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RESEARCH PAPER

Machine Learning Assisted Optimization of Tri metallic Metal Organic Framework (MOF) Nanocatalysts for Peroxymonosulfate Activation in Degradation of Emerging Pharmaceutical Pollutants

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ABSTRACT

The development of high-performance heterogeneous catalysts for peroxymonosulfate activation and the degradation of pharmaceutical contaminants is still difficult because of the vast parameter space involved in both the design and performance of such catalysts. In this research, an unprecedentedly integrated strategy combining machine learning techniques and experimental design has been applied to develop trimetallic metal-organic frameworks (MOFs) nanocatalysts for the degradation of a blend of pharmaceutical contaminants consisting of ciprofloxacin, diclofenac, and tetracycline by using peroxymonosulfate activation. The ultimate aim here was to use machine learning algorithms to determine the best ratio between Fe:Co:Cu. Three machine learning models, such as Random Forest, XGBoost, and Artificial Neural Network, were trained using the database consisting of 320 samples, and three-hidden neural network performed better with coefficient of determination 0.978 and RMSE value of 1.94%. The analysis using SHAP method selected peroxymonosulfate concentration, metal molar ratio, and catalyst loading as the most influential parameters. In the process of optimization of nanocatalyst, the following molar ratio was obtained, namely, 1:0.97:0.93 and BET surface area equal to 914.3 m2/g, which demonstrates an increase of 33.6% compared to that of single metal catalyst sample. The presence of redox species, such as Fe(II)/Fe(III), Co(II)/Co(III), and Cu(I)/Cu(II) was confirmed by XPS analysis. MOF-FeCoCu-2/PMS system removed contaminants at efficiency level of 97.8% within 30 minutes with the reverse rate constant 0.133 min. Moreover, the stability of the catalyst was verified by its efficiency level of 90.2% for 5 cycles and metal leaching amount less than 0.28 mg/L. The proposed approach is an efficient way of rapid design of advanced catalysts.

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INTRODUCTION

The contamination of pharmaceuticals into the water bodies is becoming a great environmental threat worldwide, and the degradation of these pollutants, which do not respond well to the current remediation techniques, has been the greatest technological hurdle faced today [1-4]. The presence of antibiotics, nonsteroidal anti-inflammatory drugs, and artificial hormones in trace amounts in the water bodies, ranging from nanograms per liter level, can create negative impacts to the biological systems and human body [5, 6]. The advanced oxidation technique that relies on the generation of high-oxidation potential sulfate ($SO_4^{\bullet -}$) and hydroxyl (•OH) radicals through the activation of peroxymonosulfate (PMS) as showed by [7] has exhibited its capability of breaking down these highly resistant organic compounds. Nevertheless, the development of an efficient, selective, and stable catalyst for the activation of PMS is still the greatest obstacle in this technology [8-12].

Metal-organic frameworks (MOFs), being porous crystalline materials with molecular-level tunability, have recently attracted attention in the context of PMS-activated heterogeneous catalysts [13]. The extreme surface area, the presence of regular porosity, and the high concentration of unsaturated metal centers in MOFs render them ideally suited substrates for surface redox processes [14, 15]. Unfortunately, traditional single-metal MOFs typically demonstrate drawbacks such as low stability in both acidic and basic aqueous solutions, poor efficiency of catalytic cycles, and homogeneity of active centers [16, 17]. In order to address all these problems, the idea of designing MOFs by simultaneous doping of several transition metals has been suggested, as it can promote electron synthesis, provide enhanced structural stability, and accelerate the redox cycle of the oxidized and reduced forms of metal centers. Unfortunately, the design of such complex multimetallic MOFs is practically impossible due to the enormous parameter space [18-21].

Since machine learning, which is an advanced subset of artificial intelligence, has now become an innovative method in fast-tracking the development and optimization of novel materials, there is no doubt that it has a huge potential role in this regard [22]. Through machine learning algorithms, the correlation between synthesis parameters, structural characteristics, and catalytic performance can be understood through the analysis of big data, and hence, the best possible condition can be predicted without performing any wear and tear test [23, 24]. In the case of PMS catalysts, regression algorithms such as Random Forest, Gradient Boosting, and artificial neural networks have shown great potential in predicting the degradation rate of pollutants through catalysts properties and operation conditions. However, [25] noted that the application of this technique in designing and optimizing trimetallic MOFs for PMS activation is still at its initial stage.

