



## Trends and Future Directions on Machine Learning for Enhancing Optimal Methods of Heavy Metal Ion Removal from Industrial Wastewater

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### ABSTRACT

Heavy metal contamination in industrial wastewater is a pressing environmental and public health issue, necessitating the development of innovative and efficient remediation methods. Machine learning (ML) has emerged as a promising approach for optimizing existing treatment techniques, predicting system performance, and enhancing decision-making in the removal of heavy metal ions. This study employs a bibliometric analysis to investigate research trends, influential contributions, and future directions in the application of ML for optimizing heavy metal removal methods. By analyzing scholarly publications, citation networks, and keyword trends, we identify key advancements, leading researchers, and prominent institutions shaping this interdisciplinary field. The findings underscore the integration of ML algorithms, such as artificial neural networks (ANNs), support vector machines (SVMs), and deep learning, into various remediation methods, including adsorption, membrane filtration, and bioremediation. Additionally, this study highlights challenges such as data scarcity, model generalizability, and practical implementation, while exploring opportunities for hybrid approaches, big data analytics, and interdisciplinary collaboration. The insights from this bibliometric analysis provide a comprehensive understanding of the current research landscape and offer strategic guidance for advancing ML-driven solutions for the efficient and sustainable removal of heavy metal ions from industrial wastewater.

### 1. Introduction

The contamination of industrial wastewater with heavy metals has become a critical environmental and public health challenge in recent decades[1], [2]. Industrial activities such as mining, metal plating, chemical manufacturing, and battery production frequently discharge significant amounts of heavy metals, including lead, cadmium, mercury, arsenic, and chromium, into the environment[3], [4]. These metals are highly toxic, non-biodegradable, and capable of bioaccumulation in living organisms, making them persistent pollutants with long-term detrimental effects on ecosystems and human health[5]–[7]. Exposure to heavy metals has been associated with severe health issues, including

neurological disorders, organ damage, developmental delays, and various forms of cancer[8]–[10]. Additionally, these pollutants adversely affect aquatic life, compromise soil fertility, and threaten food security by contaminating crops and water supplies[11]–[13].

The global water crisis, driven by rapid urbanization, industrial growth, population expansion, and climate change, has further exacerbated the urgency to address heavy metal contamination[14]–[16]. Industrial wastewater is one of the primary sources of water pollution, often discharged untreated or inadequately treated, contributing significantly to the degradation of water quality[17]–[20]. In many developing countries, untreated effluents from industries are directly

released into rivers, lakes, and groundwater sources, creating health risks for communities that rely on these water bodies for drinking, irrigation, and other essential activities[21]–[23]. Even in developed nations, the complexity of industrial wastewater compositions and the limitations of traditional treatment technologies pose ongoing challenges to achieving stringent water quality standards[24]–[28]. These circumstances underscore the critical need for innovative, efficient, and sustainable approaches to remove heavy metals from industrial wastewater, ensuring the protection of both water resources and public health[29]–[34].

Conventional methods for removing heavy metals from wastewater can be broadly categorized into physical, chemical, and biological techniques. Physical methods, such as filtration, sedimentation, and adsorption, rely on materials like activated carbon, biochar, or other adsorbents to capture and separate heavy metals from water[35], [36]. Chemical methods, including precipitation, ion exchange, and oxidation-reduction reactions, transform heavy metals into less toxic or insoluble forms that can be removed more effectively. Biological approaches, such as bioremediation and phytoremediation, utilize microorganisms or plants to absorb, stabilize, or degrade heavy metal pollutants[37], [38]. While these traditional methods have demonstrated varying levels of success, they are often constrained by high operational costs, energy requirements, limited scalability, and reduced efficiency when applied to wastewater with complex or mixed contaminants. Consequently, there is an urgent need to develop advanced and integrated solutions to address these limitations[39], [40].

In recent years, Machine learning (ML) has emerged as a transformative technology with the potential to revolutionize the field of wastewater treatment, particularly in the removal of heavy metals. ML, a subset of artificial intelligence (AI), employs advanced algorithms and computational models to analyze complex datasets, identify patterns, and optimize processes[41]–[44]. Unlike traditional approaches, ML enables the development of predictive models that can simulate treatment processes, monitor system performance in real time, and improve the efficiency and sustainability of heavy metal remediation[45]–[47]. Techniques such as artificial neural networks (ANNs), support vector machines (SVMs), decision trees, and deep learning have shown significant promise in addressing various

challenges associated with heavy metal removal, including process optimization, contaminant detection, and decision-making in dynamic treatment systems[48], [49].

The integration of ML into wastewater treatment offers several advantages over conventional methods. ML-driven models can analyze vast amounts of data from industrial wastewater systems, uncovering complex relationships that traditional statistical methods may overlook. These insights can be used to fine-tune treatment processes, optimize resource allocation, and reduce operational costs. Moreover, ML algorithms can adapt to changing conditions in real time, providing dynamic solutions to variations in wastewater composition and flow rates. For example, predictive models based on ML can forecast contaminant levels, enabling proactive adjustments to treatment protocols and minimizing the risk of environmental discharge violations[49]–[51].

Despite its potential, the application of ML in heavy metal removal remains an evolving field with several challenges. One significant obstacle is the availability of high-quality data for training and validating ML models[52]–[59]. Industrial wastewater systems often generate heterogeneous and incomplete datasets, which can limit the performance and generalizability of ML algorithms. Additionally, the integration of ML models into existing treatment systems requires specialized infrastructure, technical expertise, and compliance with environmental regulations. Overcoming these barriers will require interdisciplinary collaboration among researchers, engineers, industry stakeholders, and policymakers to develop robust and scalable ML solutions that align with real-world operational constraints[33], [60], [61]. This study aims to explore the current trends, advancements, and future directions in applying Machine learning to optimize methods for the removal of heavy metal ions from industrial wastewater. Through a comprehensive bibliometric analysis, the research investigates global publication trends, identifies leading researchers and institutions, and highlights key advancements and research gaps in the field. By analyzing citation patterns, keyword trends, and collaborative networks, the study provides valuable insights into the evolving research landscape and the contributions of various stakeholders to this critical area of environmental science.

