Chemosphere 362 (2024) 142792

Contents lists available at ScienceDirect

Chemosphere

journal homepage: www.elsevier.com/locate/chemosphere

Application of machine learning models to improve the prediction of pesticide photodegradation in water by ZnO-based photocatalysts

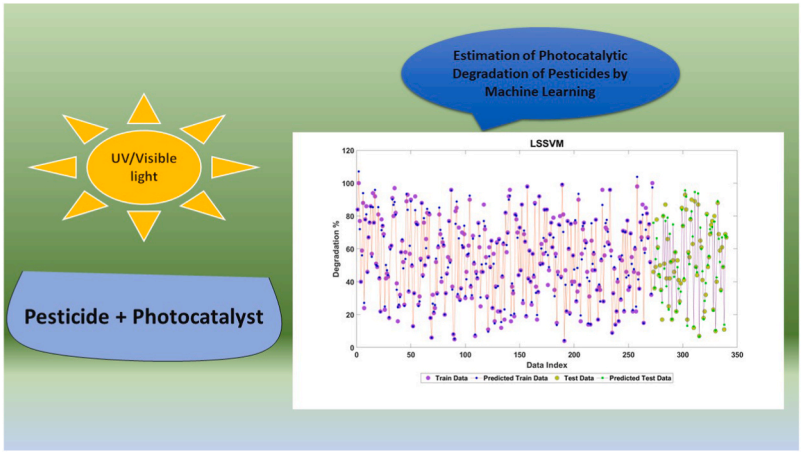
Amir Dashti, Amir Hossein Navidpour, Farid Amirkhani, John L. Zhou *, Ali Altaee

Centre for Green Technology, School of Civil and Environmental Engineering, University of Technology Sydney, 15 Broadway, NSW 2007, Australia

HIGHLIGHTS

- Photodegradation of pesticides by ZnO-based photocatalysts was reviewed as a green technology.
- Novel machine learning models were developed to predict photocatalytic process.
- RBF model showed the best performance for modeling pesticide photodegradation.
- Key parameters regulating photocatalysis process were identified by sensitivity analysis.

GRAPHICAL ABSTRACT



ARTICLE INFO

Keywords:
Machine leaning
Pesticides
Photocatalytic degradation
Wastewater treatment
ZnO

ABSTRACT

Pesticide pollution has been posing a significant risk to human and ecosystems, and photocatalysis is widely applied for the degradation of pesticides. Machine learning (ML) emerges as a powerful method for modeling complex water treatment processes. For the first time, this study developed novel ML models that improved the estimation of the photocatalytic degradation of various pesticides using ZnO-based photocatalysts. The input parameters encompassed the source of light, mass proportion of dopants to Zn, initial pesticide concentration (C_0), pH of the solution, catalyst dosage and irradiation time. Additionally, physicochemical properties such as the molecular weight of the dopants and pesticides, as well as the water solubility of both dopants and pesticides, were considered. Notably, the numerical data were extracted from the literature via relevant tables (directly) or graphs (indirectly) using the web-based tool WebPlotDigitizer. Four ML models including multi-layer perceptron artificial neural network (MLP-ANN), particle swarm optimization-adaptive neuro fuzzy inference system (PSO-ANFIS), radial basis function (RBF), and coupled simulated annealing-least squares support vector machine (CSA-LSSVM) were developed. In comparison, RBF showed the best accuracy of modeling among all models, with the highest determination coefficient (R^2) of 0.978 and average absolute relative deviation (AARD) of 4.80%. RBF model was effective in estimating the photocatalytic degradation of pesticides except for 2-chlorophenol,

* Corresponding author.
E-mail address: junliang.zhou@uts.edu.au (J.L. Zhou).

https://doi.org/10.1016/j.chemosphere.2024.142792
Received 9 January 2024; Received in revised form 16 May 2024; Accepted 4 July 2024
Available online 5 July 2024

triclopyr and lambda-cyhalothrin, where CSA-LSSVM model demonstrated superior performance. Dichlorvos was completely degraded by ZnO photocatalyst under visible light. The sensitivity analysis by relevancy factor exhibited that light irradiation time and initial pesticide concentration were the most important parameters influencing photocatalytic degradation of pesticides positively and negatively, respectively. The new ML models provide a powerful tool for predicting pesticide degradation in wastewater treatment, which will reduce photochemical experiments and promote sustainable development.

1. Introduction

There is increasing urgency for improved water security due to worldwide freshwater shortage, water pollution and climate change (Qiu et al., 2023). As a repetitive and persistent problem, the occurrence of toxic chemicals such as dyes from textile industries, pesticides generated by agriculture sector, and antimicrobials and analgesics as part of the pharmaceuticals seriously reduce water quality (Li et al., 2023). One of the most significant type of contaminants in drinking water is considered to be pesticides due to their significant global production, wide applications, and persistence (Izadifard et al., 2013; Liu et al., 2022). Nine of the twelve highly polluting and perilous chemicals in the world are pesticides or their intermediate components (Khan and Pathak, 2020), although pesticides are generally seen as a category of chemicals used for providing nutrition and fulfilling the needs of global population (Kong et al., 2022). Pesticides are complicated mixtures of chemicals with complex structures; often their intermediates or breakdown products are more toxic than the parent compounds (Schostag et al., 2022). Pesticides have a terrible effect on organisms' development, so they can influence an entire system of evolution (Hamilton et al., 2003). Many studies suggest that at the point of application, more than 98% of insecticides used in agricultural areas do not have rapid degradation and end up being absorbed into the environment (Muhamad, 2010). There are many different pesticides in the water system that come from a variety of sources, e.g. industry, agricultural sectors, and chemical spills. There has been long-term concern about pesticide toxicity, slow biodegradation and perseverance in the environment (Sakkas et al., 2005). In addition, the potential influence of pesticides on human health and quality of life has long been recognized, from skin contact, inward breath, or ingestion (Damalas and Koutroubas, 2016). Pesticide effects on the health of individuals occur after bioaccumulation followed by metabolism, removal and excretion, and shall be determined by the type, concentration, and duration of exposure as well as the individual's state of health (Kalyabina et al., 2021; Nicolopoulou-Stamati et al., 2016). Shockingly, pesticide residues have been detected in prepared food and drinks, counting cooked meals, snacks, natural products juices, drinking water, alcoholic drinks, and animal feed, as ordinary washing and peeling do not remove them efficiently (Reiler et al., 2015). Furthermore, human breast drain tests have also detected pesticide residues, which raise concerns related to fetal presentation and infant health (Brahmand et al., 2019).

Globally, approximately 2 million tons of pesticides are used annually to combat weeds, insects, and pests. Herbicides and insecticides are the predominant types, accounting for 47.5% and 29.5% of total pesticide usage, respectively (Syafrudin et al., 2021). Between 2000 and 2016, England and Wales experienced a total of 1571 instances of water quality compliance failures due to the detection of pesticides in drinking water exceeding the 0.1 μg L^{-1} limit. These compliance failures involved 35 distinct pesticides out of the 248 compounds approved for use in the UK (Cosgrove et al., 2019).

In response to the adverse effects of pesticides on human health, the Drinking Water Directive 98/83/EC establishes maximum concentration limits. Specifically, it sets a threshold of 0.1 μg L^{-1} for each individual pesticide and its degradation products, and 0.5 μg L^{-1} for the cumulative concentration of all pesticides in a sample. Additionally, the new EU directive 2020/2184 emphasizes a risk-based approach to pesticide monitoring for identifying pesticides likely to be present in a specific environment in water intended for human consumption (Kruć-Fijałkowska et al., 2022). According to European Union regulations, very low concentrations of pesticides are considered the limit values for pesticides in drinking water, with thresholds set at 5 μg L^{-1} for the sum of all pesticides and 1 μg L^{-1} for individual pesticides (Kalantary et al., 2022).

To combat water contamination, the development of water treatment methods (e.g. physical, chemical, biological) is of fundamental importance (Jia et al., 2023; Tang et al., 2022; Wu et al., 2022). Among different methods, photocatalysis is hugely popular as it can be carried out in many applications, with relatively fast degradation rates, and capacity to mineralize pollutants under ambient conditions (Ong et al., 2018).

Currently, a number of less complex ML models such as artificial neural networks (ANN) have been effectively employed in water and wastewater treatment field (Kim et al., 2016; Wan et al., 2022). With an overwhelming amount of input data with no feature engineering, ML systems are the best suited for estimating complex functions (Amirkhani et al., 2021; Dashti et al., 2020a, 2021b, 2023; Raji et al., 2019). Irfan et al. (2022) used response surface methodology (RSM) and ANN to optimize the permeability of the membranes in membrane rotating biological contactors. They managed to increase the productivity of the treatment by significantly reducing membrane fouling. Artificial Intelligence strategies are robust and reliable, and they have been used widely in different areas of research such as wastewater treatment (Wang et al., 2021).