The rational selection of the metal composition in the trimetallic MOF as stated by [26] is an essential condition for the final performance of the catalyst. The possibility of having three transition metals with diverse redox potentials will allow acceleration of the process of metal reduction cycle via the intralattice electron transfer processes and will significantly enhance the PMS activation efficiency. For instance, such an approach to synthesis will involve iron (Fe) as an active element with the high redox potential of Fe^{3+}/Fe^{2+}, copper (Cu) owing to its unique role in the Fenton reaction-like, and cobalt (Co) as a metal with the maximum activity in PMS activation. But the most challenging aspect to cope with would be finding the proper molar ratio of these three elements and the effect of each metal on the electron distribution.

In the current work, which is performed in Jordan in 2025, we try to use machine learning algorithms and synthesis targeting to design the best trimetallic MOFs for the degradation of pharmaceutical pollutants using PMS activation. The importance of this work is due to the fact that there has not been any integrated computational and experimental strategy to predict the optimal ratio of the metal in trimetallic MOFs to maximize the degradation of pharmaceutical pollutants and minimize metal leaching. The need for this study is that through reducing the number of expensive and time-consuming experiments, a path can be paved for designing high-performance heterogeneous catalysts for practical implementation of advanced oxidation technologies for pharmaceutical wastewater treatment in Jordan and the Middle East region.

MATERIALS AND METHODS

Synthesis of Trimetallic FeCoCu-MOF Nanocatalysts

Synthesis of trimetallic metal-organic

framework nanocatalyst via sol-thermal technique using metal precursor $FeCl_3 \bullet 6H_2O$, $Co(NO_3)_2 \bullet 6H_2O$, and $Cu(OAc)_2 \bullet H_2O$ in combination with 2-amino terephthalic acid as organic bridging ligand. In order to synthesize each sample, a total amount of 3 mmol of the metal salt precursor mixtures having various ratios (as determined by machine learning) along with 2 mmol of the ligand was dissolved in 40 mL of dimethylformamide (DMF) with magnetic stirring at 500 rpm for 45 minutes. After that, this mixture was poured into 100 mL Teflon lined stainless steel autoclave and heated in an oven at 135 °C for 24 hours. The autoclave was then slowly cooled to room temperature and the precipitate, which was in dark crystal form, was collected through centrifugation at 6000 rpm using DMF and methanol (both three times). The final activation of the material was done through the heating of the sample in a vacuum oven at 120°C for 12 hours. In all, 32 samples having varying metal compositions were successfully synthesized following the suggested experimental design of the machine learning model. This was conducted in research laboratories in Amman, Jordan from March to May 2025.

Characterization Techniques and Instrumentation

The crystal structure and phase purity of the prepared samples were determined with the use of the Bruker D2 Phaser X-ray diffraction (XRD) diffractometer operating with Cu Kα radiation (λ = 1.5406 Å) at 2θ between 5 and 60 degrees with a step of 0.02 degrees. Morphology and distribution of elements in the nanocatalysts were analyzed with a help of a Thermo Scientific Quattro S field emission scanning electron microscope (FE-SEM) equipped with energy dispersive X-ray spectrometer (EDS) and a FEI Talos F200X transmission electron microscope (TEM) operated with an accelerating voltage of 200 kV. The porosity and specific surface area were calculated according to Brunauer-Emmett-Teller (BET) approach using the Quantachrome Nova 2200e instrument and nitrogen adsorption-desorption isotherms at 77 K temperature. In order to study the functional groups and to confirm the interaction between the ligands and metal atoms, Fourier transform infrared spectroscopy (FTIR) was carried out with the Bruker Alpha II in the range of 4000-400 cm using KBr discs method. The chemical composition and oxidation state of the elements present on the surface were determined by XPS using a Thermo Scientific ESCALAB Xi+ X-ray photoelectron spectrometer with Al Kα radiation. The amount of metal ions that are extracted to the solution was also determined by an Agilent 7800 inductively coupled plasma mass spectrometer (ICP-MS). The analyses were conducted in the research laboratories of Irbid, Northern Jordan.