The findings of this study emphasize the growing role of ML in enhancing traditional remediation methods and driving innovation in hybrid approaches. For

instance, ML techniques can be combined with physical, chemical, and biological processes to improve their efficiency, scalability, and environmental sustainability. Big data analytics and AI-driven decision-making tools offer additional opportunities to refine treatment strategies, monitor system performance, and ensure compliance with stringent regulatory standards. These advancements hold the potential to revolutionize wastewater management, paving the way for more effective and sustainable solutions to tackle heavy metal pollution. By providing a detailed overview of the current research landscape and future prospects, this study contributes to the understanding of the transformative potential of ML in industrial wastewater treatment. It underscores the importance of interdisciplinary collaboration, international partnerships, and innovative approaches in addressing the complex challenges posed by heavy metal contamination. Ultimately, the research aims to guide future advancements in Machine learning applications for heavy metal remediation, ensuring the development of efficient, resilient, and sustainable strategies to protect water resources, ecosystems, and public health.

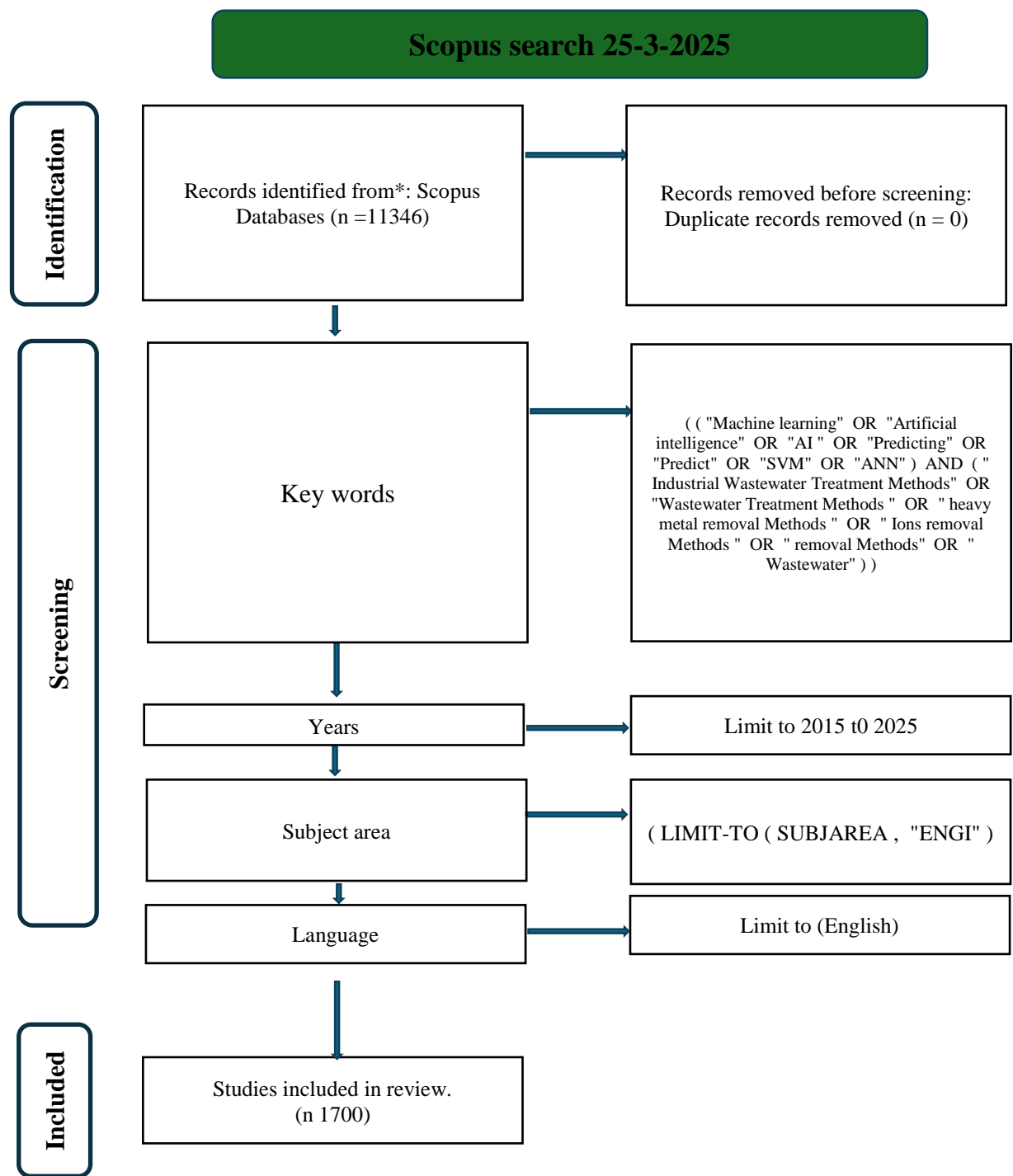
## 2. Methodology

This study aims to investigate research on the application of Machine learning (ML) for enhancing optimal methods of heavy metal ion removal from industrial wastewater using a bibliometric analysis approach. It seeks to identify key trends, influential

publications, leading institutions, prominent researchers, and contributing countries in this evolving field. Additionally, the study focuses on uncovering research gaps and providing strategic insights to guide future advancements in integrating ML technologies with innovative and effective remediation methods. The methodology encompasses three main stages: data collection and selection, application of scientific mapping techniques, and execution of a comprehensive bibliometric analysis. This systematic approach provides a detailed overview of the current research landscape and highlights future directions for advancing data-driven, sustainable, and efficient solutions for heavy metal ion removal from industrial wastewater.

### 2.1. Bibliometric Analysis

This review highlights the trends and future directions in the application of Machine learning for optimizing methods of heavy metal ion removal from industrial wastewater between 2015 and 2025. To achieve this, a bibliometric analysis approach was utilized. The study also utilizes the PRISMA framework [62], depicted in Fig. 1, to guide its methodology. Bibliometric analysis involves examining research papers on a specific topic and extracting meaningful insights by analyzing them across multiple parameters [63]. To identify relevant publications, the search within the Scopus database covered fields such as Title, Abstract, Author Keywords, and Keywords Plus.



**Fig. 1:** PRISMA Framework-Based Review of Machine learning approaches for optimizing heavy metal ion removal from industrial wastewater.