To design a photocatalytic process for the effective degradation of pesticides, it is important to understand the complex and often nonlinear relationships which exist between the process variables (e.g. light intensity, catalyst dosage, and pollutant concentration) and photocatalysis results, as well as the interactions between different variables (Ayodele et al., 2021). The relationships between these factors are not always linear, meaning that small changes in one parameter can have an important impact on the overall process efficiency. By understanding the relationships between the process variables, photocatalytic reactors can be better designed to optimize the photocatalytic degradation process and maximize the removal efficiency. Therefore, this research aimed to develop novel ML methods (MLP-ANN, PSO-ANFIS, RBF, CSA-LSSVM) for the estimation of the photocatalytic degradation of different types of pesticides over ZnO-based photocatalyst. The input parameters were light source (UV/visible light), mass proportion of the dopants to Zn, initial concentration of pesticide (C_0), pH of the solution, and irradiation time which were considered the process parameters, while the molecular weight of dopants and pesticides, and water dissolvability of dopants and pesticides were regarded as the structural parameters of materials. The estimation of the photocatalytic degradation of each pesticide was carried out by collecting a set of data for the input parameters. A systematic literature review identified relevant research on ZnO photocatalysts for pesticide removal. Studies with all the above-mentioned input and output data, demonstrating strong correlations, were chosen for further analysis. It is hypothesized that the ML models will demonstrate high-performance prediction of pesticide photocatalysis in water and wastewater. To evaluate the prediction strength of these models, the modeling results were compared with experimental values through a variety of statistic and visual analyses.

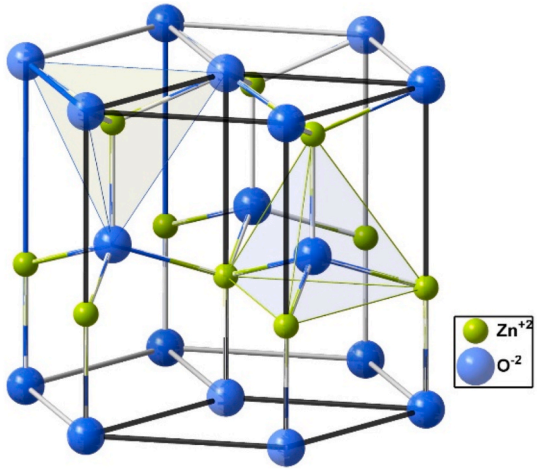


Fig. 1. Wurtzite (hexagonal) crystalline structure of ZnO. Reproduced with permission from (Escudero and Escamilla, 2011). Copyright 2011 Elsevier.

2. Review and data selection

Different semiconductors such as TiO_2 (Navidpour et al., 2023a), ZnO (Navidpour et al., 2023d), and g-C_3N_4 (Navidpour et al., 2023b) have been used for the photocatalytic degradation of organic contaminants. Although TiO_2 or P25 is known as a benchmark semiconductor in photocatalysis (Navidpour et al., 2023a), wurtzite ZnO provides a more superior photocatalytic activity than TiO_2 in some cases and is an under-explored alternative to TiO_2 (Navidpour et al., 2023c; Sakthivel et al., 2003). Zinc oxide is odorless and insoluble in water (Lee et al., 2016), and crystallizes in three different crystal structures including Wurtzite (hexagonal), zinc blende (cubic), and rocksalt (cubic) (Espitia et al., 2012). Notably, ZnO is considered a multifunctional material with extensive usages in various fields such as sensors, catalysts, environmental remediation, pharmaceutical drugs, and biological applications (Rahman et al., 2021). Generally, wurtzite ZnO (Fig. 1) is considered the most common crystalline structure of ZnO used in photocatalysis with ease of synthesis (Rajbongshi and Samdarshi, 2014).

ZnO has many promising features such as versatile synthetic conditions for different morphologies, high photocatalytic properties, non-toxicity, abundance, sufficient electron mobility, low cost, high absorption coefficient, large exciton binding energy of 60 meV at room temperature, and high redox potential (Abbas and Bidin, 2017; Ansari et al., 2015). The wide band gap energy of ZnO (~3.37 eV) restricts its application under visible light irradiation (Rahman et al., 2021). Several strategies have been considered to improve the photocatalytic activity of ZnO. Among those, element doping is a widely used method that can change morphological, structural, and optical features of ZnO nanoparticles (Rahman et al., 2021).

The photodegradation effectiveness is affected by the characteristics of photocatalysts like surface area and pore volume, properties of pesticides (e.g. initial concentration, chemical structure) and photocatalytic reaction including intensity of light, catalyst dose, pH, and operation time, which should all be carefully examined (Derikvandi and Nezamzadeh-Ejhieh, 2017). In most cases, a few days or even months are needed for full optimization of these preparatory conditions by carrying out carefully designed and lengthy tests. Using conventional photocatalytic testing, the optimum values of these parameters for photodegradation have been explored to a large extent (Bassi et al., 2022; Sekar and Yadav, 2021). Alternative methods like machine learning (ML) techniques can recognize the relationship between different process parameters and their corresponding targets (Amirkhani et al., 2022, 2023). ML approaches have many unique features, such as the estimation of nonlinear and complex systems, the ability to distinguish each parameter's impact, and the discovery of optimum values for each parameter (Tabatabai-Yazdi et al., 2021). Yadav and colleagues (Yadav et al., 2021) fabricated light-responsive nanostructures of ZnO doped with lithium using various lithium concentrations through a simple combustion method at low temperatures. The findings of their investigation illustrate that during Triclopyr degradation through photodegradation, a robust electronic bonding between lithium and ZnO enhances the efficacy of charge transfer and delays their recombination. The modification in the optical and surface characteristics of ZnO due to the incorporation of lithium into its lattice also contributed to the heightened performance of lithium-doped ZnO.

Peng and collaborators (Peng et al., 2019) crafted Ag/ZnO nanocomposites and utilized them in the photocatalytic breakdown of phenol with ozone. Subsequently, they noted a marked advancement in the photocatalytic breakdown of phenol catalyzed by Ag/ZnO substances. Furthermore, they detected a collaborative influence between photocatalysis and ozonation. Benhebal and co-authors (Benhebal et al., 2013) investigated the photocatalytic breakdown of phenol and benzoic acid in water utilizing ZnO powder synthesized via the sol-gel technique. Daneshvar and colleagues (Daneshvar et al., 2007) synthesized ZnO nanocrystals through a precipitation method for the decomposition of diazinon in aqueous solution. The findings indicated that the photocatalytic process with ZnO nanoparticles, having an average size of 14 nm, exhibited the highest energy efficiency. Consequently, it could be inferred that around 80% elimination of the pesticide, upon optimizing operational conditions, could be accomplished in a relatively short period, approximately 80 min.

Evgenidou and colleagues (Evgenidou et al., 2005) explored the photocatalytic breakdown of an organophosphorus insecticide, dichlorvos, employing two distinct photocatalysts (TiO_2 and ZnO). The exposure of zinc oxide suspensions resulted in the disappearance of dichlorvos, although complete mineralization was not achieved, leading to the formation of intermediates. Premalatha and co-researchers (Benhebal et al., 2013) investigated the photocatalytic efficacy of ZnO and ZnO–Bi2O3 using Lambda-Cyhalothrin (LCHT), a pyrethroid pesticide detrimental to humans and animals, under visible light irradiation. Anju and colleagues (Anju et al., 2012) explored the degradation of trace levels of phenol pollutants in water utilizing Zinc oxide catalyst under UV), Ultrasonic (US), and a combination of UV and US irradiation.

In the case of ZnO photocatalysts with dopant, Shirzad and Siboni (Shirzad-Siboni et al., 2017) scrutinized the photocatalytic disintegration of organophosphorus pesticide diazinon using ZnO nanorods infused with copper. They fabricated Cu-doped ZnO nanorods employing a simple co-precipitation method. Cu-doped ZnO nanorods had significantly higher photocatalytic degradation rather than ZnO photocatalysts in diazinon degradation. Rani and colleagues (Rani et al., 2023) synthesized nanostructured ZnO and Zinc Oxide doped with Lanthanum (La) via the hydrothermal synthesis method, resulting in highly effective photocatalytic materials. They examined the degradation of 2-chlorophenol (2-CP) using both ZnO and La-doped ZnO photocatalysts under optimal pH, irradiation duration, and catalytic dosage conditions. Remarkably, ZnO achieved a maximum degradation efficiency of 75.85%, while La-doped ZnO exhibited even higher efficiency at 83.92%.

Machine learning methodologies can be effectively applied in modeling the photocatalytic degradation process. Salahshoori et al. (2024) employed utilized various ML models to predict the elimination of tetracycline (TC) via photocatalysis using Metal-Organic Frameworks (MOFs). Among these models, the GAPSO-LSSVM model emerged as the accurate one.

Gheytanzadeh et al. (2022) compiled an extensive database consisting of 374 data points sourced from previous experiments. They introduced a robust machine learning approach, Gaussian process regression (GPR) model, incorporating four kernel functions to predict the photodegradation of tetracycline (TC) based on features of Metal-Organic Frameworks (MOFs) such as surface area and pore volume, along with process parameters including radiation time, catalyst

Table 1
Physicochemical properties of the target pesticides and dopants for ZnO.