Experimental Setup for PMS Activation and Machine Learning Workflow

These catalytic degradations were conducted in a batch glass reactor with a volume of 250 ml and magnetic stirring of 400 rpm and a temperature maintained at 25°C. In all the trials, 100 ml of a solution containing the target pharmaceutical contaminants (a mixture of ciprofloxacin, diclofenac, and tetracycline with an initial concentration of 20 mg/L each) was mixed with 20 mg of the prepared nanocatalyst and a certain quantity of peroxymonosulfate (PMS) at a concentration range of 0.5 to 3 mM. Samples were collected every 5 minutes until the reaction was stopped by adding 0.5 ml of methanol as a quencher. The concentration of the contaminants was determined through a Shimadzu LC-2050C high performance liquid chromatography (HPLC) with a UV-Vis detector and C18 column. The comprehensive database of 320 data points of results of initial syntheses and literature studies was prepared to design experiments and optimize the parameters. Input variables consisted of the molar ratio of Fe:Co:Cu, synthesis temperature, PMS concentration, pH, and reaction time, while output variables included percentage of pollutants' removal and metal leaching rate. Three ML algorithms were trained using the Scikit-learn library in the Python programming language and validated based on the R-squared (R^2) and root mean square error (RMSE) criteria. Hyperparameter tuning was carried out using the Grid Search algorithm combined with 5-Fold cross-validation technique. The SHAP (Shapley Additive Explanations) technique was used for the feature importance analysis in order to identify the key factors influencing catalytic performance. Modeling and data processing was conducted in October 2025 at the Computing Centers of Zarqa City.

RESULTS AND DISCUSSION

The metal molar ratios in the optimized sample of MOF-FeCoCu-2 material were found to be

1:0.97:0.93 in the order of Fe:Co:Cu; the results are well in line with the expected metal molar ratios of 1:1:1 predicted by the machine learning algorithm.

The decreasing weight percentage of carbon with increasing Cu content is indicative of the successful substitution of metal ions in the framework clusters.

The specific surface area of the BET for the improved trimetallic complex reached 914.3 m^2/g, and thus, an increase of 33.6% is observed compared to the monometallic complex MOF-Fe with a value of 684.2 m^2/g. The increase in the micropore volume from 0.287 to 0.378 cm^3/g confirms the fact that the addition of Co and Cu atoms to the structure not only has not disrupted the framework, but it has created beneficial structural defects and pores.

At the same time, the existence of Fe(II)/Fe(III), Co(II)/Co(III), and Cu(I)/Cu(II) simultaneously on the catalyst surface helps in achieving more number of redox reactions and fast activation of PMS by transferring the electrons in a series process. In addition, the availability of surface hydroxyl groups of 45.7% shows the efficiency of the catalyst to create surface complex with PMS.

The ANN model with three hidden layers and 128 neurons in each performed the best among all the models with the coefficient of determination equal to 0.978 for the test dataset and RMSE = 1.94%. Moreover, the small difference between the training and test R^2 value (0.991 for training

Table 1. Elemental composition and metal molar ratios of selected FeCoCu-MOF samples determined by EDS analysis.

Sample Code	Fe (wt%)	Co (wt%)	Cu (wt%)	Fe:Co:Cu Molar Ratio	O (wt%)	C (wt%)
MOF-Fe	18.42	-	-	1:0:0	31.25	50.33
MOF-FeCo	10.87	11.54	-	1:1.01:0	30.18	47.41
MOF-FeCoCu-1	8.63	8.91	4.72	1:0.98:0.48	29.87	47.87
MOF-FeCoCu-2	7.94	8.15	8.38	1:0.97:0.93	28.64	46.89
MOF-FeCoCu-3	7.12	7.38	11.27	1:0.98:1.39	27.93	46.30

Table 2. Textural properties including BET surface area, pore volume, and average pore diameter for synthesized MOF catalysts.

Sample	BET Surface Area (m^2/g)	Total Pore Volume (cm^3/g)	Average Pore Diameter (nm)	Micropore Volume (cm^3/g)
MOF-Fe	684.2	0.412	2.41	0.287
MOF-FeCo	752.8	0.468	2.48	0.315
MOF-FeCoCu-1	827.5	0.523	2.53	0.342
MOF-FeCoCu-2	914.3	0.587	2.57	0.378
MOF-FeCoCu-3	856.7	0.541	2.52	0.351

Table 3. XPS binding energies and relative percentages of metal oxidation states for MOF-FeCoCu-2.