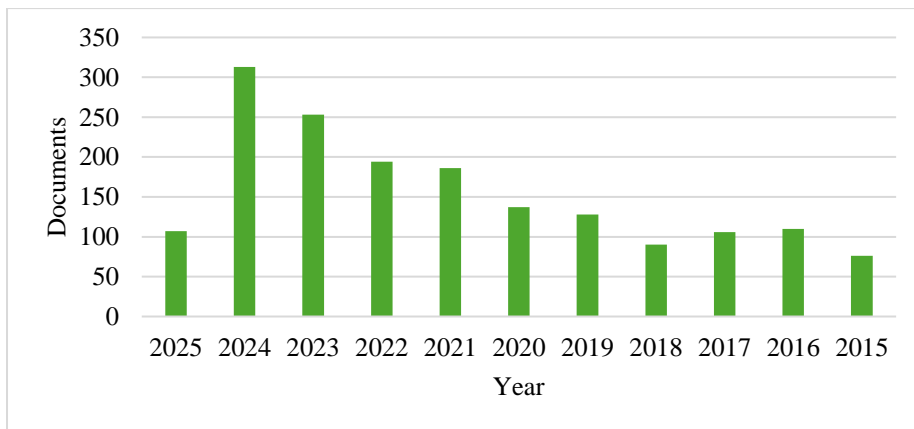
### 3. Results

Bibliometric analysis is a statistical approach used to quantify and evaluate the emerging trends within a particular field of study [64], [65]. Bibliometric analysis has been applied to evaluate academic outputs across multiple disciplines [66]. The search, conducted on the Scopus database from 2015 to 2025, utilized various search fields such as Author keywords, Title, Abstract, Author, and Keywords Plus. The search employed a combination of keywords using AND/OR logic, including terms like ( "Machine learning" OR "Artificial intelligence" OR "AI" OR "Predicting" OR "Predict" OR "SVM" OR "ANN" ) AND ( "Industrial Wastewater Treatment Methods" OR "Wastewater Treatment Methods" OR "heavy metal removal Methods" OR "Ions removal Methods" OR "removal Methods" OR "Wastewater" ). The results were assessed based on titles and abstracts to ensure coherence with the article's theme and core topic.

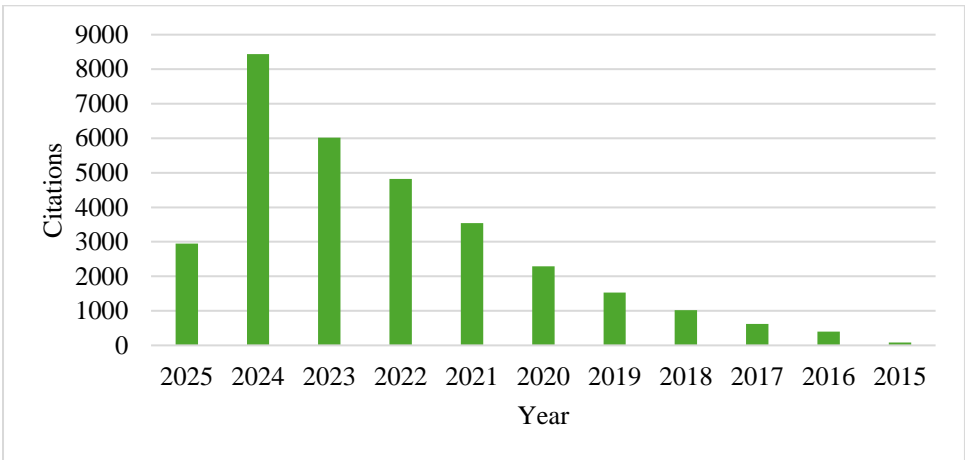
The analysis utilized Scopus analysis and VOS viewer for data visualization. Graphs were generated using Microsoft Excel. Various details were extracted for each document, including (1) the number of documents per year, (2) average citations of articles per year, (3) author keywords and frequently used words in titles, (4) journals of publication for each article, (5) science categories, (6) most cited articles, (7) authors and coauthors for each article, (8) H-index for top 30 authors, (9) affiliation details for authors and coauthors, (30) countries of the authors, and (11)

H-index for top 20 journals,. Bibliographic maps were generated using VOS viewer software, encompassing keywords co-occurrence, countries co-authorship maps, and bibliographic coupling for countries and affiliations.

11346 documents were initially identified, with 1700 aligning with the study's theme. These documents were then categorized as follows: 1383 research articles, 210 conference papers, and 107 documents falling into other categories. The dataset comprises 120 sources and 1449 keywords. The publications obtained showed an average growth rate of 18.20% per year. The most notable increase was observed between 2020 and 2024, reaching its peak with 313 publications in 2024, as shown in Fig. 2. The average annual citation was 28.73%, reported in 2024, as illustrated in Fig. 3. Only 8438 articles were cited for that particular year. Fig. 3 illustrates the fluctuation of journals over the years. Until 2024, the journal "Water Research" held the top position, but it was surpassed by the "Desalination And Water Treatment" which accumulated a total of 182 articles. In terms of the Cite Score (2023) of journals, the "Water Research" led the rankings with a score of 20.8, followed by "Journal of Cleaner Production" and "Desalination" with scores of 20.4 and 14.6, respectively, as detailed in **Table 1**.



**Fig. 2.** Yearly Publication Trends on Machine learning techniques for enhancing heavy metal ion removal from industrial wastewater.



**Fig. 3.** early Average Citations per Article on Machine learning applications for heavy metal ion removal from industrial wastewater.

**Table 1.** The Top 10 Highly Productive Journals on Machine learning applications for heavy metal ion removal from industrial wastewater.

