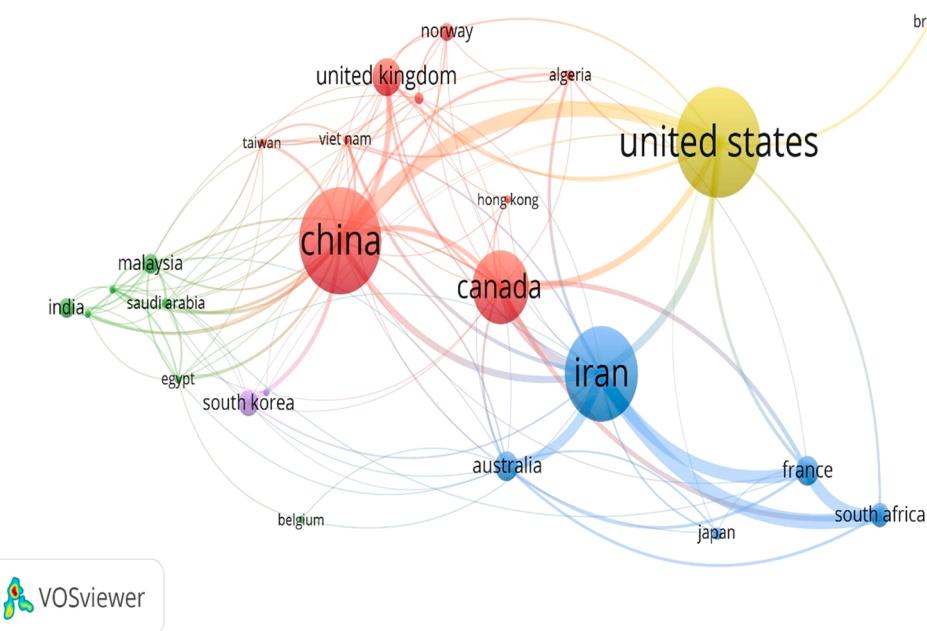


Fig. 4. : Co-authorship of countries from Scopus database between 1999 and 2022 (minimum number of publications = 3 and citations = 1).

Table 6

List of top 20 keywords that were utilized by the researchers for over 20 years (1999–2022).

Rank	Keywords	Occurrences	Total link strength
1	CO ₂ capture	40	69
2	machine learning	36	51
3	carbon capture	21	38
4	artificial intelligence	19	38
5	Carbon dioxide	17	27
6	Artificial neural network	16	22
7	Deep learning	16	10
8	CO ₂	15	35
9	Solubility	14	37
10	Carbon capture and storage	14	18
11	CO ₂ solubility	13	27
12	Modelling	9	24
13	Neural networks	9	10
14	Ionic liquids	8	16
15	Neural network	8	10
16	Prediction	7	21
17	ANN	7	17
18	Ionic liquid	6	16
19	Adsorption	6	9
20	Absorption	5	17

into 6 clusters. Clusters 1, 2, 3, 4, 5, and 6 are presented in the respective colors of red, green, dark blue, yellow, purple, and light blue. In Cluster 1, the keywords were related to the CO₂ capture in the absorption and adsorption process for predicting CO₂ solubility and adsorption capacity using machine learning. This cluster had a strong connection with Clusters 3, 4, and 5, especially ionic liquids that had the thickest curve line with the solubility keyword. The machine learning with common types of models that were used for the CO₂ absorption technology existed in Clusters 3, 4, and 5 as the relevant keywords of the artificial neural network, deep learning, and genetic algorithm were encompassed. While Cluster 2 consisted of the CO₂ capture and storage area since it can be figured out from the keywords such as CO₂ sequestration and optimization. Clusters 2 and 3 also had a sturdy relationship in the CO₂ capture and storage area. The keywords of CO₂ storage, pipeline network, carbon capture and storage, machine learning, and CO₂ absorption ensued in Cluster 3. Meanwhile, Cluster 4 emphasized the prediction of CO₂ solubility in ionic liquids and amino acids using an

artificial neural network. The machine learning models of artificial intelligence, artificial neural networks, fuzzy logic, multi-objective optimization, and genetic programming that were employed in CO₂ capture and storage were constituted in Cluster 5. This fact was supported by the carbon capture and storage keyword being found in the same cluster. Lastly, the prediction of CO₂ absorption solubility in aqueous amine using an artificial neural network is highlighted in Cluster 6. To sum up, all these clusters revealed the main areas of machine learning for CO₂ capture from 1999 to June 2022 through co-occurrence and visibility of keywords. It is also critical to mention that the keywords such as “CO₂ adsorption”, “carbon capture by adsorption” “metal organic frameworks”, and “carbon sequestration” are apparent recently in small frequencies indicating them as new areas in this field. This is because CO₂ adsorption only emerged after 2014 (Section 4.1, Table 2 and Fig. 2).