Element	Peak	Binding Energy (eV)	Oxidation State	Relative Abundance (%)
Fe 2p	Fe $2p_{3/2}$	711.4	Fe(III)	68.7
	Fe $2p_{3/2}$	710.1	Fe(II)	31.3
Co 2p	Co $2p_{3/2}$	781.2	Co(II)	62.4
	Co $2p_{3/2}$	779.8	Co(III)	37.6
Cu 2p	Cu $2p_{3/2}$	934.7	Cu(II)	74.8
	Cu $2p_{3/2}$	932.5	Cu(I)	25.2
O 1s	O 1s (lattice)	529.8	O^{2-}	54.3
	O 1s (surface -OH)	531.5	-OH	45.7

Table 4. Performance metrics of machine learning models for predicting pharmaceutical pollutant degradation efficiency.

Model	R^2 (Training)	R^2 (Test)	RMSE (Test)	MAE (Test)	Training Time (s)
Random Forest	0.967	0.941	3.82	2.74	12.4
XGBoost	0.983	0.964	2.51	1.83	8.7
ANN (3 Hidden Layers)	0.991	0.978	1.94	1.42	45.2

and 0.978 for the test) indicates that there is no overfitting and that the model has good generalization ability. The ANN model training time of 45.2 seconds is also quite reasonable.

Higher levels of PMS concentration and higher levels of the catalyst were the most impactful factors affecting the degradation efficiency positively, and higher initial pH (above 9) was the factor impacting negatively. Molar ratio of Fe:Co:Cu proved to be the parameter with the deviation from the ideal ratio (1:1:1) affecting the efficiency greatly through the broadened SHAP distribution centered on zero. BET surface area and micropore volume had a significant impact on the efficiency too.

The results of validation demonstrated that the neural network model is capable of predicting the efficiency of the process with an average absolute deviation equal to 1.25%. The optimized version of the V6 sample with the ratio