Pesticide/Dopant	MW (g mol^{-1})	Solubility in water (mg L^{-1})
2-Chlorophenol	128.556	5165
Diazinon	304.345	6.456
Dichlorvos	220.976	1889
Triclopyr	256.471	374.9
Trifluralin	335.279	0.209
Lambda-cyhalothrin	449.850	0.001
Phenol	94.111	26160
La	138.906	53940
Cu	63.546	420800

dosage, TC concentration, and pH. The GPR models exhibited strong performance, with the GPR-Matern model demonstrating the most precise accuracy. Navidpour and co-authors (Navidpour et al., 2024) investigated the use of Adaptive Boosting (AdaBoost), Gradient Boosting Machine (GBM), and Random Forest (RF) machine learning algorithms to simulate and predict the photocatalytic degradation of perfluorooctanoic acid (PFOA). Their modeling results indicated that both the GBM and RF models outperformed the AdaBoost model in terms of predictive performance.

Deylami and colleagues (Deylami et al., 2023) examined the photodegradation of disulfine blue dye and tetracycline over g-CN/Ag3-VO4/PAN nanofibers using Response Surface Methodology (RSM), RBF-NN) and ANFIS modeling. Their findings suggest that the ANFIS model provides more accurate predictions for the degradation of TC. Jaffari and colleagues (Jaffari et al., 2023) delved into the capabilities of multiple machine learning models to forecast the photocatalytic breakdown of malachite green in wastewater using diverse NM-BiFeO3 composites. They assembled an extensive databank containing 1200 data points gathered from diverse experimental setups. Evaluation metrics revealed that the CatBoost model attained the highest test coefficient of determination (0.99).

The search for relevant experimental data was through the Scopus database. Extensive research in pesticide photodegradation has been reported in different studies (Anju et al., 2012; Benhebal et al., 2013; Daneshvar et al., 2007; Evgenidou et al., 2005; Peng et al., 2019; Premalatha and Miranda, 2019; Rani et al., 2023; Sadeghi et al., 2021; Shirzad-Siboni et al., 2017; Yadav et al., 2021), which allow its deep analysis and forecast. With respect to the accessible information in literature for the photocatalytic treatment of different pesticides, the photocatalytic parameters, and physiochemical parameters of pesticides and dopants of ZnO were assembled. The source of light (UV (1) and visible light (2)), mass proportion of the dopants to Zn, initial pesticide concentration (C_0), pH of the solution, and irradiation time were considered as the process parameters. The physicochemical properties such as the molecular weight of the dopants and pesticides, and water dissolvability of dopants and pesticides, were obtained from the predicted values using the US Environmental Protection Agency EPISuite™, which is available in Chemspider website (www.chemspider.com). The details of these parameters are shown in Table 1.

A comprehensive dataset was obtained by considering seven distinctive pesticides (diazinon, dichlorvos, triclopyr, trifluralin, lambda-cyhalothrin, phenol, 2-chlorophenol), in their photocatalytic degradation by ZnO-based photocatalysts with and without dopants. It should be noted that Cu and La were considered as dopants, while impurities were not regarded as doping elements. The numerical data were gathered and extracted directly via tables or indirectly via graphs from the publications using the web-based tool WebPlotDigitizer 4.7 (https://apps.automeris.io/wpd/). The extracted data are presented in Table S1 (Supplementary Material). Notably, the gathered data have common input parameters. Characteristics of the photocatalysts, techniques used for the pollutant analysis, detection limits of the analysis methods, and the number of experimental repetitions for the publications used to gather data are provided in Table S2. Table 2 provides the details of the experimental conditions and the degradation performance for the target pesticides.

To set up precise ML models, 80% of the datapoints were randomly isolated as the train set and the remaining (20%) were regarded as the test data to assess the accuracy of the models. Statistical analysis was measured by the calculation of measurable variables such as the determination coefficient (R^2), average absolute relative deviation (AARD), root-mean-square error (RMSE), and the standard deviation (STD), which are described in equations (1)–(4):

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left[x_i^{predicted} - x_i^{experimental}\right]^2}{\sum_{i=1}^{n}\left[x_i^{predicted} - x^m\right]^2}, x_m = \frac{\sum_{i=1}^{n} x_i^{experimental}}{n} \quad (1)$$

$$AARD\ (\%) = \frac{100}{n}\sum_{i=1}^{n}\frac{\left|x_i^{predicted} - x_i^{experimental}\right|}{x_i^{experimental}} \quad (2)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(x_i^{experimental} - x_i^{predicted}\right)^2} \quad (3)$$

$$STD = \sqrt{\sum_{i=1}^{n}\left(\frac{\left(x_i^{predicted} - x_m\right)^2}{n}\right)} \quad (4)$$

Table 2
A summary of experimental conditions and degradation efficiency from the photocatalytic treatment of water by ZnO-based photocatalysts.

Pesticide	Type of dopant	Irradiation time (h)	Catalyst dosage (mg L^{-1})	Solution pH	Initial pesticide concentration (mg L^{-1})	Degradation (%)	Number of data	Ref.
2-Chlorophenol	La[a]	0.30–2.00	333–1667	2.0–10.0	10.0	64.39–84.00	14	Rani et al. (2023)
2-Chlorophenol	–	0.30–2.00	333–1667	2.0–10.0	10.0	33.71–77.00	14	Rani et al. (2023)
Diazinon	Cu[b]	0.25–2.00	10–1000	3.0–11.0	10.0–50.0	4.00–99.00	100	Shirzad-Siboni et al. (2017)
Diazinon	–	0.17–2.00	25–200	3.5–11.3	16.0–30.0	7.00–88.00	52	(Daneshvar et al., 2007; Shirzad-Siboni et al., 2017)
Dichlorvos	–	0.03–2.00	100–500	7.0–7.2	10.0–50.0	16.00–100	73	Evgenidou et al. (2005)
Triclopyr		0.25–2.00	1000	7.0	10.0	6.00–17.00	8	Yadav et al. (2021)
Trifluralin	–	0.33–1.00	50–150	9.0	0.6	58.00–92.00	9	Sadeghi et al. (2021)
Lambda-cyhalothrin	–	0.50–3.00	1200	7.0	50.0	33.00–69.47	6	Premalatha and Miranda (2019)
Phenol	–	0.25–2.00	20–2500	2.5–12.5	40.0–250.0	12.00–87.00	64	(Anju et al., 2012; Benhebal et al., 2013; Peng et al., 2019)
–	–	0.03–3.00	10–2500	2.0–12.5	0.6–250.0	4.00–100	340	–

[a] Mass ratio of doping element to Zn: 0.123.
[b] Mass ratio of doping element to Zn: 0.007.

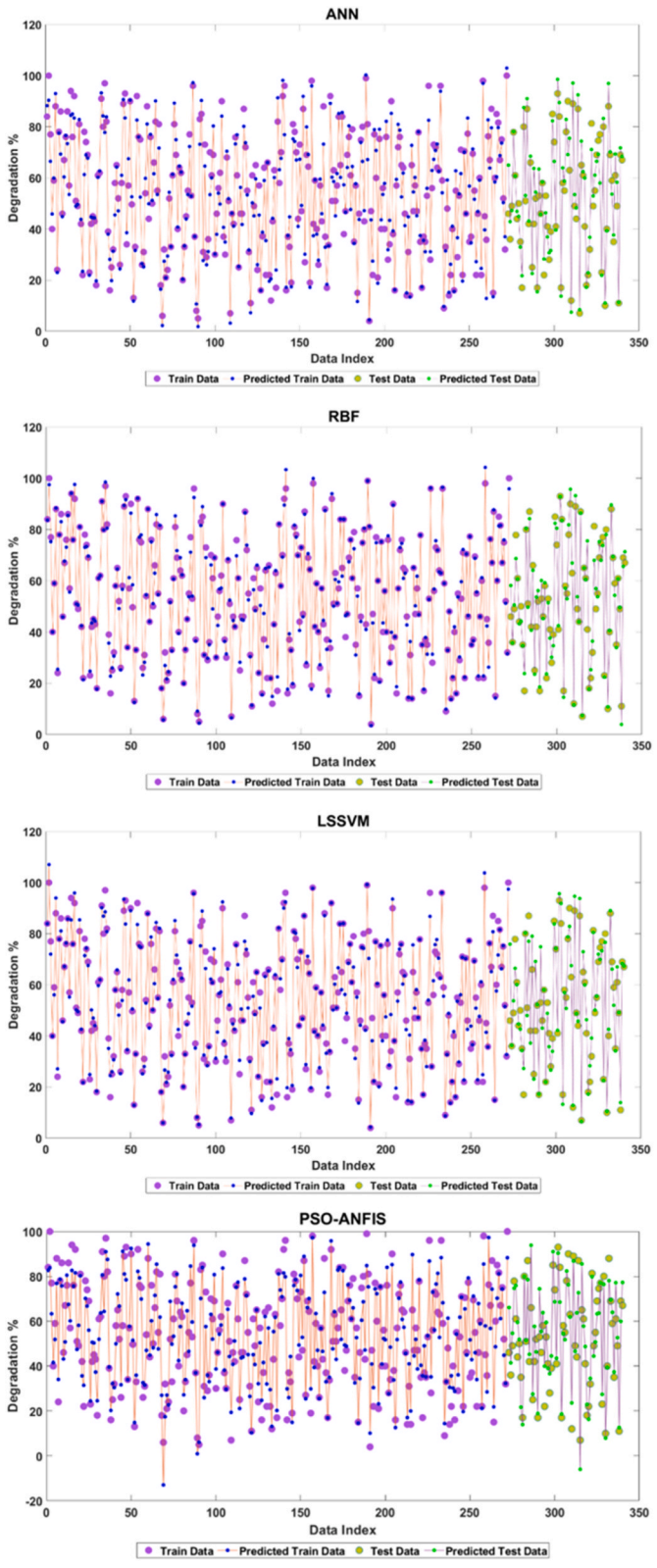


Fig. 2. Comparison between experimental results and estimated values from the developed models against index of data points.