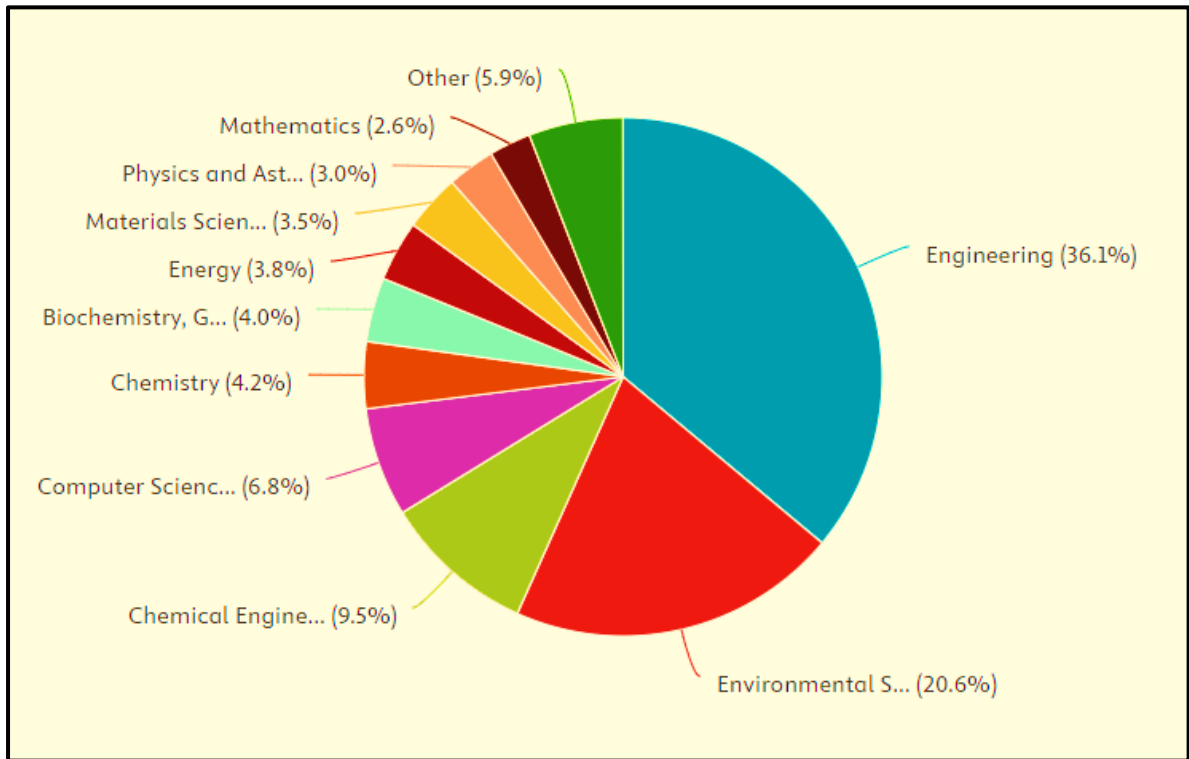
Journal	TP	TC	Cite Score (2023)	Most cited publication	Times Cited	Publisher
Water Research	4,826	100,330	20.8	Li, Ning, et al. (2023).	169	Elsevier
Desalination and Water Treatment	4,385	9,714	2.2	Xu, Peilong, et al. (2023)	56	Elsevier
Journal Of Water Process Engineering	3,477	37,357	10.7	Khan, Mohammad Danish, et al. (2023)	170	Elsevier
Chemical Engineering Journal	-	-	-	-	-	Elsevier
Journal of Cleaner Production	19,382	394,597	20.4	Mujtaba, Muhammad, et al. (2023)	429	Elsevier
Process Safety and Environmental Protection	3,065	34,855	11.4	Aljohani, Meshari M., et al. (2023)	172	Institution of Chemical Engineers
Journal of Environmental Engineering (United States)	571	2,505	4.4	Reinhart, Debra R., Stephanie C. Bolyard, and Jiannan Chen. (2023)	12	American Society of Civil Engineers
Biochemical Engineering Journal	1,299	9,160	7.1	Kulkarni, Madhusudan B., et al. (2023)	32	Elsevier
IEEE Access	49,687	484,743	9.8	Gupta, Maanak, et al. (2023)	286	IEEE
Desalination	2,082	30,471	14.6	Li, Ning, et al. (2023)		Elsevier

TP= Total Publications, TC= Total Citation  
Concerning scientific categories, 36.1% of total articles were categorized under Engineering, followed

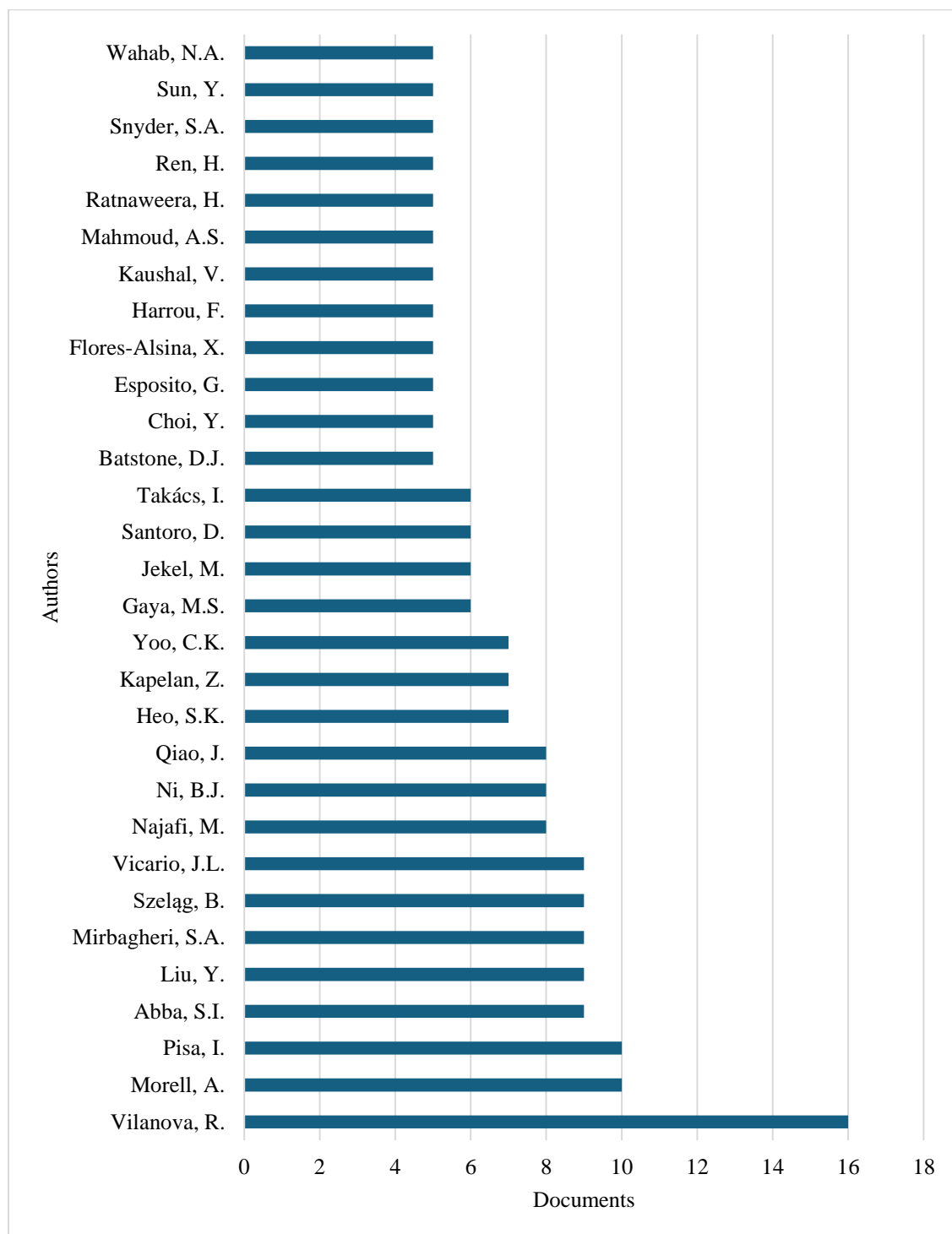
by Environmental Science and Chemical Engineering with 20.6% and 9.5% of the total articles, respectively

as illustrated in **Fig. 4**. The total number of authors across all articles amounted to 159. Notably, "Vilanova, R." authored the superior number of articles, with 16 articles. Following closely, "Morell, A.", and "Pisa, I." contributed 10 articles, while "Abba, S.I.", "Liu, Y.", and "Mirbagheri,

S.A." authored 9 articles as shown in **Fig. 5**. In terms of the authors' H-index, " Ni, B.J." achieved the highest score of 93, followed by " Batstone, D.J.." with an H-index of 77, and " Jekel, M." attained an H-index of 73, as detailed in **Table 2**.