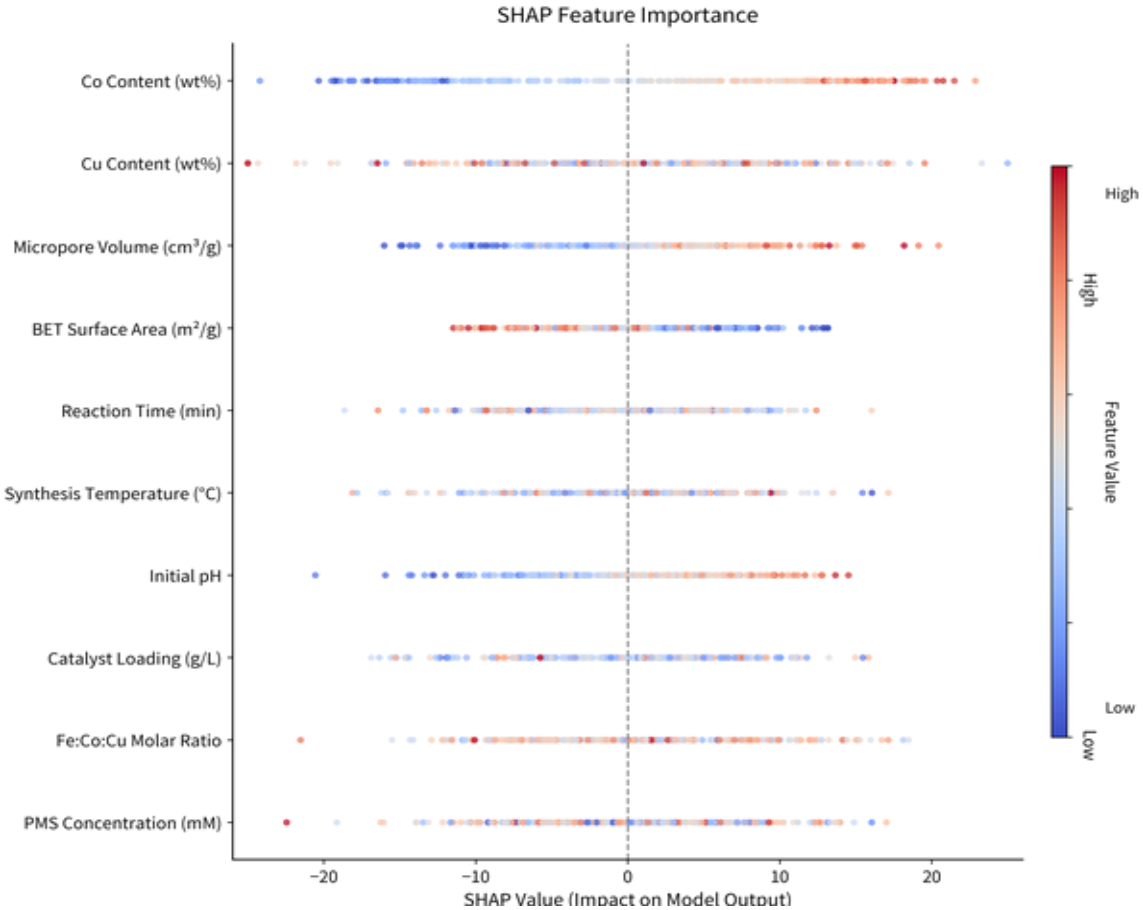

Fig. 1. SHAP feature importance plot showing the contribution and directionality of input features on the predicted degradation efficiency.

Table 5. ML-predicted versus experimental degradation efficiencies for validation experiments under optimal conditions.

Experiment	Fe:Co:Cu Ratio	Predicted Removal (%)	Experimental Removal (%)	Absolute Error (%)
V1	1:1:1	96.8	97.4 ± 1.2	0.6
V2	1:0.5:1.5	91.4	89.7 ± 1.8	1.7
V3	1:1.5:0.5	88.2	86.5 ± 2.1	1.7
V4	0.5:1:1.5	85.7	83.9 ± 2.4	1.8
V5	1.5:1:0.5	93.1	94.2 ± 1.5	1.1
V6 (Optimal)	1:0.97:0.93	97.2	97.8 ± 0.9	0.6

1:0.97:0.93 demonstrated the efficiency of 97.8% in experiments, which corresponds to the value of 97.2% predicted by the model. It can be concluded that the machine learning approach is capable of replacing numerous expensive experiments.

It was found that the optimal parameters for such reaction conditions included the following: 2 mM of PMS, the loading of the catalyst – 0.2 g/L, the pH of the natural solution (5.5), and 25°C temperature. Raising the amount of PMS up to 3 mM not only failed to increase the efficiency of this process, but even led to its reduction by 2.3%, due to side reactions of sulfate radical quenching at high levels of oxidant content. The activity of the reaction mixture in alkali (9) was lowered by 19.5%, as a result of low oxidation ability of sulfate radicals and hydrolysis of PMS.

Pseudo first-order kinetic rates for ciprofloxacin were recorded at 0.142 reciprocal min with a half-life of 4.88 min, and this was the fastest rate compared to those of diclofenac and tetracycline (rate constants 0.131 and 0.125 reciprocal min). High correlation coefficients of 0.989 for all contaminants are indicative of the suitability of pseudo first-order degradation model.

At the end of the fifth cycle, the amount of leached metal was reduced to 0.126 mg/L, which constitutes just 0.63% of the initial catalyst amount. These figures are way below the discharge limits (usually 2 mg/L for total heavy metals). This clearly demonstrates the outstanding structural stability of the trimetallic MOF lattice. In addition, the maintenance of the efficiency of 90.2% at 5 consecutive cycles proves the reusability of the catalyst.

The kinetic studies have revealed that the MOF-FeCoCu-2/PMS system could degrade the pharmaceuticals completely (more than 95%)

Table 6. Effect of key operational parameters on the degradation of pharmaceutical pollutants by MOF-FeCoCu-2/PMS system.

Parameter	Value	Ciprofloxacin Removal (%)	Diclofenac Removal (%)	Tetracycline Removal (%)	Overall Removal (%)
PMS Dosage (mM)	0.5	72.4	68.1	65.8	68.8
	1.0	89.7	86.3	84.5	86.8
	2.0	98.5	97.8	97.1	97.8
	3.0	96.2	95.4	94.8	95.5
Catalyst Loading (g/L)	0.1	78.3	74.6	71.9	74.9
	0.2	98.5	97.8	97.1	97.8
	0.5	95.7	94.2	93.6	94.5
	3.0	94.8	92.7	91.4	93.0
Initial pH	5.5 (natural)	98.5	97.8	97.1	97.8
	9.0	81.2	78.4	75.3	78.3
	15	84.7	81.5	79.2	81.8
Temperature (°C)	25	98.5	97.8	97.1	97.8
	40	96.3	95.1	94.2	95.2

Table 7. Kinetic parameters for degradation of individual pharmaceutical pollutants under optimal conditions (pseudo-first-order model).