3. Results and discussion

3.1. Model development

The details of ML methods are presented in the Supplementary Material. In this study, the RBF kernel was utilized to propose CSA-LSSVM. CSA used two variables of γ (389.4) and σ^2 (2.7496). In expansion, particle swarm optimization (PSO) (Eberhart and Kennedy, 1995; Kıran et al., 2012; Kuo et al., 2010) was connected to optimize the ANFIS structure and to determine the ideal values of ANFIS variables. The Generalized Gaussian sort was accomplished by MFs within the fuzzy sub-domain, as exhorted in the literature (Amirkhani et al., 2021; Dashti et al. 2020a, 2020b, 2021b, 2021c, 2023). PSO parameters were changed by trial and error to obtain the highest accuracy for PSO-ANFIS model. Table S3 records the details of the PSO-ANFIS models utilized to compute photocatalytic degradation of pesticides by ZnO-based materials.

To improve the MLP models, the number of neurons in a hidden layer were changed. The RMSE of the tested data decided the accuracy of the model. The Levenberg-Marquardt (LM) training approach empowered us to prepare and control the weight values as the method showed excellent stability in the training stage and presented a sharp convergence in training process (Yadav et al., 2021). In order to find the optimal neuron for the MLP-ANN show, a trial and error approach was used. The results showed that a layer of 25 neurons covered by the MLP-ANN appeared to generate the best design.

In the RBF model, tuning variables, and counting spread and the maximum number of neurons (MNN) are necessary to be decided (Barati-Harooni et al., 2017; Tatar et al., 2016). To obtain an accurate model effectively, the optimization of these parameters is crucial. Through trial and error operation (Tatar et al., 2016), the optimum values were obtained in the 28 to 201 range for Spread MNN and maximum number of neurons.

3.2. Modeling results and validation

Several evaluation methods have been carried out to assess the estimation capability of proposed artificial intelligence models for photodegrading pesticides using ZnO-based photocatalysts. Two basic approaches, statistical and visual comparison plots, were used for assessing the approval. The statistical parameters show the degree to which the actual and expected values are aligned. For the training and testing datasets, these parameters were recorded in Table S4. For the test data that were used in the ANN, RBF, PSO-ANFIS and CSA-LSSVM models on a case-by-case basis, the R^2 values achieved were 0.912, 0.935, 0.841, and 0.911, respectively. Such results confirmed that the estimation of photocatalytic degradation of pesticides was sufficiently precise by RBF and CSA-LSSVM with their comparative statistics for AARD, RMSE and STD. RBF with AARD of 4.80% for total data, as shown in Table S4, appeared to be the most precise model for photocatalytic pesticide degradation by ZnO-based photocatalysts. Fig. 2 shows that pesticide photodegradation values from experiments were accurately estimated. Thus, the created ML models show dependable expectation execution for the pesticides photodegradation framework. In addition, in expansion the real efficiencies of photodegradation for pesticides were compared to model output obtained by ML (Fig. 3). The closer the data is to the bisector line, the more accurate the recommended models are. For all the ML models, especially the RBF, the estimated data points were closely following the experimental data points with a R^2 value of 0.978. The results therefore confirmed that ML models were able to estimate the real dataset in this analysis.

Table S5 shows the accuracy of the ML models in terms of AARD for the estimation of photocatalytic degradation of the considered pesticides. As the results show, RBF can estimate the photocatalytic degradation of all pesticides except 2-chlorophenol/La, 2-chlorophenol, triclopyr and lambda-cyhalothrin, for which CSA-LSSVM model demonstrated better performance.

3.3. Effect of input parameters on photocatalytic degradation of pesticides

Fig. 4 shows the impact of process variables on the photodegradation

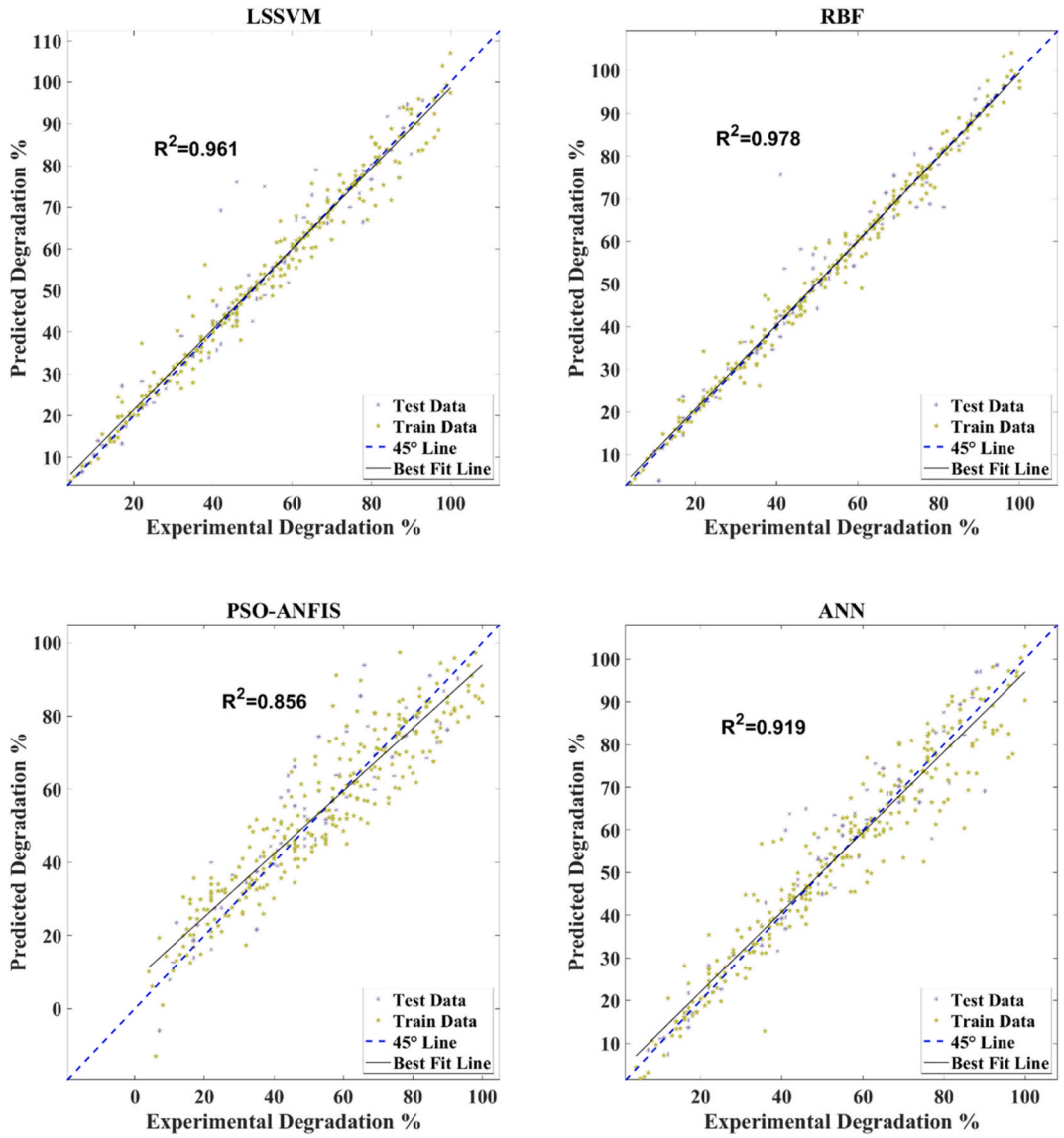


Fig. 3. Predictions of pesticide photodegradation (%) by ML models in comparison to experimental results.

of pesticides using ZnO-based photocatalyst. Undoubtedly, the irradiation time is considered an important factor in photocatalysis process. Generally, the more the time of irritation, the higher degradation is expected. However, the rate of degradation depends on several parameters including type of photocatalyst, type of pollutant, dosages of photocatalyst and pollutant, type of reactor, solution pH, and source of light. Notably, the vital impact of time on the photocatalytic degradation of pesticides is evidenced in Fig. 4(a) and (e).