**Fig. 4.** Research field base publication on Machine learning applications for heavy metal ion removal from industrial wastewater.



**Fig. 5.** Top 30 authors based on the number of articles on Machine learning applications for heavy metal ion removal from industrial wastewater.



**Table 2.** List of the 25 Most Prolific Authors in Machine learning applications for heavy metal ion removal from industrial wastewater.

No	author	TP*	h-index	Current affiliation	Country
1.	Vilanova, R.	407	32	Universitat Autònoma de BarcelonaThe institution will open in a new tab, Cerdanyola del Valles, Spain	Spain
2.	Morell, A.	84	20	Universitat Autònoma de BarcelonaThe institution will open in a new tab, Cerdanyola del Valles, Spain	Spain
3.	Pisa, I.	20	8	Universitat Oberta de CatalunyaThe institution will open in a new tab, Barcelona, Spain	Spain
4.	Abba, S.I.	214	34	King Fahd University of Petroleum and MineralsThe institution will open in a new tab, Dhahran, Saudi Arabia	Saudi Arabia
5.	Liu, Y.	121	32	South China University of TechnologyThe institution will open in a new tab, Guangzhou, China	China
6.	Mirbagheri, S.A.	139	27	K. N. Toosi University of TechnologyThe institution will open in a new tab, Tehran, Iran	Iran
7.	Szeląg, B.	100	15	Politechnika Swietokrzyska w KielcachThe institution will open in a new tab, Kielce, Poland	Poland
8.	Vicario, J.L.	106	23	Universitat Autònoma de BarcelonaThe institution will open in a new tab, Cerdanyola del Valles, Spain	Spain
9.	Najafi, M.	224	19	College of EngineeringThe institution will open in a new tab, Arlington, United States	United States
10	Ni, B.J.	618	93	UNSW SydneyThe institution will open in a new tab, Sydney, Australia	Australia
11	Qiao, J.	877	58	Beijing University of TechnologyThe institution will open in a new tab, Beijing, China	China
12	Heo, S.K.	57	19	Imperial College LondonThe institution will open in a new tab, London, United Kingdom	United Kingdom
13	Kapelan, Z.	347	56	Department of Water Management, TU DelftThe institution will open in a new tab, Delft, Netherlands	Netherlands
14	Yoo, C.K.	400	51	Kyung Hee UniversityThe institution will open in a new tab, Seoul, South Korea	South Korea
15	Gaya, M.S.	39	11	Kano University of Science and TechnologyThe institution will open in a new tab, Wudil, Nigeria	Nigeria

16	Jekel, M.	302	73	Technische Universität BerlinThe institution will open in a new tab, Berlin, Germany	Germany
17	Santoro, D.	122	27	USP Technologies, Atlanta, United States	United States
18	Takács, I.	122	33	Dynamita SARL, Sigale, France	France
19	Batstone, D.J.	268	77	The University of QueenslandThe institution will open in a new tab, Brisbane, Australia	Australia
20	Choi, Y.	87	20	Kookmin UniversityThe institution will open in a new tab, Seoul, South Korea	South Korea
21	Esposito, G.	321	63	Università degli Studi di Napoli Federico IIThe institution will open in a new tab, Naples, Italy	Italy
22	Flores-Alsina, X.	97	32	Department of Chemical and Biochemical Engineering, Lyngby, Denmark	Denmark
23	Harrou, F.	213	42	King Abdullah University of Science and TechnologyThe institution will open in a new tab, Thuwal, Saudi Arabia	Saudi Arabia
24	Kaushal, V.	54	11	College of EngineeringThe institution will open in a new tab, Arlington, United States	United States
25	Mahmoud, A.S.	41	16	Arish UniversityThe institution will open in a new tab, El-Arish, Egypt	Egypt

\*TP= Total Publications.

The total number of keywords used in the articles was 1449. "Wastewater Treatment" emerged as the most frequently utilized keyword, appearing 1011 times, as depicted in **Fig. 6**. This was followed by "Machine Learning" observed 346 times, and "Wastewater" documented 341 times. As shown in **Table 3**, the frequently occurring keywords in the articles are