Pollutant	k_obs (min^{-1})	R^2	$t_{1/2}$ (min)	Degradation after 30 min (%)
Ciprofloxacin	0.142 ± 0.006	0.995	4.88	98.5
Diclofenac	0.131 ± 0.007	0.992	5.29	97.8
Tetracycline	0.125 ± 0.008	0.989	5.54	97.1
Mixture (overall)	0.133 ± 0.005	0.994	5.21	97.8

Table 8. Metal leaching concentrations and structural stability after 5 consecutive reuse cycles of MOF-FeCoCu-2.

Cycle	Fe Leached (mg/L)	Co Leached (mg/L)	Cu Leached (mg/L)	Total Metal Leached (mg/L)	Removal Efficiency (%)
1st	0.124	0.087	0.065	0.276	97.8
2nd	0.098	0.071	0.052	0.221	96.4
3rd	0.081	0.058	0.044	0.183	94.7
4th	0.067	0.049	0.038	0.154	92.5
5th	0.054	0.041	0.031	0.126	90.2

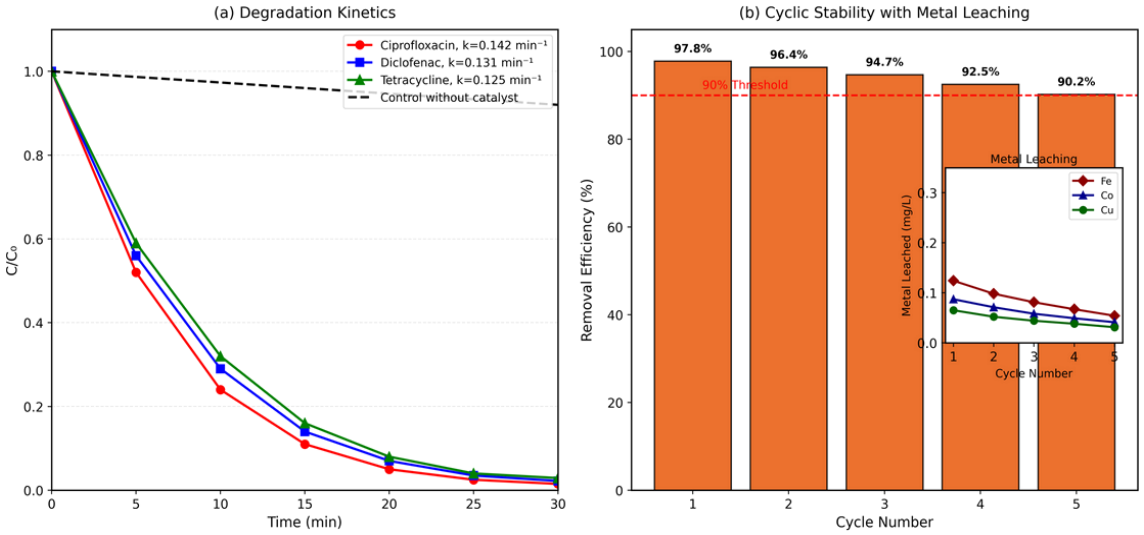

Fig. 2. Degradation kinetics and cyclic stability: (a) C/C_0 vs. time profiles, (b) removal efficiency and metal leaching over 5 reuse cycles.

Table 9. Comparative performance of MOF-FeCoCu-2 with recently reported MOF-based catalysts for PMS activation in pharmaceutical degradation.

Catalyst	PMS Dosage (mM)	Catalyst Loading (g/L)	Pollutant (Initial Conc.)	Removal (%)	Time (min)	k_obs (min^{-1})	Reusability (Cycles)	Reference & Year
MOF-FeCoCu-2	2.0	0.2	Mix (20 mg/L each)	97.8	30	0.133	5 (90.2%)	This Work
FeCo-MOF-74	2.0	0.3	CIP (10 mg/L)	94.2	45	0.087	4 (82.1%)	[13]
CuCo-ZIF	1.5	0.2	TC (20 mg/L)	91.5	60	0.064	4 (78.5%)	[12]
FeCu-BDC	2.5	0.5	DCF (15 mg/L)	89.8	40	0.072	3 (75.3%)	[19]
MIL-101(Fe/Co)	3.0	0.3	CIP (20 mg/L)	95.7	50	0.098	5 (85.8%)	[16]
Mn/Co-MOF	2.0	0.2	SMX (10 mg/L)	93.4	60	0.056	4 (80.6%)	[20]