Solution pH is an important parameter affecting the photocatalytic performance (Rani et al., 2023). Notably, the electrostatic interaction between the catalyst and the pollutant depends on solution pH and the catalyst pH_{zpc} values. At pH higher than pH_{zpc}, the catalyst surface is negatively charged, whereas it is positively charged at pH lower than pH_{zpc} (Rani et al., 2023). Rani et al., (2023) evaluated the effect of pH (2–10) on the photocatalytic degradation of 2-chlorophenol over ZnO and La-doped ZnO under UV and visible light irradiation, respectively, where acidic medium generally yielded higher efficiency than basic medium for both photocatalysts (with the highest efficiency at pH 2). Considering their findings, the effect of solution pH on the photocatalytic degradation of 2-chlorophenol (experimental and estimated values) using La-doped ZnO under visible light irradiation is shown in Fig. 4b. The superior efficiency of ZnO and La-doped ZnO at acid medium (specifically at pH 2) has been attributed to the electrostatic interaction between phenolate anions and positively charged surface of the photocatalysts. Formation of carbonate anions, acting as scavengers for OH^- anions, could also be responsible for the reduced photocatalytic degradation of 2-chlorophenol at basic medium (Rani et al., 2023). Shirzad-Siboni et al. (Shirzad-Siboni et al. (2017) evaluated the effect of pH (3–11) on the photocatalytic degradation of diazinon over Cu-doped ZnO nanorods. Similarly, acidic medium yielded higher efficiency than basic medium, but the best efficiency was obtained at neutral pH (i.e. 7) due to the photo-corrosion of ZnO in basic and acidic solutions. In addition, considering the electrostatic interaction between the catalyst and the pollutant, the optimal pH was expected to be in the range of 2.6 (pK_a value of diazinon) and 7.8 (pH_{zpc} value of Cu-doped ZnO) where negatively charged diazinon could readily react with positively charged Cu-doped ZnO nanorods.

The photocatalyst dosage is considered another important factor in photocatalytic reactions. Usually, increasing the amount of photocatalyst, up to an optimum level which corresponds to the optimum of light absorption, can improve the degradation efficiency. Hence, dosages higher than the optimum value cannot be effective due to the blocked passage of light and the increased light scattering (Evgenidou et al., 2005). For instance, Shirzad-Siboni et al. (Shirzad-Siboni et al.

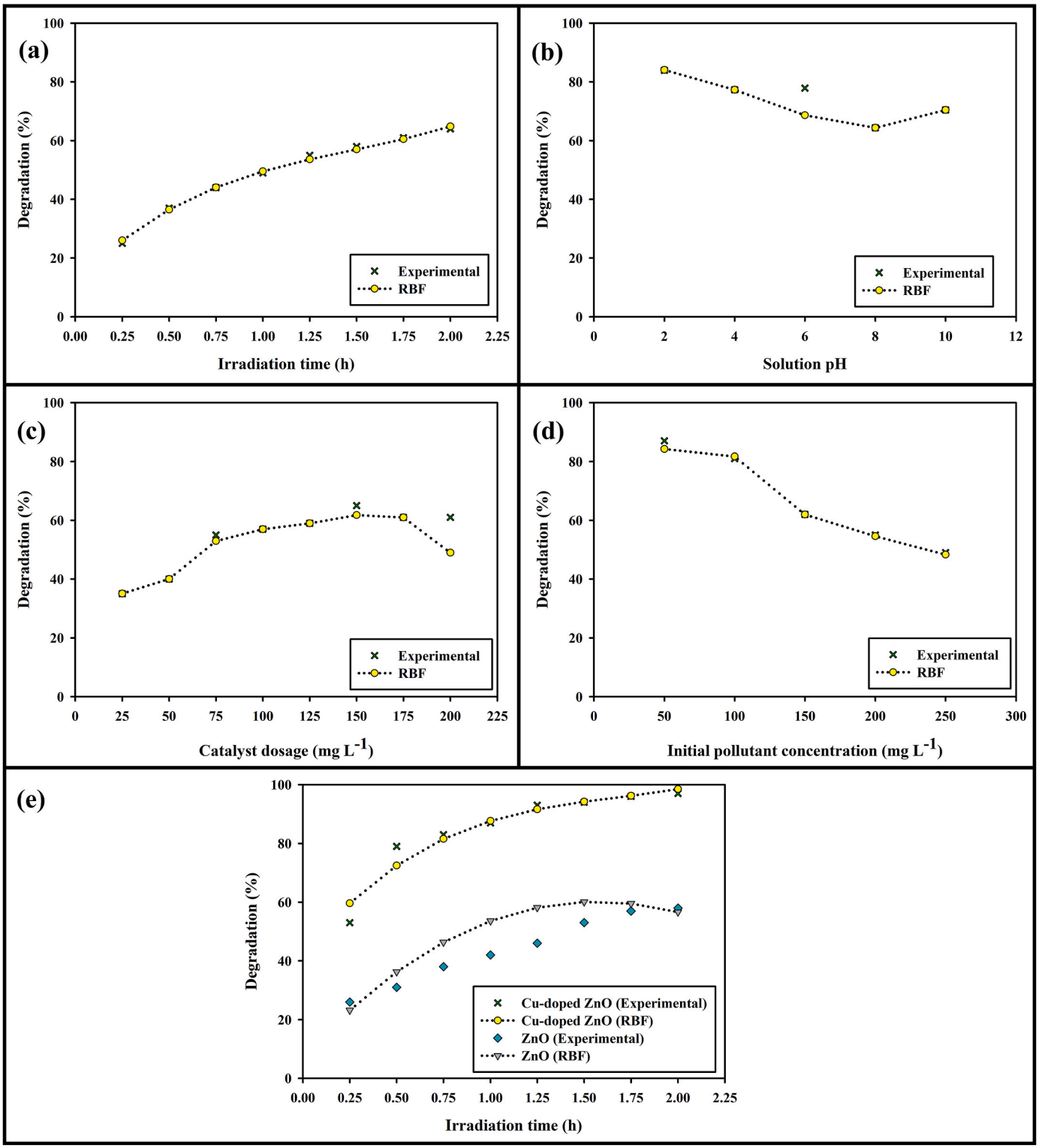


Fig. 4. Comparing the experimental and the estimated values of photocatalytic degradation of pesticides. (a) effect of irradiation time (Cu-doped ZnO catalyst, 0.007 mass ratio of Cu to Zn, initial diazinon concentration of 20 mg L^{-1}, UV light, catalyst dosage of 200 mg L^{-1}, solution pH 3) (Shirzad-Siboni et al., 2017), (b) effect of solution pH (La-doped ZnO catalyst, 0.123 mass ratio of La to Zn, initial 2-chlorophenol concentration of 10 mg L^{-1}, visible light, catalyst dosage of 333.33 mg L^{-1}, irradiation time of 2 h) (Rani et al., 2023), (c) effect of catalyst dosage (ZnO catalyst, initial diazinon concentration of 20 mg L^{-1}, UV light, solution pH 7, irradiation time of 0.83 h) (Daneshvar et al., 2007), (d) effect of initial phenol concentration (ZnO catalyst, catalyst dosage of 1000 mg L^{-1}, UV light, solution pH 2.5, irradiation time of 2 h) (Benhebal et al., 2013), and (e) effect of element doping (ZnO and Cu-doped ZnO catalysts, mass ratio of Cu to Zn at 0.007, initial diazinon concentration of 20 mg L^{-1}, UV light, catalyst dosage of 200 mg L^{-1}, solution pH 7) (Shirzad-Siboni et al., 2017).

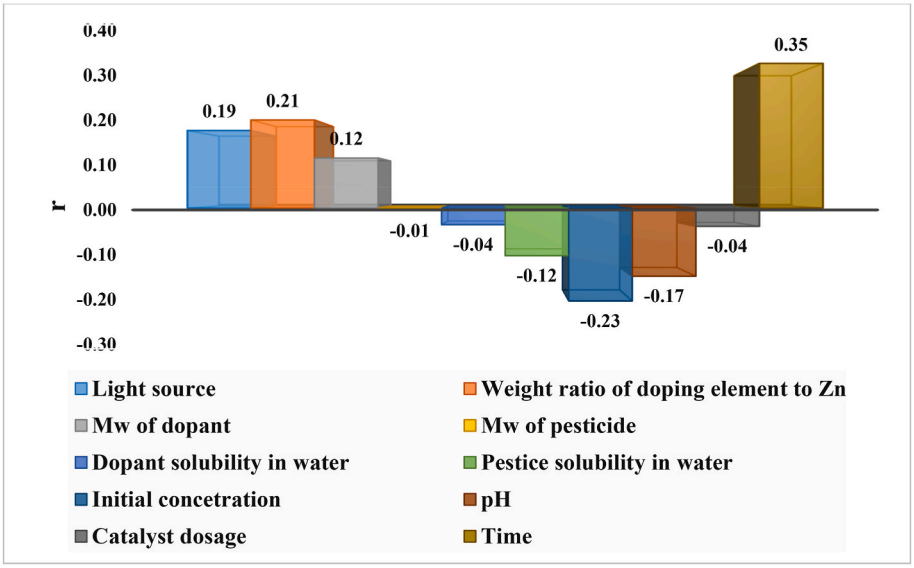


Fig. 5. Sensitivity analysis of input parameters in the ML models.