4.2.3. Trend topic on machine learning in carbon capture application

Fig. 6 shows the trending topic of machine learning in carbon capture applications from 2011 to 2022, with a minimum frequency of 5 citations. Based on Fig. 6, from 2011 to 2016, topics related to the modeling, simulation and sensitivity analysis obtained a high frequency of citation and become a hot topic within that year. Meanwhile, starting from 2018 machine learning has been used in carbon capture and storage application with topics related to CO₂ solubility, ionic liquid, absorption, CO₂ capture, and carbon capture being dominant in 2020. From 2020–2022, topics related to adsorption, metal organic framework, machine learning, carbon capture and storage have become hot topics, and many publications focus on this area. For example, in 2000 many articles published on MOFs. This is because MOFs are a unique class of porous material with high surface area which suitable to be used for CO₂ adsorption process [125]. The use of ionic liquids as the absorbent (solvent) to capture CO₂ offers several advantages such as high thermal stability, low vapor pressure, high solubility and non-corrosivity [126]. Ionic liquids have become a hot topic since 2000. Research trends with a timeline are important to identify the current technology and this information is useful for future research in this area.

4.2.4. Sankey diagram (three-field plot)

The Sankey diagrams (three-field plots) were used to evaluate the relationship between co-authorship between countries, keywords, and sources (journals). This plot was analyzed using a Bibliometrix R-

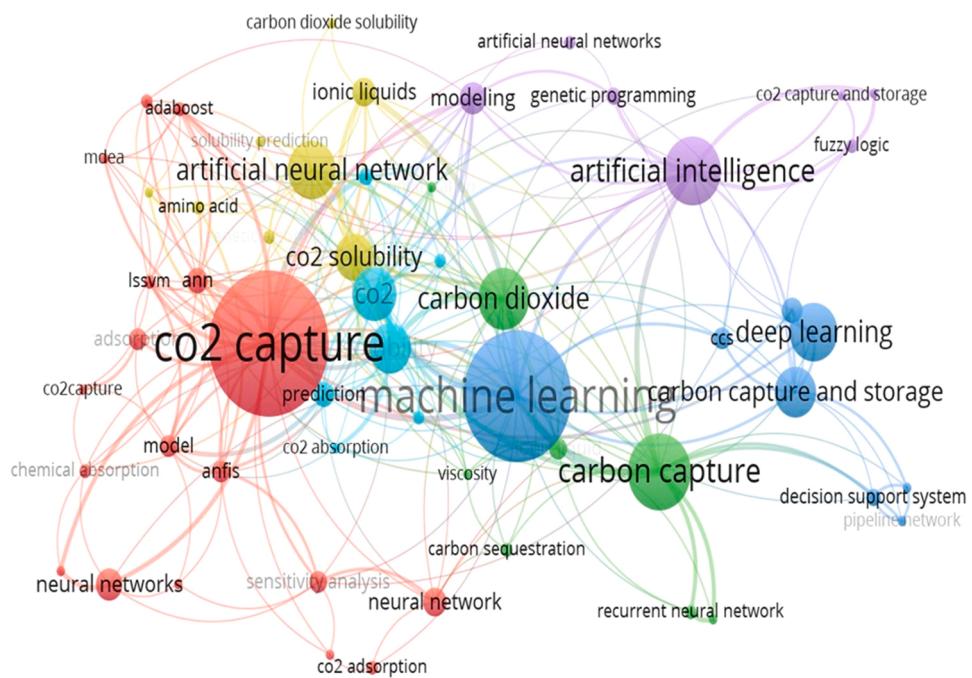


Fig. 5. : The networks of a) co-occurrence of authors' keywords between 1999 and 2022 (minimum number of occurrence keywords = 3)..

