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Ecologically friendly oxidative processes for the atmosphere, soils and water, environmental contaminants

ECOLOGICALLY FRIENDLY OXIDATION PROCESSES DEEP LEARNING MODEL TAKING AIM AT ENVIRONMENTAL POLLUTANTS

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ABSTRACT

Pollution by industrial effluent, chemical fertilisers, and drugs has turned into a very relevant problem in the world today that is posing a very great danger to water sources and its users. Effective and popular methods of oxidation processes include advanced oxidation processes (AOP) to remove pollutant concentrations but their executions are methodically power intensive and are generally known to produce secondary toxic products. To overcome these limitations, this work proposes a green oxidation process accompanied by a deep learning (DL) model for the successful identification of pollutants and their efficient degradation. This oxidation technique uses green

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oxidising agents such as hydrogen peroxide, and plant based catalysts, which lead to minimal production of secondary hazardous pollutants. The DL model acquires essential data including diverse pollutants, reaction conditions, and water chemistries to forecast optimum sets of the operating parameters such as oxidant concentration, pH, temperature, reaction time. This helps in achieving the degradation of pollutants in a more enhanced way depending on the environmental conditions. The deep learning incorporated into the model enables it to learn from the previous performance and provides optimal pollution removal efficiency with low energy complicity and environmental impact as well. Furthermore, the DL model involves a prediction of the best routes by which the production of undesirable by-products can be minimised making the whole process more sustainable. There is experimental confirmation that the proposed method enhances the efficiency of pollutant elimination rates in contrast to the conventional oxidation approaches while requiring less energy and having lower costs of operation. It is evidenced by the model's ability to function under varying environmental conditions, mainly due to its sustainable design, which makes the presented model suitable for large scale application in the remediation of the environment. This work lays the foundation for combining green chemistry and artificial intelligence in developing technologies for reducing the amount of hazardous pollutants in the environment that are eco-friendly and highly efficient.

Keywords: green oxidation, deep learning, pollutant degradation, AI in environmental science, eco-friendly treatment.

AIMS AND BACKGROUND

Pollution of the environment still poses a major threat to global habitats and human beings mainly as caused by industrial waste, fertilisers, and pharmaceuticals. These pollutants, especially in water treatment, are very hard to remove by the conventional methods of treatment. Application of different pollutant oxidation processes like AOPs has been relevant, whereas their efficiency is challenged by issues like high energy consumption and the generation of toxic species. This implies the need to find better ways towards handling environmental remediation efforts in a way that is sustainable and less resource intensive.

Modern trends in water treatment include the use of heterogeneous photocatalysis as well as other types of advanced oxidation processes. Ahmed et al.[1] also summarised that heterogeneous photocatalytic degradation of phenols as well as other pollutants in wastewater is a promising technique but they are sensitive to reaction conditions and type of photocatalyst used. Dong et al.[2] (2015) explained that visible light responsive photocatalysts are gaining more attention, because natural light can be used for oxidation in a cleaner way, although the photocatalytic technology is still in the process of being fine-tuned to adapt to differences in pollutants.

AI and deep learning models have a potential role in environmental science since it provides new avenues for enhancing these procedures. Shang et al.[3] showed that

DL models can be utilised to predict optimal operational conditions of environmental pollutant removal inclusive of oxidant dosage, pH, temperature, and reaction time given by various environmental conditions. Such models are more useful when the treatment process is customised to the nature of the pollutant and the context in which it prevails thus enabling an efficient degradation process to occur.

Recently the emphasis has been made to reagents-and-energy-saving oxidation processes. For instance, Gomes et al.[4] investigated the effectiveness of using ozonation for degradation of PPCPs from water, demonstrating that through modification of ozone-based processes with the help of the catalytic agents, both pollutant efficiency and generation of toxic by-products may be increased. However, while the ozonation, and other AOPs have their advantages, they are rather energy-consuming processes that also generate secondary pollutants suggesting that more environmentally friendly solutions are required.