(2017) assessed the impact of catalyst dosage, for the photocatalytic degradation of diazinon over Cu-doped ZnO nanorods (under UV irradiation), where the optimum catalyst dosage was 0.2 g L^{-1} among the range of 0.1–1.0 g L^{-1}. Considering the results reported by Daneshvar et al., (2007), the effect of the catalyst dosage on the photocatalytic degradation of diazinon using ZnO (under UV irradiation) is shown in Fig. 4c, where increasing the catalyst dosage, from 25 to 150 mg L^{-1}, gradually improved the degradation efficiency of diazinon, but further increase in the catalyst dosage, from 150 to 200 mg L^{-1}, suppressed the photocatalytic activity.

Shirzad-Siboni et al. (Shirzad-Siboni et al., (2017) evaluated the effect of initial diazinon concentration, in the range of 10–50 mg L^{-1}, where increase of the initial diazinon concentration reduced its degradation efficiency gradually, (Similar to Fig. 4d) and has been mainly related to the blockage effect of adsorption of diazinon molecules on the surface of catalysts. An approximately similar trend was observed by Zhu et al., (2020), where the effect of different initial concentrations of dimethoate, in the range of 1–20 mg L^{-1}, have been evaluated in their research. On the other hand, increasing the initial concentration of dyes has improved their degradation efficiency in some cases (Hanafi and Sapawe, 2020), and therefore the effect of the initial pollutant concentration on the photocatalytic degradation relies on several factors in the photocatalytic process (e.g. type of pollutant/photocatalyst and dosage of photocatalyst).

The source of light (UV or visible light) is another factor affecting the photocatalytic activity of semiconductors. Notably, ZnO and TiO_2 are among semiconductors with wide band gap energies, however, ZnO can provide higher photo-absorption ability than TiO_2. Metal doping is among the methods which can be used to improve the photocatalytic activity of ZnO. Due to their ability in trapping the photogenerated e^-, rare earth metals such as La, Nd, Sm, and Dy have been effectively used to increase the photocatalytic efficiency of ZnO (Alam et al., 2018). Notably, it has been reported that substitution of Cu into ZnO lattice could modify its photocatalytic performance, and its optical and magnetic properties (Shirzad-Siboni et al., 2017). For instance as shown in Fig. 4e, the photocatalytic degradation of diazinon significantly increased from 58.52% to 96.97% for ZnO and Cu-doped ZnO, respectively, under UV irradiation (C_0 = 20 ppm, pH = 7, and catalyst dosage = 0.2 g L^{-1}) (Shirzad-Siboni et al., 2017).

3.4. Sensitivity analysis

For analysts and engineers in water and wastewater treatment, it is critical to make clear recommendations as to the impact that various operating parameters have on the process performance. To this end, an investigation was carried out on the impact of each input variable in order to calculate its significance by equation (5) (Amirkhani et al., 2024; Dashti et al., 2021a):

$$r = \frac{\sum_{i=1}^{n}\left(X_{k,i}-\overline{X}_k\right)\left(Y_i-\overline{Y}\right)}{\sqrt{\sum_{i=1}^{n}\left(X_{k,i}-\overline{X}_k\right)^2\sum_{i=1}^{n}\left(Y_i-\overline{Y}\right)^2}} \quad (5)$$

where $X_{k,i}$ and Y_i stand the 'k' th input and 'i' th output while $\overline{X}_k$ and $\overline{Y}$ indicate the average values of input and outputs, respectively.

A more significant impact on the yield is included in each input with a more significant r value. The negative values signify that the comparing parameter adversely influences the target (photocatalytic degradation). As it is shown in Fig. 5, all process variables including irradiation time, mass ratio of doping element to Zn, light source and MW of dopant had positive impacts on degradation of pesticides by ZnO based photocatalyst. In comparison, initial pesticide concentration, solution pH, pesticide solubility in water, catalyst dosage, dopant solubility in water, and pesticide MW had the decreasing negative effects on the modeling output. Therefore, among all the variables, the light irradiation time demonstrated to be the most effective parameter in the photocatalytic decomposition of pesticides over ZnO-based semiconductors.

It is obvious that the photocatalytic degradation of pollutants highly depended on operation time from a kinetic control point of view. During the photocatalytic degradation of dichlorvos (10 mg L^{-1}) over ZnO (100 mg L^{-1}) at pH 7, the photodegradation efficiency was significantly increased from 17% to 26%, 37%, 46%, 57%, 63%, 72%, 81%, 88%, 92%, and finally 96%, respectively at different times (0.03, 0.06, 0.1, 0.17, 0.28, 0.33, 0.5, 0.75, 1, 1.33, 2 h) (Evgenidou et al., 2005). In addition, the photocatalytic degradation of 2-chlorophenol (10 mg L^{-1}) at pH 2 over La-doped ZnO (~333.3 mg L^{-1}) was increasing from 77%, 78%, 80%, 82%, to 84% at different operation time of 0.3, 0.7, 1, 1.3, and 1.7 h respectively (Rani et al., 2023).

Besides, Fig. 4 shows that the initial concentration of pesticide has the most negative effect on the photocatalytic degradation. Such an

adverse effect can be related to the blockage impact of adsorption of pesticide molecules on the surface of photocatalysts, which caused a reduction of surface active sites in the photocatalyst (Shirzad-Siboni et al., 2017).

4. Conclusions

The reliable estimation of the photodegradation of pesticides by ZnO photocatalysts is of vital significance to improve photocatalysis process design and performance. Four ML models were developed, namely ANN, RBF, PSO-ANFIS and CSA-LSSVM. The RBF model showed the most promising modeling power, and exhibited the highest modeling accuracy, achieving a R^2 value of 0.978 and AARD value of 4.80%. The RBF model was successful in predicting the photocatalytic degradation of all pesticides expect 2-chlorophenol, triclopyr, and lambda-cyhalothrin, for which CSA-LSSVM model provided a better fit. The most positive and negative effects on photocatalytic degradation of the pesticides by ZnO-based photocatalysts were light illumination time and initial pesticide concentration, based on their relative importance in sensitivity analysis. Future research should study the performance of different types of photocatalysts in the degradation of highly persistent organic contaminants, and develop new types of ML models.

CRediT authorship contribution statement

Amir Dashti: Writing – original draft, Software, Methodology, Conceptualization. **Amir Hossein Navidpour:** Writing – original draft, Resources, Data curation. **Farid Amirkhani:** Writing – original draft, Visualization, Validation, Investigation. **John L. Zhou:** Writing – review & editing, Supervision. **Ali Altaee:** Writing – review & editing, Supervision.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the author(s) used Grammarly, Gemini and ChatGPT in order to check the grammar and improve clarity. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

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.

Acknowledgements

The authors thank the University of Technology Sydney (UTS) for the International Research Scholarship and UTS President's Scholarship.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.chemosphere.2024.142792.