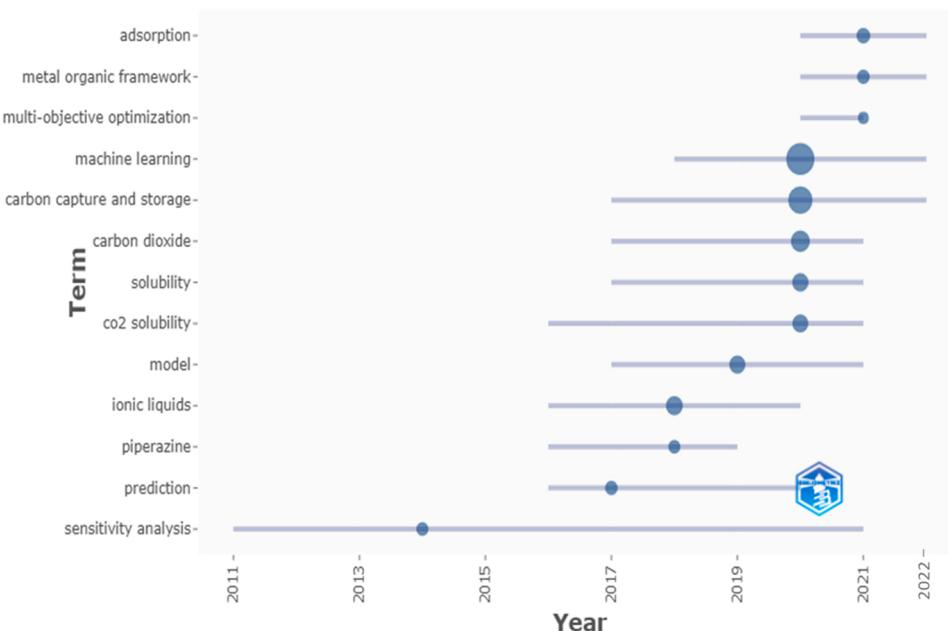


Fig. 6. Trend topic of machine learning for carbon capture application between 2011 and 2022.

Package via Biblioshiny App (for non-coders). Fig. 7 shows the three-field plot on machine learning in carbon capture application with the top ten most cited articles. This diagram shows the relationship between countries (left), keywords (middle), and sources/journals (right). For example, in the country column, the height of the box shows the highest publication and frequency of the document. Similarly, the thickness of connection between country, keyword and sources (journal) shows the capacity of the publication and citations. As shown in Fig. 7, the top 3 countries such as Iran, the United States and China, published articles mainly on machine learning in CO₂ capture, and carbon dioxide application. The top 5 keywords were carbon capture and storage, ANN, machine learning, carbon dioxide, and solubility, and these were

published in sources such as the International Journal of Greenhouse Gas Control, Fuel, the Journal of CO₂ Utilization, Applied Energy, and the Journal of Natural Gas Science and Engineering.

5. Future recommendations

In the past 7 years, due to the Fourth Industrial Revolution (IR 4.0), many manufacturing companies have been converting their manual processes into digitalized or automated system. They used computing power such as machine learning to improve productivity. Machine learning is useful for a wide range of applications. Nowadays, most of the manual processes are transformed into automatic processes and this

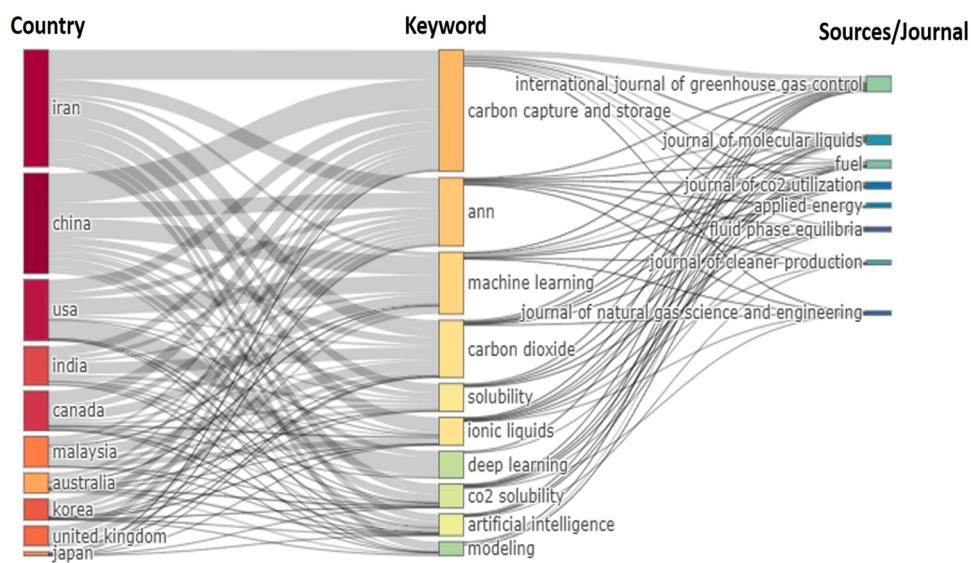


Fig. 7. : Sankey diagram, a three-field plot of the top 10 ten most cited articles between 1999 and 2022.

transformation has become a standard practice for manufacturers around the world. Machine learning is an effective and efficient tool to predict and make decisions on material, properties or processes. In R&D area, machine learning is able to reduce experimental time and cost.