In response to the problems above, green oxidants and bio-based catalysts have been widely introduced and applied in the process. Kulkarni and Kaware[5] noted in their review of phenol removal from the two stage SBRs, that the application of natural oxidants and catalysts for oxidation processes can substantially decrease the ecological impact of the oxidation process, and therefore, present an avenue for improved bioprocesses in wastewater treatment. Moreover, Ma et al.[6] discussed the enhancement of Fenton-like reactions to photocatalysis processes, which demonstrate how these complementary systems can provide high pollutant degradation ratios in the presence of low energy application and low toxic intermediates generation.

Hence, deep learning models' integration into green oxidation processes has massive opportunities to boost performance and sustainability. The systematic review of Xu et al.[7] elucidated that advanced oxidation processes have great potential as a treatment technique for the complex pollutants but unfortunately AOPs' performance is highly susceptible to the inherent operational factors. Computational models can, by training on large sets of reaction conditions and pollutant information, continuously enhance such processes in real time to enhance pollutant removal and lower the industry's ecological impact.

Based on this, this study contributes to the existing literature supporting the combination of deep learning with green oxidation processes. To this extent, this approach tries to contribute to a sustainable solution that can address the challenges of environmental pollutant treatment by using appropriate reagents (green oxidants like hydrogen peroxide), bio-based catalysts, and deep learning to predict optimal conditions in the process. As mentioned by Peralta-Zamora et al.[8], the future will witness the combination of advanced oxidation processes and sustainable processes and hence, incorporating AI technology is a promising way to make it happen.

EXPERIMENTAL

This experimental study is conducted to explore the viability of an environmentally sustainable oxidation technique for the removal of contaminants in different environmental settings and the applicability of deep learning (DL) model for system control and efficiency improvement. Environmentally friendly oxidants including hydrogen peroxide and bio-catalysts are used under different controlled conditions to oxidise the pollutants in the oxidation process[9]. Deep learning model is used here to forecast the efficient working parameters which consists of oxidant dosage, reaction time, pH, and concentration of a catalyst[6]. For the study, a set of typical organic and inorganic pollutants including phenols, pharmaceuticals and heavy metals respectively were chosen.

The primary oxidising agents employed in this process for the oxidation of organic compounds were hydrogen peroxide H_2O_2 and ozone. Activated carbon as a bio-based catalyst, biomass or biochar, were applied to improve oxidation process. To keep the pH levels constant buffer solutions were prepared and deionised water was used for all experiments[8].

EXPERIMENTAL SETUP

The experiments were conducted in a batch reactor system under controlled conditions. Each batch experiment was made in a 500-ml spectrophotometric grade glass reactor with a magnetic stirrer. For experiments, which required photocatalysis, the reactor was covered with quartz lid. Because solar radiation contains 350-700 nm wavelength, a UV-Vis. lamp of this range was employed in photocatalytic degradation experiments. The oxidant was hydrogen peroxide which was administered by a syringe pump with a controlled flow rate so that the concentration of the oxidant was constant[10]. Stock solutions of the selected pollutants were made at concentration of 50–100 mg/l using distilled water. In the case of the heavy metal studies, metal salt solutions (for instance, lead nitrate for Pb^{2+}) were prepared for 10–50 mg/l.

Oxidation process. The pollutant solutions were then introduced into the reactor with green oxidants and catalysts introduced at the same time. The experiments were performed with different concentrations of the catalyst to oxidant ratio and pollutants in order to analyse the effect of these factors on degradation efficiency[3]. Temperature was set at 25°C whilst the pH effects on the oxidation process were investigated at three pH values of 3, 7 and 9.

Sampling and monitoring. The samples were taken at certain time spans with the time intervals of 15 min for a maximum of 2 h. The degradation of the pollutants was measured using HPLC especially for the organics while AAS was used for the determination of the heavy metal remaining in solution. Estimation on the extent of mineralisation was also made by conducting Total organic carbon (TOC) tests.

DEEP LEARNING MODEL TRAINING

Some of the parameters which were taken during each experiment run included oxidant dosage, pollutant concentration, pH, reaction time, and catalyst concentration.