References

Abbas, K.N., Bidin, N., 2017. Morphological driven photocatalytic activity of ZnO nanostructures. Appl. Surf. Sci. 394, 498–508.
Alam, U., Khan, A., Ali, D., Bahnemann, D., Muneer, M., 2018. Comparative photocatalytic activity of sol–gel derived rare earth metal (La, Nd, Sm and Dy)-doped ZnO photocatalysts for degradation of dyes. RSC Adv. 8 (31), 17582–17594.
Amirkhani, F., Dashti, A., Abedsoltan, H., Mohammadi, A.H., 2024. Estimation of CO2 absorption by a hybrid aqueous solution of amino acid salt with amine. Chem. Eng. Technol. 47 (2), 253–261.
Amirkhani, F., Dashti, A., Abedsoltan, H., Mohammadi, A.H., Chau, K.-W., 2021. Towards estimating absorption of major air pollutant gasses in ionic liquids using soft computing methods. J. Taiwan Inst. Chem. Eng. 127, 109–118.
Amirkhani, F., Dashti, A., Abedsoltan, H., Mohammadi, A.H., Chofreh, A.G., Goni, F.A., Klemeš, J.J., 2022. Estimating flashpoints of fuels and chemical compounds using hybrid machine-learning techniques. Fuel 323, 124292.
Amirkhani, F., Dashti, A., Jokar, M., Mohammadi, A.H., Chofreh, A.G., Varbanov, P.S., Zhou, J.L., 2023. Estimation of CO2 solubility in aqueous solutions of commonly used blended amines: application to optimised greenhouse gas capture. J. Clean. Prod. 430, 139435.
Anju, S., Yesodharan, S., Yesodharan, E., 2012. Zinc oxide mediated sonophotocatalytic degradation of phenol in water. Chem. Eng. J. 189, 84–93.
Ansari, S.A., Khan, M.M., Ansari, M.O., Cho, M.H., 2015. Silver nanoparticles and defect-induced visible light photocatalytic and photoelectrochemical performance of Ag@m-TiO2 nanocomposite. Sol. Energy Mater. Sol. Cell. 141, 162–170.
Ayodele, B.V., Alsaffar, M.A., Mustapa, S.I., Cheng, C.K., Witoon, T., 2021. Modeling the effect of process parameters on the photocatalytic degradation of organic pollutants using artificial neural networks. Process Saf. Environ. Protect. 145, 120–132.
Barati-Harooni, A., Najafi-Marghmaleki, A., Mohammadi, A.H., 2017. A reliable radial basis function neural network model (RBF-NN) for the prediction of densities of ionic liquids. J. Mol. Liq. 231, 462–473.
Bassi, A., Hasan, I., Qanungo, K., Koo, B.H., Khan, R.A., 2022. Visible light assisted mineralization of malachite green dye by green synthesized xanthan gum/agar@ZnO bionanocomposite. J. Mol. Struct. 1256, 132518.
Benhebal, H., Chaib, M., Salmon, T., Geens, J., Leonard, A., Lambert, S.D., Crine, M., Heinrichs, B., 2013. Photocatalytic degradation of phenol and benzoic acid using zinc oxide powders prepared by the sol–gel process. Alex. Eng. J. 52 (3), 517–523.
Brahmand, M.B., Yunesian, M., Nabizadeh, R., Nasseri, S., Alimohammadi, M., Rastkari, N., 2019. Evaluation of chlorpyrifos residue in breast milk and its metabolite in urine of mothers and their infants feeding exclusively by breast milk in north of Iran. Journal of Environmental Health Science and Engineering 17, 817–825.
Cosgrove, S., Jefferson, B., Jarvis, P., 2019. Pesticide removal from drinking water sources by adsorption: a review. Environmental Technology Reviews 8 (1), 1–24.
Damalas, C.A., Koutroubas, S.D., 2016. Farmers' Exposure to Pesticides: Toxicity Types and Ways of Prevention. MDPI, p. 1.
Daneshvar, N., Aber, S., Dorraji, M.S., Khataee, A., Rasoulifard, M., 2007. Photocatalytic degradation of the insecticide diazinon in the presence of prepared nanocrystalline ZnO powders under irradiation of UV-C light. Separ. Purif. Technol. 58 (1), 91–98.
Dashti, A., Amirkhani, F., Hamedi, A.-S., Mohammadi, A.H., 2021a. Evaluation of CO2 absorption by amino acid salt aqueous solution using hybrid soft computing methods. ACS Omega 6 (19), 12459–12469.
Dashti, A., Amirkhani, F., Jokar, M., Mohammadi, A., Chau, K.-W., 2021b. Insights into the estimation of heavy metals ions sorption from aqueous environment onto natural zeolite. Int. J. Environ. Sci. Technol. 18, 1773–1784.
Dashti, A., Jokar, M., Amirkhani, F., Mohammadi, A.H., 2020a. Quantitative structure property relationship schemes for estimation of autoignition temperatures of organic compounds. J. Mol. Liq. 300, 111797.
Dashti, A., Noushabadi, A.S., Asadi, J., Raji, M., Chofreh, A.G., Klemeš, J.J., Mohammadi, A.H., 2021c. Review of higher heating value of municipal solid waste based on analysis and smart modelling. Renew. Sustain. Energy Rev. 151, 111591.
Dashti, A., Raji, M., Alivand, M.S., Mohammadi, A.H., 2020b. Estimation of CO2 equilibrium absorption in aqueous solutions of commonly used amines using different computational schemes. Fuel 264, 116616.
Dashti, A., Raji, M., Harami, H.R., Zhou, J.L., Asghari, M., 2023. Biochar performance evaluation for heavy metals removal from industrial wastewater based on machine learning: application for environmental protection. Separ. Purif. Technol. 312, 123399.
Derikvandi, H., Nezamzadeh-Ejhieh, A., 2017. Increased photocatalytic activity of NiO and ZnO in photodegradation of a model drug aqueous solution: effect of coupling, supporting, particles size and calcination temperature. J. Hazard Mater. 321, 629–638.
Deylami, S., Sabzevari, M.H., Ghaedi, M., Azqhandi, M.A., Marahel, F., 2023. Efficient photodegradation of disulfine blue dye and Tetracycline over Robust and Green g-CN/Ag3VO4/PAN nanofibers: experimental design, RSM, RBF-NN and ANFIS modeling. Process Saf. Environ. Protect. 169, 71–81.
Eberhart, R., Kennedy, J., 1995. A New Optimizer Using Particle Swarm Theory. Ieee, pp. 39–43.
Escudero, R., Escamilla, R., 2011. Ferromagnetic behavior of high-purity ZnO nanoparticles. Solid State Commun. 151 (2), 97–101.
Espitia, P.J.P., Soares, N.d.F.F., Coimbra, J.S.d.R., de Andrade, N.J., Cruz, R.S., Medeiros, E.A.A., 2012. Zinc oxide nanoparticles: synthesis, antimicrobial activity and food packaging applications. Food Bioprocess Technol. 5, 1447–1464.
Evgenidou, E., Fytianos, K., Poulios, I., 2005. Semiconductor-sensitized photodegradation of dichlorvos in water using TiO2 and ZnO as catalysts. Appl. Catal. B Environ. 59 (1–2), 81–89.
Gheytanzadeh, M., Baghban, A., Habibzadeh, S., Jabbour, K., Esmaeili, A., Mohaddespour, A., Abida, O., 2022. An insight into tetracycline photocatalytic degradation by MOFs using the artificial intelligence technique. Sci. Rep. 12 (1), 6615.