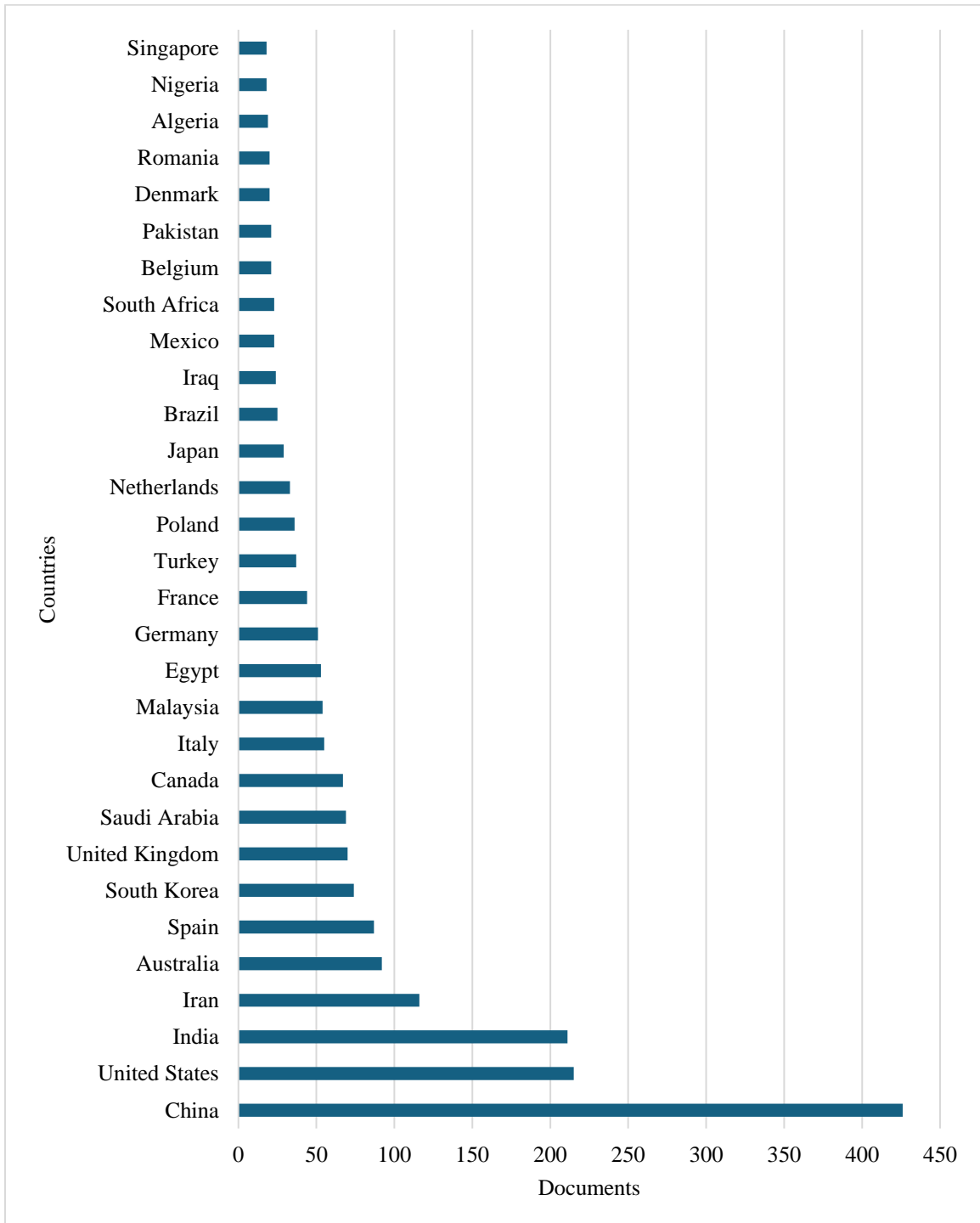
grouped into four primary subject areas: Wastewater Treatment, Modeling and Analysis Approaches, Wastewater Treatment Methods, and other related topics. These classifications highlight the most emphasized areas in Machine learning in industrial wastewater treatment and the commonly used analytical methods.

**Table 3.** Categorization of Recurring Terms in Articles on Machine learning applications for heavy metal ion removal from industrial wastewater.

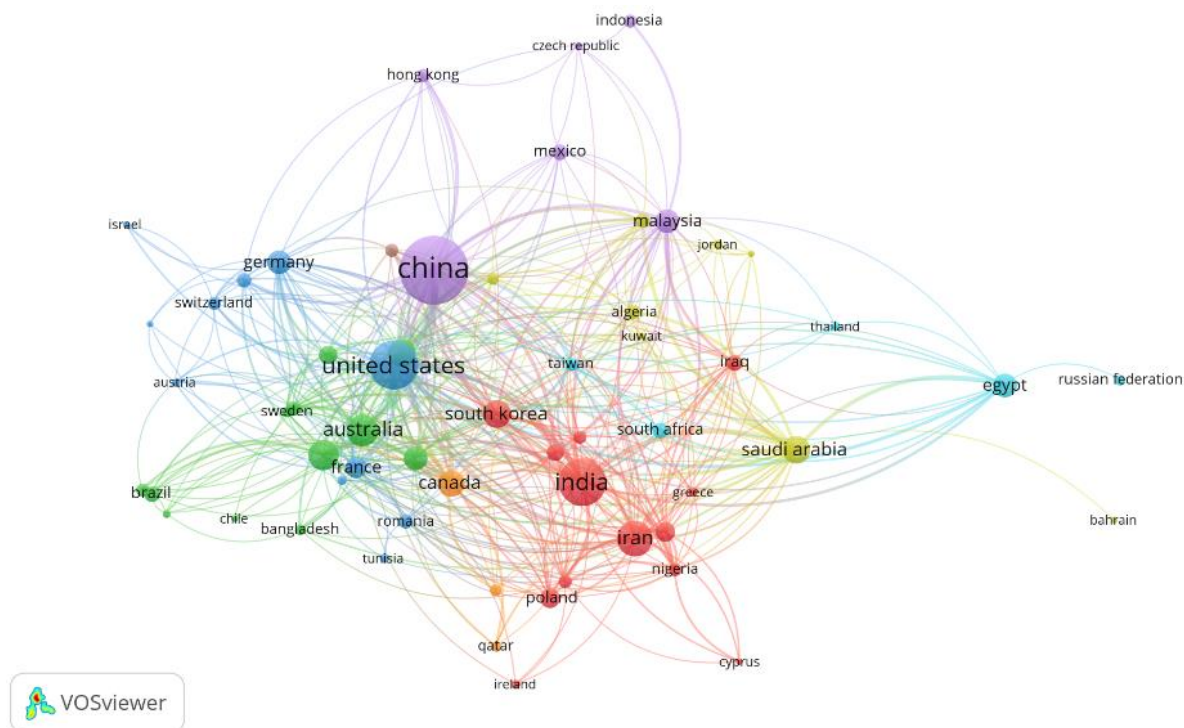
ID	Keywords	Subject Areas	Occurrences
1.	Wastewater Treatment	Wastewater Treatment	1011
2.	Wastewater		341
3.	Waste Water		117
4.	Water Treatment		117
5.	Pollutant Removal		99
6.	Water Pollutant		81

7.	Chemicals Removal (water Treatment)		45
8.	Heavy Metals		43
9.	Waste Treatment		43
10.	Industrial Water Treatment		36
11.	Machine Learning	Modeling and Analysis Approaches	346
12.	Forecasting		256
13.	Artificial Intelligence		171
14.	Artificial Neural Network		171
15.	Neural Networks		170
16.	Machine-learning		168
17.	Prediction		161
18.	Learning Systems		116
19.	Modeling		107
20.	Deep Learning		94
21.	Numerical Model		78
22.	Mean Square Error		72
23.	Regression Analysis		69
24.	Learning Algorithms		67
25.	Decision Trees		55
26.	Support Vector Machines		54
27.	Algorithm		52
28.	Random Forest		41
29.	Genetic Algorithms		40
30.	Adsorption		162
31.	Procedures		86
32.	Bioreactors	Wastewater Treatment Methods	78
33.	Biochemical Oxygen Demand		77
34.	Biological Water Treatment		75
35.	Nitrogen		66
36.	Oxidation		64
37.	Wastewater Treatment Process		63
38.	Bioreactor		58
39.	Bioremediation		46
40.	Nitrogen Removal		43
41.	Membranes		35
42.	Water Treatment Plants	Other topics	132
43.	Waste Water Management		119
44.	Wastewater Treatment Plants		105
45.	Energy Utilization		57
46.	Sustainable Developmen		51
47.	Desalination		37





**Fig. 7.** Most productive countries on Machine learning applications for heavy metal ion removal from industrial wastewater.