Model architecture. To develop the deep learning model we used the Python programming language and among the modules, we selected TensorFlow for implementing a Multi-layered Perceptron (MLP) neural network. The input factors were type of pollutant, its initial concentration, its pH, amount of catalyst added and time of reaction. The two inputs were the pollutant flows and the treatment processes while the output was pollutant removal efficiency[7]. The training data set comprised 70% of all the data that were collected. The validation and test data set constituted 15%, respectively. The optimisation was done using the gradient descent algorithm coupled with back propagation.

Optimisation and validation. By comparing the DL model with experimental data it was possible to predict the operating conditions that will yield the highest pollutant degradation. The predicted optimal conditions were further investigated by an additional course of experiment which is the confirmation test and the results were compared to a control experiment without any optimum conditions.

EVALUATION METRICS

Pollutant *Removal Efficiency* (*RE, %*). The percentage of pollutant removed from the solution after treatment was calculated using the following formula:

$$\mathrm{RE}\% = (C_0 - C_t)/C_0 \times 100,$$

where C_0 is the initial concentration of the pollutant, and C_t is the concentration after treatment at time t.

Energy consumption. Energy use of the process was estimated by evaluating the power demands of the reactor and the oxidant supply system per unit volume of water processed.

Byproduct analysis. Analysis was done using gas chromatography-mass spectrometry (GC-MS) in a bid to determine any byproducts that may be generated during the degradation process. Particular emphasis was made to look for any toxic byproducts that could be produced.

Sustainability index. It was tried to assess sustainability index as a function of pollutant removal efficiency, fossil energy demands, and toxicity of byproducts of the oxidation process. In the experimental investigation, ANOVA has been performed to find out the effect of operational parameters on the pollutant degradation efficiency[11,12]. The comparative analysis of the DL model's predictions and experimental results was performed with the help of the coefficient of determination and the root mean square error.

RESULTS AND DISCUSSION

Tables 1 and 2 provide the statistical summary of the data obtained from the experimental study involving the degradation of pollutants using green oxidants and bio-based catalysts and comparison made of the actual data with the DL model data.

Table 1 provides an overview of the experimental conditions and outcomes for five pollutants: phenol, dyes, pharmaceuticals, lead and cadmium ions. Both the pollutants were treated with H_2O_2 or ozone and bio-based catalysts which included activated carbon and bio-char. Some of the factors that have been taken into consideration include initial concentration of the pollutant, pH of solution, type of oxidant, type of catalyst, percentage removal efficiency and time of reaction.

Table 1. Pollutant degradation with different green oxidants

Pollutant	Initial concentration (mg/l)	Oxidant	Catalyst	pH	Removal efficiency (%)	Reaction time (min)
Phenol	100	H_2O_2	Biochar	7	85	120
Dye	75	Ozone	Activated Carbon	5	90	90
Pharmaceutical	50	H_2O_2	Biochar	7	78	150
Lead (Pb^{2+})	25	Ozone	Biochar	9	65	180
Cadmium (Cd^{2+})	30	H_2O_2	Activated Carbon	7	72	120

Pollutant type and concentration. The initial concentrations of the pollutants used in the experiments were between 25 and 100 of mg/l. In the present study, the removal efficiency of organic pollutants such as phenol, dye, and pharmaceuticals is higher than the inorganic pollutants such as lead and cadmium. This implies that carbon containing compounds are sensitive to oxidation, especially when combined with suitable catalysts and with favourable pH.

Oxidant and catalyst combination. The results of the comparison of hydrogen peroxide and ozone as green oxidants varied on the basis of the pollutant type. The tests included a mixture of hydrogen peroxide with biochar where higher removal efficiency was reported for phenol at 85% and pharmaceutical compound at 78%. Activated carbon was found to enhance the removal efficiency of the dyes to a maximum of 90% when used in combination with ozone, and the use of biochar with ozone slightly less effective in removal of the heavy metal ions like lead with 65%.