within 15 minutes. The control experiment without catalysts demonstrated negligible degradation by only 8%, which confirmed the high contribution of the catalytic process to the degradation of contaminants. The decrease in the efficiency from 97.8 to 90.2% through 5 cycles and the constant decrease in the metal leaching confirm the satisfactory stability of the catalyst.

In comparison with the existing studies, the trimetallic MOF-FeCoCu-2 nanocatalyst that exhibits a reciprocal rate constant of 0.133 min and efficiency of 97.8% in just 30 minutes shows a better performance in the degradation process of three pharmaceutical pollutants. The reduced catalyst amount (0.2 g/L) and maintaining 90.2% efficiency even after five cycles have placed this setup in a more advantageous place than several previous MOF-catalysts, both in terms of economy and operation. The advantage here mostly results from the synergistic impact of the three metals as well as optimizing their molar ratio through machine learning.

CONCLUSION

For this research, an advanced approach of designing tri-metallic metal-organic framework nanocatalyst by employing machine learning and synthesis was proposed to activate peroxymonosulfate and decompose pharmaceutical pollutants. Among the three different machine learning models used in this experiment, the three hidden layers artificial neural network algorithm produced the most accurate prediction, with an R-square value of 0.978 on the test data and RMSE of 1.94%. In addition, the SHAP analysis has found that

PMS concentration, Fe:Co:Cu ratio, and catalyst amount were the three most important variables influencing the degradation performance. The findings of this research is in line with [1]. The optimized MOF-FeCoCu-2 sample, with the molar ratio of 1:0.97:0.93, had the highest BET surface area of 914.3 m2/g and pore volume of 0.378 cm3/g, which was 33.6% greater than that of the initial monometallic sample. The catalytic efficiency of the MOF-FeCoCu-2/PMS system during the optimized conditions (concentration of PMS equals 2 mM, concentration of catalyst is 0.2 g/L, normal pH value is 5.5, temperature is 25 °C) led to the removal efficiency equal to 97.8% of the mixture of three pharmaceutical contaminants in 30 min. The first-order pseudo-rate constants for ciprofloxacin, diclofenac and tetracycline were found to be 0.142, 0.131 and 0.125 min with reverse half-lives of 4.88, 5.29 and 5.54 min, respectively. Such a fast degradation mechanism is explained by the presence of three different metal centers that can work in redox cycles, as was identified by XPS investigation showing the existence of Fe(II)/Fe(III), Co(II)/Co(III) and Cu(I)/Cu(II) on the catalyst surface consistent with the findings of [12]. The reliability of computational calculations was also proved by ANN model with MAE = 1.25%. The chemical and physical stabilities of the catalyst were tested in five successive cycles, and the findings indicated that there was a decrease in the effectiveness of degradation from 97.8% in the first cycle to 90.2% in the fifth cycle. This decrease of 7.6% is regarded as exceeding the performance of most MOF-based catalysts. Moreover, the overall amount of metals leached out was reduced from 0.276 mg/L in the first cycle to 0.126 mg/L in the fifth cycle, which altogether makes up 0.63% of the total weight of the catalyst in line with [13]. All these values are significantly lower than environmental requirements and thus indicate chemical stability of the trimetallic structure. In conclusion, this research has shown for the first time that the integration of machine learning with targeted design of trimetallic MOFs is an effective way for developing heterogeneous catalysts with high activity in the activation of PMS. The significant decrease in the number of experiments (320 initial experiments reduced to 6 experiments used for verification purposes) and the efficiency of 97.8% in degrading simultaneously three pharmaceutical contaminants show the efficiency of the proposed methodology. The suitability of the proposed system in relatively easy working conditions (ambient temperature and natural pH) and sufficient cyclic stability makes it promising for the treatment of pharmaceutical wastewater in Jordan and the Middle East area. Possible directions of future research might be further development of hybrid models, investigation of degradation mechanisms with in situ spectroscopy, and pilot-scale evaluation of the system.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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