Based on bibliometric analysis, the publication trend increased drastically from 50 publications in 2020–94 publications in December, 2022. This is evident that machine learning in CO₂ capture and storage has become a widely discussed topic. From the keyword analysis, it indicates that not much studies have reported on pre-combustion, post-combustion (particularly on different type of adsorbents such as activated carbon, molecular sieve, porous carbon and graphene), material synthesis (amino acid and deep eutectic solvent), adsorption design ((pressure swing adsorption (PSA), temperature swing adsorption (TSA), vacuum swing adsorption (VSA), vacuum pressure swing adsorption (VPSA), temperature vacuum swing adsorption (TVSA) and pressure vacuum swing adsorption (PVSA)) and characterization (textural and thermal properties such as surface area, pore volume, elemental composition and heat capacity). However, there are still many areas on machine learning in CO₂ capture and storage that require an in-depth understanding and exploration. Several possible future research directions are listed below:

i. Step by step or complete guidelines to apply machine learning algorithm models in CO₂ capture and storage application. Most published articles on machine learning did not discuss and elaborate in details the model of the machine learning. Therefore, other researchers who have tried to reproduce the results from the literature find it difficult to get results with high accuracy. All input files and scripts are recommended to be discussed in the research article.

ii. To develop a comprehensive machine learning tools that can effectively model and subsequently optimize the process to reduce the energy penalty and maximize the CO₂ capture yield.

iii. Study on techno-economic analysis. A detailed study on cost analysis and the impact of machine learning to reduce production cost, particularly in large-scale process is an area that can be explored. Machine learning is potential for industrial applications. Therefore, applying machine learning in techno-economic analysis is needed for large-scale of carbon capture. By integrating techno-economic and machine learning to determine the economy impact of the process, it can make the process more efficient and effective. This can be applied for different industrial application to reduce CO₂ emission. An in-depth understanding and comprehensive study can help researcher and industry player to obtain a better picture on cost-effectiveness of production.

iv. A comprehensive study is needed to predict CO₂ adsorption capacity through various textural and thermal properties data using machine learning, combined with density functional theory calculations, and experimental studies.

v. Membrane-based technology has not been studied much and therefore, this area can be further explored as this specific area of research requires urgent attention.

vi. A compilation of database on potential application of machine learning in CO₂ capture and storage, particularly in large-scale production can be a guideline for researcher and industry player.

vii. The data generated from experiments can be used as an input and this input has significant impacts on data-driven material science. To predict the output, the input data is very important in machine learning. Machine learning require abundant data for model training, but some processes have insufficient data information and they become an obstacle to apply machine learning particularly in large-scale process of carbon capture and storage.

viii. The life cycle is important for large-scale application. Life cycle assessment (LCA) is an environmental assessment tool that studies the environmental impact of a product and process. Applying machine learning in LCA can predict various important parameters such as energy consumption, CO₂ emissions and disposal processes effectively.

6. Conclusion

Integrating Industry 4.0 and Industry 5.0 to solve environmental issues (such as reducing carbon emissions) has become an important topic. Smart technologies, such as machine learning (Industry 4.0 – digital technology) and creating or developing technology by R&D teams (Industry 5.0 - interaction between humans and smart machines technology) could help to cater to climate issues related to carbon emission. Therefore, this study aims to present a comprehensive analysis of research trend on the topic of machine learning in carbon capture applications. The bibliometric method was used to analyze the research trend based on several criteria such as co-authorship country, citation or the number of publications, keywords and trending topics. For bibliometric analysis, choosing a suitable keyword may be challenging. To get relevant information (such as journal articles on a specific topic) from the Scopus database, a keyword search string is used. Approximately 314 articles from the Scopus database were compiled from 1999 to June 2022. The relationship between co-authorship in terms of country, collaboration network and hot keywords were performed using VOS-viewer. The relationship between keywords and timeline, as well as the

trending topics, were analyzed using Biblioshiny App (for non-coders). The findings obtained from the bibliometric analysis can provide a robust roadmap for potential future research on this topic. For instance, China, the United States, and Iran are the main countries that contributed to the research topic of machine learning for CO₂ capture. The topic related to CO₂ adsorption, deep learning, machine learning, artificial intelligence, genetic programming, carbon capture, and CO₂ storage have become a hot topic from 2020 to 2022. In recent years, there have been very few articles investigating the prediction of CO₂ adsorption capacity using various machine learning method. Therefore, a comprehensive bibliometric analysis is important to identify research gaps, current technology, and hot spots for the research topic.

CRediT authorship contribution statement

Farihahusnah Hussin: Writing - original draft. **Siti Aqilah Nadhirah Md Rahim:** Data collection, and methodology. **Nur Syahirah Mohamed Hatta:** Data analysis. **Mohamed Kheireddine Aroua:** Supervision, Reviewing. **Shaukat Ali Mazari:** Reviewing and Editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Data will be made available on request.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.jcou.2023.102474](https://doi.org/10.1016/j.jcou.2023.102474).

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