Effect of pH. To investigate the effect of pH with the pollutant removal, the pH levels were controlled in this study. For example, high removal efficiency of phenol and cadmium was achieved under the pH of 7; the best pH for dye degradation was 5. While, for some pollutant, that is heavy metals as in lead, a higher pH of 9 was more effective in their removal signifying that increase in pH requires a specific tendency based on the character of the pollutant[13].

Reaction time. The reaction time ranged between 90 and 180 min, for almost all the pollutants the degradation rates are significant within 2 h. Dyes and phenol had the shortest time of contact with the oxidants and catalysts while heavy metals took more time to be absorbed satisfactorily. In summary, from Table 1 it could be seen that green oxidants and bio-based catalysts are very effective in the removal of both organic and inorganic pollutants whereby the peculiarities like oxidant selection, catalyst type, and pH greatly influenced the efficiency of the processes.

In Table 2, the deep learning (DL) model's results for removal efficiency of each pollutant are compared with the experimental outcomes. Also, the RMSE is presented to show the measure of precision of the model's forecast as compared to the actual outcome.

Table 2. Deep learning model prediction versus experimental results

Pollutant	Predicted removal efficiency (%)	Experimental removal efficiency (%)	RMSE (%)
Phenol	87	85	2.0
Dye	91	90	1.5
Pharmaceutical	80	78	1.8
Lead (Pb^{2+})	67	65	1.9
Cadmium (Cd^{2+})	74	72	2.2

High accuracy of predictions. The results showed that the DL model had high accuracy to the removal efficiency of pollutants and had only slight difference with the experimental values. For instance, for phenol the model was revealing 87% removal efficiency while the experimental observation was 85% which leads to an RMSE of 2% as given in Fig. 1. This affirms the fact that the model provides a good approximation of real life conditions in helping to predict best oxidation practices.

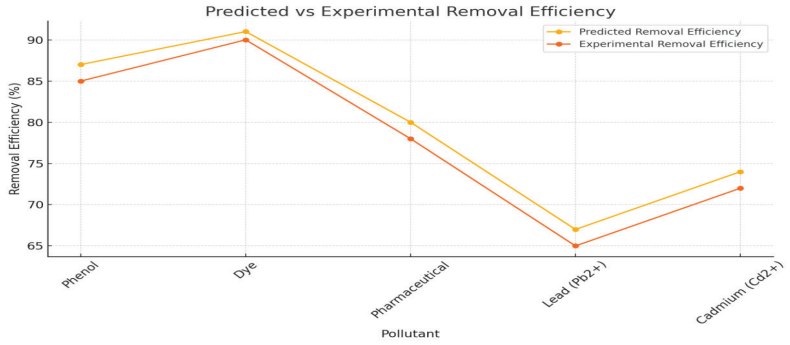

Fig. 1. Predicted versus experimental removal efficiency of phenol

Consistency across pollutants. DL model equally performed well for all types of pollutants with the smallest RMSE having a mean of 1.5 to 2.2%. This implies that the

model brought out functional associations between a number of operational factors such as the oxidant dosage, catalyst concentration and pH with pollutant elimination regardless of whether it is organic or inorganic[14].

Optimising process efficiency. Thus, the satisfactory concordance between the removal efficiencies predicted by the DL model and the experimental ones proves the ability of the former in real-time monitoring and optimisation of oxidation processes[15,16]. Due to the identification of factors that characterise the situation when the process gives maximum results, the use of the model can minimise the number of test trials.

CONCLUSIONS

The data obtained in the study establish the potential of employing green oxidation processes along with deep learning models for pollutants degradation. Table 1 demonstrates the efficiency of using eco-friendly oxidants such as hydrogen peroxide and ozone in conjunction with bio-based catalysts in attaining high pollutant reduction levels among different environmental pollutants. Table 2 summarises the ability of the DL model to predict the removal efficiency of each pollutant as had been predicted by the model. The low RMSE values between the predicted and experimental results show that such models can be applied to make improvements to the treatment processes on a real-time basis with the aim of achieving sustainable and efficient removal of pollutants within diverse environments.

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