Hamilton, D., Ambrus, A., Dieterle, R., Felsot, A., Harris, C., Holland, P., Katayama, A., Kurihara, N., Linders, J., Unsworth, J., 2003. Regulatory limits for pesticide residues in water (IUPAC Technical Report). Pure Appl. Chem. 75 (8), 1123–1155.
Hanafi, M.F., Sapawe, N., 2020. Effect of initial concentration on the photocatalytic degradation of remazol brilliant blue dye using nickel catalyst. Mater. Today: Proc. 31, 318–320.
Irfan, M., Waqas, S., Arshad, U., Khan, J.A., Legutko, S., Kruszelnicka, I., Ginter-Kramarczyk, D., Rahman, S., Skrzypczak, A., 2022. Response surface methodology and artificial neural network modelling of membrane rotating biological contactors for wastewater treatment. Materials 15 (5), 1932.
Izadifard, M., Achari, G., Langford, C.H., 2013. Application of photocatalysts and LED light sources in drinking water treatment. Catalysts 3 (3), 726–743.
Jaffari, Z.H., Abbas, A., Lam, S.-M., Park, S., Chon, K., Kim, E.-S., Cho, K.H., 2023. Machine learning approaches to predict the photocatalytic performance of bismuth ferrite-based materials in the removal of malachite green. J. Hazard Mater. 442, 130031.
Jia, M., Farid, M.U., Kharraz, J.A., Kumar, N.M., Chopra, S.S., Jang, A., Chew, J., Khanal, S.K., Chen, G., An, A.K., 2023. Nanobubbles in water and wastewater treatment systems: small bubbles making a big difference. Water Res., 120613
Kalantary, R.R., Barzegar, G., Jorfi, S., 2022. Monitoring of pesticides in surface water, pesticides removal efficiency in drinking water treatment plant and potential health risk to consumers using Monte Carlo simulation in Behbahan City, Iran. Chemosphere 286, 131667.
Kalyabina, V.P., Esimbekova, E.N., Kopylova, K.V., Kratasyuk, V.A., 2021. Pesticides: formulants, distribution pathways and effects on human health–a review. Toxicol Rep 8, 1179–1192.
Khan, S.H., Pathak, B., 2020. Zinc oxide based photocatalytic degradation of persistent pesticides: a comprehensive review. Environ. Nanotechnol. Monit. Manag. 13, 100290.
Kim, M., Kim, Y., Kim, H., Piao, W., Kim, C., 2016. Evaluation of the k-nearest neighbor method for forecasting the influent characteristics of wastewater treatment plant. Front. Environ. Sci. Eng. 10, 299–310.
Kıran, M.S., Özceylan, E., Gündüz, M., Paksoy, T., 2012. A novel hybrid approach based on particle swarm optimization and ant colony algorithm to forecast energy demand of Turkey. Energy Convers. Manag. 53 (1), 75–83.
Kong, R., Yang, C., Huang, K., Han, G., Sun, Q., Zhang, Y., Zhang, H., Letcher, R.J., Liu, C., 2022. Application of agricultural pesticides in a peak period induces an abundance decline of metazoan zooplankton in a lake ecosystem. Water Res. 224, 119040.
Kruć-Fijałkowska, R., Dragon, K., Drożdżyński, D., Górski, J., 2022. Seasonal variation of pesticides in surface water and drinking water wells in the annual cycle in western Poland, and potential health risk assessment. Sci. Rep. 12 (1), 3317.
Kuo, R., Hong, S., Huang, Y., 2010. Integration of particle swarm optimization-based fuzzy neural network and artificial neural network for supplier selection. Appl. Math. Model. 34 (12), 3976–3990.
Lee, K.M., Lai, C.W., Ngai, K.S., Juan, J.C., 2016. Recent developments of zinc oxide based photocatalyst in water treatment technology: a review. Water Res. 88, 428–448.
Li, W., Xin, S., Deng, W., Wang, B., Liu, X., Yuan, Y., Wang, S., 2023. Occurrence, spatiotemporal distribution patterns, partitioning and risk assessments of multiple pesticide residues in typical estuarine water environments in eastern China. Water Res. 245, 120570.
Liu, P., Zhang, L., Li, H., Wei, Y., Wu, F., You, J., 2022. Reduced concentrations and toxicity of sediment-associated pesticides from vegetable planting field to surrounding waterways: impacts of chemical properties and intrinsic toxicity. J. Hazard Mater. 436, 129292.
Muhamad, S.G., 2010. Kinetic studies of catalytic photodegradation of chlorpyrifos insecticide in various natural waters. Arab. J. Chem. 3 (2), 127–133.
Navidpour, A.H., Abbasi, S., Li, D., Mojiri, A., Zhou, J.L., 2023a. Investigation of advanced oxidation process in the presence of TiO2 semiconductor as photocatalyst: property, principle, kinetic analysis, and photocatalytic activity. Catalysts 13 (2), 232.
Navidpour, A.H., Hao, D., Li, X., Li, D., Huang, Z., Zhou, J.L., 2023b. Key factors in improving the synthesis and properties of visible-light activated g-C3N4 for photocatalytic hydrogen production and organic pollutant decomposition. Catal. Rev. 1–72. https://doi.org/10.1080/01614940.2023.2228130.
Navidpour, A.H., Hosseinzadeh, A., Huang, Z., Li, D., Zhou, J.L., 2024. Application of machine learning algorithms in predicting the photocatalytic degradation of perfluorooctanoic acid. Catal. Rev. 66 (2), 687–712.
Navidpour, A.H., Hosseinzadeh, A., Zhou, J.L., Huang, Z., 2023c. Progress in the application of surface engineering methods in immobilizing TiO2 and ZnO coatings for environmental photocatalysis. Catal. Rev. 65 (3), 822–873.
Navidpour, A.H., Safaei, J., Zhang, G., Mojiri, A., Ni, B.-J., Huang, Z., Zhou, J.L., 2023d. Photocatalytic and photoelectrocatalytic degradation of perfluorooctanoic acid by immobilised ZnO nanoparticles using electrophoretic deposition. Environ. Sci.: Nano 10 (8), 1955–1965.
Nicolopoulou-Stamati, P., Maipas, S., Kotampasi, C., Stamatis, P., Hens, L., 2016. Chemical pesticides and human health: the urgent need for a new concept in agriculture. Front. Public Health 4, 148.
Ong, C.B., Ng, L.Y., Mohammad, A.W., 2018. A review of ZnO nanoparticles as solar photocatalysts: synthesis, mechanisms and applications. Renew. Sustain. Energy Rev. 81, 536–551.
Peng, J., Lu, T., Ming, H., Ding, Z., Yu, Z., Zhang, J., Hou, Y., 2019. Enhanced photocatalytic ozonation of phenol by Ag/ZnO nanocomposites. Catalysts 9 (12), 1006.
Premalatha, N., Miranda, L.R., 2019. Surfactant modified ZnO–Bi2O3 nanocomposite for degradation of lambda-cyhalothrin pesticide in visible light: a study of reaction kinetics and intermediates. J. Environ. Manag. 246, 259–266.
Qiu, Y., Wu, S., Xia, L., Ren, L.-F., Shao, J., Shen, J., Yang, Z., Tang, C.Y., Wu, C., Van der Bruggen, B., 2023. Ionic resource recovery for carbon neutral papermaking wastewater reclamation by a chemical self-sufficiency zero liquid discharge system. Water Res. 229, 119451.
Rahman, A., Harunsani, M.H., Tan, A.L., Khan, M.M., 2021. Zinc oxide and zinc oxide-based nanostructures: biogenic and phytogenic synthesis, properties and applications. Bioproc. Biosyst. Eng. 44, 1333–1372.
Rajbongshi, B.M., Samdarshi, S., 2014. Cobalt-doped zincblende–wurtzite mixed-phase ZnO photocatalyst nanoparticles with high activity in visible spectrum. Appl. Catal. B Environ. 144, 435–441.
Raji, M., Dashti, A., Amani, P., Mohammadi, A.H., 2019. Efficient estimation of CO2 solubility in aqueous salt solutions. J. Mol. Liq. 283, 804–815.
Rani, S., Sharma, A., Tabasum, S., Malik, A.Q., Chaudhary, S., Kumar, D., Singh, H., Singh, P.P., 2023. Highly efficient photocatalytic properties of La-doped ZnO over pristine ZnO for degradation of 2-chlorophenol from aquatic agriculture waste. Chemistry Africa 1–10.
Reiler, E., Jørs, E., Bælum, J., Huici, O., Caero, M.M.A., Cedergreen, N., 2015. The influence of tomato processing on residues of organochlorine and organophosphate insecticides and their associated dietary risk. Sci. Total Environ. 527, 262–269.
Sadeghi, F., Fadaei, A., Mohammadi-Moghadam, F., Hemati, S., Mardani, G., 2021. Photocatalytic degradation of trifluralin in aqueous solutions by UV/S2O82− and UV/ZnO processes: a comparison of removal efficiency and cost estimation. Int. J. Chem. Eng. 2021, 1–10.
Sakkas, V., Dimou, A., Pitarakis, K., Mantis, G., Albanis, T., 2005. TiO 2 photocatalyzed degradation of diazinon in an aqueous medium. Environ. Chem. Lett. 3, 57–61.
Sakthivel, S., Neppolian, B., Shankar, M., Arabindoo, B., Palanichamy, M., Murugesan, V., 2003. Solar photocatalytic degradation of azo dye: comparison of photocatalytic efficiency of ZnO and TiO2. Sol. Energy Mater. Sol. Cell. 77 (1), 65–82.
Salahshoori, I., Jorabchi, M.N., Baghban, A., Khonakdar, H.A., 2024. Integrative analysis of multi machine learning models for tetracycline photocatalytic degradation with MOFs in wastewater treatment. Chemosphere 350, 141010.
Schostag, M.D., Gobbi, A., Fini, M.N., Ellegaard-Jensen, L., Aamand, J., Hansen, L.H., Muff, J., Albers, C.N., 2022. Combining reverse osmosis and microbial degradation for remediation of drinking water contaminated with recalcitrant pesticide residue. Water Res. 216, 118352.
Sekar, A., Yadav, R., 2021. Green fabrication of zinc oxide supported carbon dots for visible light-responsive photocatalytic decolourization of Malachite Green dye: optimization and kinetic studies. Optik 242, 167311.
Shirzad-Siboni, M., Jonidi-Jafari, A., Farzadkia, M., Esrafili, A., Gholami, M., 2017. Enhancement of photocatalytic activity of Cu-doped ZnO nanorods for the degradation of an insecticide: kinetics and reaction pathways. J. Environ. Manag. 186, 1–11.
Syafrudin, M., Kristanti, R.A., Yuniarto, A., Hadibarata, T., Rhee, J., Al-Onazi, W.A., Algarni, T.S., Almarri, A.H., Al-Mohaimeed, A.M., 2021. Pesticides in drinking water—a review. Int. J. Environ. Res. Publ. Health 18 (2), 468.
Tabatabai-Yazdi, F.-S., Pirbazari, A.E., Saraei, F.E.K., Gilani, N., 2021. Construction of graphene based photocatalysts for photocatalytic degradation of organic pollutant and modeling using artificial intelligence techniques. Phys. B Condens. Matter 608, 412869.
Tang, X., Fan, C., Zeng, G., Zhong, L., Li, C., Ren, X., Song, B., Liu, X., 2022. Phage-host interactions: the neglected part of biological wastewater treatment. Water Res., 119183
Tatar, A., Naseri, S., Bahadori, M., Hezave, A.Z., Kashiwao, T., Bahadori, A., Darvish, H., 2016. Prediction of carbon dioxide solubility in ionic liquids using MLP and radial basis function (RBF) neural networks. J. Taiwan Inst. Chem. Eng. 60, 151–164.
Wan, X., Li, X., Wang, X., Yi, X., Zhao, Y., He, X., Wu, R., Huang, M., 2022. Water quality prediction model using Gaussian process regression based on deep learning for carbon neutrality in papermaking wastewater treatment system. Environ. Res. 211, 112942.
Wang, Y., Peng, G., Sharshir, S.W., Yang, N., 2021. The weighted values of solar evaporation's environment factors obtained by machine learning. ES Materials & Manufacturing 14, 87–94.
Wu, X., Zhao, X., Chen, R., Liu, P., Liang, W., Wang, J., Teng, M., Wang, X., Gao, S., 2022. Wastewater treatment plants act as essential sources of microplastic formation in aquatic environments: a critical review. Water Res. 221, 118825. www.chemspider.com.
Yadav, S., Jindal, J., Mittal, A., Sharma, S., Kumari, K., Kumar, N., 2021. Facile solution combustion synthesized, Li doped ZnO nanostructures for removal of abiotic contaminants. J. Phys. Chem. Solid. 157, 110217.
Zhu, Z., Guo, F., Xu, Z., Di, X., Zhang, Q., 2020. Photocatalytic degradation of an organophosphorus pesticide using a ZnO/rGO composite. RSC Adv. 10 (20), 11929–11938.