**Fig. 8.** Co-authorship map of countries on Machine learning applications for heavy metal ion removal from industrial wastewater.

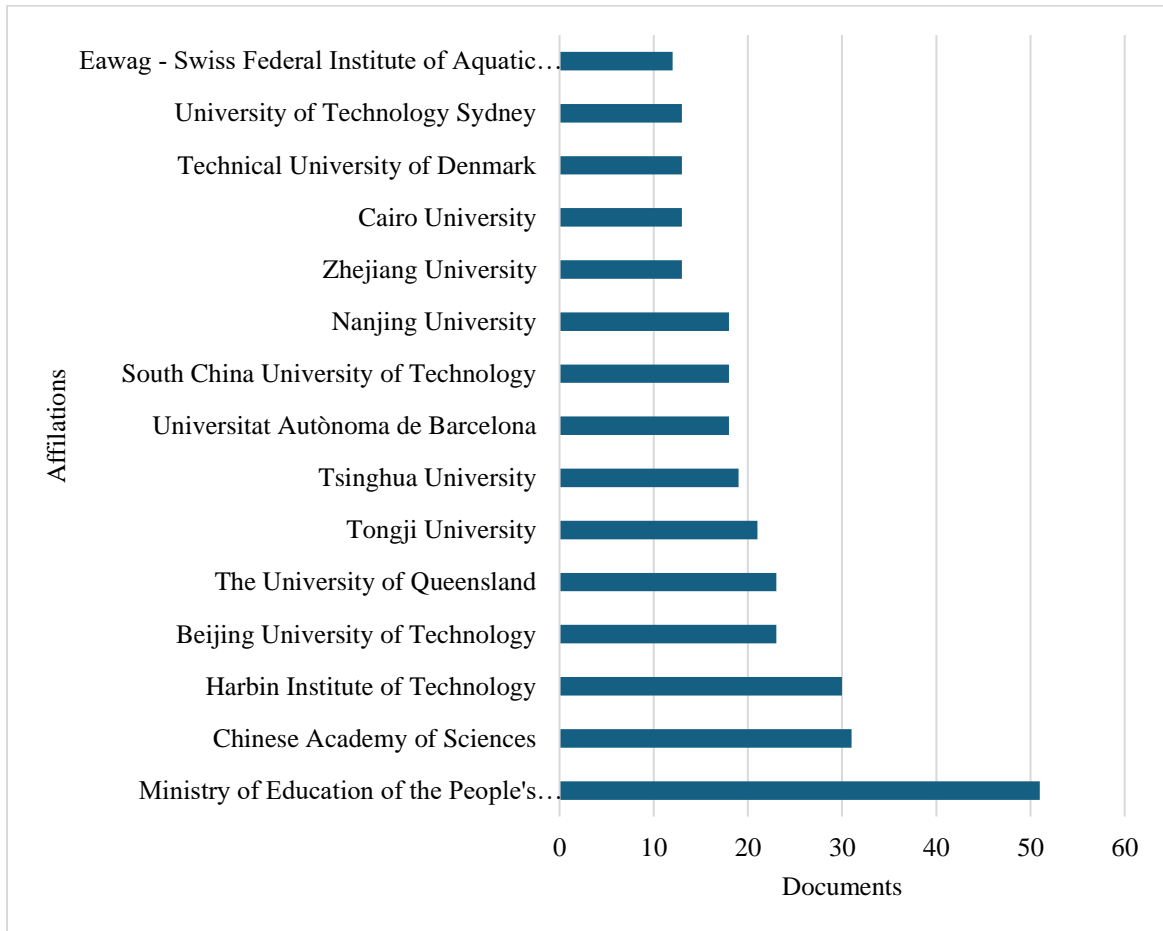
**Table 4.** Most Productive Countries on Machine learning applications for heavy metal ion removal from industrial wastewater.

COUNTRY	No of articles
China	426
United States	215
India	211
Iran	116
Australia	92
Spain	87
South Korea	74
United Kingdom	70
Saudi Arabia	69
Canada	67
Italy	55
Malaysia	54
Egypt	53
Germany	51
France	44

Turkey	37
Poland	36
Netherlands	33
Japan	29
Brazil	25
Iraq	24
Mexico	23
South Africa	23
Belgium	21
Pakistan	21
Denmark	20
Romania	20
Algeria	19
Nigeria	18
Singapore	18

The most productive affiliation was “Ministry of Education of the People's Republic of China” with 51 articles, followed by “Chinese Academy of Sciences”

with 31 articles and “Harbin Institute of Technology” with 30 articles as shown in **Fig. 9**.



**Fig. 9.** Top 15 affiliations based on the number of documents on Machine learning applications for heavy metal ion removal from industrial wastewater.

#### 4. Discussion

Heavy metal ion contamination in industrial wastewater poses a significant threat to environmental sustainability and public health. Due to the toxicity, persistence, and bio accumulative nature of heavy metals, developing effective and efficient removal methods is critical[2]–[5], [7], [55], [56]. As treatment challenges grow more complex and environmental regulations become increasingly stringent, Machine learning (ML) has emerged as a powerful tool for enhancing the optimization and control of heavy metal removal processes. Understanding the diverse factors affecting treatment efficiency such as metal ion characteristics, treatment technologies, operational parameters, and environmental conditions is essential for advancing both research and practical applications[39], [40], [43], [44], [46].

The removal of heavy metal ions is influenced by numerous material and process variables, including wastewater composition, chemical dosage, adsorbent

properties, microbial involvement, treatment duration, and environmental parameters like pH and temperature. The interplay of these factors significantly impacts removal efficiency, highlighting the importance of predictive modeling. While traditional systems rely on empirical methods and trial-and-error optimization, ML enables more advanced predictive analytics and dynamic process control, offering improved precision and adaptability[11], [13], [19].

This study conducts a bibliometric analysis using VOSviewer to investigate global research trends in applying ML to heavy metal ion removal from industrial wastewater. Among the 1700 research articles published from 2015 to March 25, 2025, a significant portion originated from countries with strong industrial activity and investment in environmental research namely China, the United States, India, Iran, and Australia.



The bibliometric insights reveal four primary subject areas: Wastewater Treatment, Modeling and Analysis Approaches, Wastewater Treatment Methods, and other related topics. These areas collectively contribute to the advancement of treatment strategies by enhancing removal efficiency, minimizing costs, and reducing environmental impact. Investigating the influence of operational conditions, material interactions, and treatment innovations such as biosorption, ion exchange, membrane filtration, and electrochemical methods is vital for achieving optimal results.

Conventional studies in heavy metal treatment typically use physicochemical properties and experimental variables as model inputs, with metal removal efficiency as the target output. ML techniques, however, facilitate the modeling of complex, nonlinear relationships, enabling more accurate forecasting and real-time process adjustments. Commonly used ML methods include Multiple Linear Regression (MLR), Random Forest (RF), Support Vector Regression (SVR), Decision Tree (DT), Gradient Boosting Regression (GBR), Artificial Neural Networks (ANN), Adaptive Neuro-Fuzzy Inference System (ANFIS), and Gene Expression Programming (GEP)[33], [48], [51], [54], [61]. Each offers distinct capabilities:

- MLR is suitable for linear relationships but limited in modeling complex, nonlinear systems.
- RF improves accuracy by aggregating multiple decision trees but is computationally intensive.
- SVR captures complex nonlinearities but lacks model transparency.
- DT offers interpretability but is prone to overfitting in high-variability datasets.
- GBR boosts model accuracy via iterative learning but requires significant computation.
- ANN models intricate nonlinear patterns but needs large datasets and careful tuning.
- ANFIS integrates fuzzy logic with neural networks for hybrid solutions, albeit with higher processing needs.
- GEP effectively models complex systems but requires careful parameter calibration.

The study emphasizes the importance of comprehensive datasets both in scale and diversity to improve the predictive accuracy of ML models. Future

research should prioritize enhancing model transparency, developing standardized datasets, and integrating ML with real-time monitoring systems. The emergence of smart sensing technologies, IoT-enabled wastewater infrastructure, and AI-driven automation is poised to revolutionize heavy metal treatment in industrial contexts.

By harnessing ML techniques, the removal of heavy metal ions from industrial wastewater can become more efficient, precise, and sustainable. Continued innovation in AI, data science, and intelligent process control will drive the development of next-generation treatment systems, supporting cleaner industrial practices and better environmental stewardship.

## 5. Conclusion

- This study presents a comprehensive bibliometric analysis of research on applying machine learning (ML) to enhance heavy metal ion removal from industrial wastewater.
- The annual publication trend demonstrates rapid growth in this interdisciplinary field, particularly after 2020, reflecting increasing global interest.
- China, the United States, and India are the most productive countries in this domain, supported by strong institutional research output and collaboration.
- Leading ML techniques identified include artificial neural networks (ANN), support vector machines (SVM), decision trees (DT), and hybrid models, which are commonly used to optimize treatment efficiency and predict removal performance.
- Keyword analysis and bibliographic mapping revealed four major research clusters: Wastewater Treatment, ML Modeling and Analysis Approaches, Treatment Methods, and Related Emerging Topics.

- Key challenges include limited access to high-quality datasets, lack of model interpretability, and barriers to integrating ML with operational systems.
- The study emphasizes the need for interdisciplinary collaboration, development of real-time ML-integrated systems, and a focus on explainable AI to drive future innovation.

### 5.1. Study Contributions

This study conducts an in-depth bibliometric and literature review on the application of Machine learning (ML) for enhancing the removal of heavy metal ions from industrial wastewater. Research in this area is categorized into four primary domains: Wastewater Treatment, Modeling and Analysis Approaches, Wastewater Treatment Methods, and other related topics. These thematic classifications offer insight into current research priorities, prevalent methodologies, and the evolving landscape of ML integration in industrial wastewater treatment. The volume of related publications has grown significantly since 2020, peaking in 2024, with projections indicating continued momentum in 2025 and beyond.

Key contributors to this field include China, the United States, India, Iran, and Australia, underscoring their strong focus on environmental engineering, pollution mitigation, and AI-driven innovations. Among the most influential researchers are those affiliated with institutions such as Ministry of Education of the People's Republic of China, Chinese Academy of Sciences, articles and Harbin Institute of Technology reflecting the global scope and collaborative nature of this research. Leading journals like *Water Research*, *Desalination* and *Journal Of Water Process Engineering* have emerged as central platforms for disseminating advancements in AI-powered wastewater treatment technologies.

The analysis further highlights the growing impact of ML techniques in predicting and optimizing heavy metal ion removal. Models such as artificial neural networks (ANN), support vector regression (SVR), random forests (RF), gradient boosting regression

(GBR), multiple linear regression (MLR), and decision trees (DT) are frequently employed due to their ability to capture complex interactions between treatment parameters and pollutant behavior. More sophisticated approaches, including adaptive neuro-fuzzy inference systems (ANFIS) and gene expression programming (GEP), are particularly valuable for modeling nonlinear relationships and system uncertainties. Despite their effectiveness, challenges such as computational intensity, overfitting risks, data scarcity, and lack of model interpretability remain. The selection and tuning of ML models, therefore, play a critical role in achieving optimal performance for specific treatment scenarios.

### 5.2. Suggestions for Academia and Industry Practice

This study is expected to accelerate progress in industrial wastewater management by emphasizing the critical role of Machine learning (ML) in optimizing heavy metal ion removal processes. Based on the findings, the following key recommendations are proposed to guide both academic research and practical applications in the field:

- ML models will form the backbone of predictive frameworks for assessing and enhancing the efficiency of heavy metal ion removal methods.
- Continuous refinement of these models will improve accuracy, adaptability, and real-time decision-making in diverse industrial treatment settings.
- This research supports the development of intelligent, automated treatment systems, facilitating smart monitoring and control of heavy metal remediation processes.
- ML-enabled simulations will allow for the optimization of treatment parameters, such as pH, dosage, contact time, and temperature, reducing trial-and-error experimentation.
- Future studies should explore ML-driven optimization for emerging green adsorbents like biochar, modified clays, and nanomaterials to support eco-friendly wastewater treatment solutions.
- Quality control strategies empowered by ML will help industries meet regulatory standards while maintaining cost-effectiveness.
- Expanding and diversifying datasets—including data from various industries and

effluent compositions—is essential for building more generalizable and robust ML models.

- Time-dependent and real-time modeling techniques will be essential for capturing dynamic treatment behaviors and long-term performance trends.
- Interdisciplinary collaboration between environmental science, AI, and chemical engineering will be key to developing hybrid models and intelligent treatment frameworks.
- Integrating ML with smart sensors, IoT devices, and automation systems will enable adaptive, self-regulating treatment operations.
- Greater focus on explainable AI (XAI) will improve model interpretability, fostering trust and transparency in regulatory and operational environments.
- Future research should emphasize sustainability by minimizing energy consumption, chemical usage, and waste generation through AI-optimized treatment design.

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