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Modeling Methodology Based on Stacked Neural Networks Applied to the Photocatalytic Degradation of Triclopyr

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In the present paper, we propose a modeling methodology based on stacked neural networks by combining several individual networks in parallel, whose outputs are weighted to provide the output of the stack. Also, a procedure was included for finding the optimal set of weights that leads to the best performance of modeling, on both training and validation data. As a case study, we consider the photocatalytic oxidation of triclopyr where the final concentration was evaluated depending on the reaction conditions, irradiation time and amounts of reactants. We show that the performance of the stack is better than those of individual networks, especially for the validation phase.

Keywords decomposition; modeling; neural network; photocatalysis; triclopyr

INTRODUCTION

Pesticides and agrochemical compounds in general have been detected in water since the 1950s. The United Nations estimates that less than 1% of all pesticides used in agriculture actually reach the crops. The remainder ends up contaminating the land, the air, and particularly the water (1–3). As these contaminants in many cases are toxic and non-biodegradable, they tend to accumulate in the environment with unpredictable consequences for the mid-term future (4). An ideal treatment method for pesticide wastes would be a non-selective one that could achieve rapid and complete degradation to inorganic products and could be suitable for small-scale wastes (5).

Possible advanced treatment methods that are used at the present time include advanced chemical oxidation,

adsorption on granulated active carbon, incineration, etc. Among the so-called Advanced Oxidation Processes (AOP), solar photocatalytic methods like heterogeneous photocatalysis ($TiO_2/UV-A$) or photo-Fenton reagent ($Fe^{3+}/H_2O_2/UV-A, Vis$) have proven to be effective for a variety of chemicals (pesticides, dyes, etc.) and different types of wastewater (industrial, municipal, etc.) (5–7). A variety of toxic agrochemical substances, such as insecticides and pesticides, have also been studied with regard to their photocatalytic degradation, in the presence of artificial or solar illumination, with very encouraging results, while studies dealing with real or simulated wastewater have revealed that their complete or partial degradation is possible via the above-mentioned methods (5,8–11).

The phenomenological treatment of such photochemical systems is very complex. In general, the rate of reaction in heterogeneous photocatalytic systems is a complex non-linear function of catalyst loading, light intensity, initial solution pH, reactant, and oxidants concentration, etc. Due to these reasons, the ability of systems such as artificial neural networks (ANN) to recognize and reproduce cause–effect relationships through training, for multiple input–output mappings, has gained popularity in various areas of chemical engineering, and also in the field of photocatalytic treatment of wastewater (12–17).

Artificial neural networks (ANN) represent promising alternative tools for classical process modeling. The role of an artificial neural network is to discover the relationships that link patterns of input data to the associated output data. Numerous types of problems in science can be cast in the form of a pattern-matching problem, and artificial neural networks are among the most effective methods within machine learning for revealing these links. Once trained, artificial neural networks are fast in operation and are particularly valuable in circumstances where

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the volume of available raw data is large, but not enough is known about the relationships within the data to allow the scientist to build an analytical model (18).

Among the existing numerous neural networks paradigms, the feed-forward neural networks are the most popular due to their flexibility in structure, good representational capabilities, and large number of available training algorithms (19). In general, there is no certainty that any individual model can extract all relevant information from the data set. The idea of combining neural network models is based on the premise that different neural networks can capture different aspects of process behavior and aggregating this information should reduce uncertainty and provide more accurate predictions. It is always possible that a stacked network could outperform a single-best trained network for the following reasons:

1. Optimal network architecture cannot always be guaranteed.
2. The optimization of network parameters is a problem with many local minima. Even for a given architecture, final network parameters can differ between one run of the algorithm and another.
3. Different activation functions and learning algorithms can also lead to different generalization characteristics, and no one activation function or learning algorithm is the best in all cases.
4. Convergence criteria used for network training can lead to very different solutions for a given network architecture (20).

Stacked neural networks designed to improve predictive modeling, have been increasingly used in the chemical processes, especially for dealing with some complex nonlinear processes where the understanding of the phenomena is limited. Some examples are presented in references (20–24).

Our paper presents a neural networks modeling methodology applied to the heterogeneous photocatalytic decomposition of triclopyr in the presence of TiO_2 as photocatalyst and is based on our experimental data obtained earlier (25). The heterogeneous photocatalytic oxidation of organic pollutants in the presence of TiO_2 as catalyst, under artificial or solar irradiation, is a well known methodology, the description of which is presented in several excellent review articles (5,26,27). Therefore, in this paper, the various stages of the photocatalytic process will not be further presented.

This methodology includes simple and stacked feed-forward neural networks and a technique of optimizing the weights of the stack to obtain the best performance of the neural models. The developed models, especially stacked neural networks, accurately predict the final concentration of triclopyr as a function of reaction conditions.

NEURAL NETWORK MODELING

Individual Neural Networks

A good process model—accurate model with a short simulation time—is a prerequisite for application in the optimal control strategy. A phenomenological model of a chemical process is difficult to obtain, especially when limited knowledge about the process is available. Neural networks could overcome these difficulties because they have a series of advantages, such as the possibility to be applied to complex nonlinear processes, the ease in using neural models, the possibility of substituting experiments with predictions. Neural models need only input-output data (experimental data), so their advantages are evident against the complexity of the computations.

The most common neural network architecture is the multi-layer feed-forward neural network (often called multi-layer perceptron, MLP) which has a layered structure, consisting of input, hidden, and output layers. The number of neurons in input and output layers corresponds to the independent and dependent variables in the modeling and hidden neurons will be established within the best topologies of the neural networks.

The neural network modeling implies several stages—collecting the training data by experiments, choosing training and testing data sets, developing the neural network topology, training, and, finally, establishing the performance of the model by evaluating the network predictions for new, unseen data.

For our case study, the photocatalytic degradation of triclopyr, we follow the final concentration of this compound as a function of process conditions. The neural models consider the irradiation time (t), the initial concentration of triclopyr (C_0), the concentration of TiO_2 used as a catalyst (C_{TiO_2}), and the concentration of H_2O_2 ($C_{\text{H}_2\text{O}_2}$) as inputs, and the final concentration of triclopyr (C) as the output.

First, the data (368 in total) were split into training and validation data sets, about 15% being the test data set used to evaluate the performance of the neural network to data not being used in the training process. In this way, we can evaluate the most important feature of a neural model—the generalization capability.

The number of hidden layers and units was established by training a different range of networks and selecting the one that best balanced generalization performance against network size. The best network topology was determined based on the mean of squared errors (MSE) of the training data. Hidden neurons, as well as the output layer neuron, use hyperbolic tangent as the nonlinear activation function. The network was trained using the well-known back-propagation algorithm. We consider that training ends when the network error (MSE) on the testing set becomes sufficiently small and does not increase.

TABLE 1
Different neural networks developed with experimental data

Network type	MSE	r	E_p %
MLP(4:5:1)	0.0012	0.988230	19.2430
MLP(4:10:1)	0.0004	0.998497	13.1822
MLP(4:15:1)	0.000354	0.998669	9.9729
MLP(4:20:1)	0.000375	0.99859	13.5923
MLP(4:12:4:1)	0.000756	0.997156	17.9502
MLP(4:24:8:1)	0.00058	0.997816	11.6835
MLP(4:25:20:1)	0.000079	0.999702	3.8722
MLP(4:30:25:1)	0.000106	0.999599	5.5637
MLP(4:42:14:1)	0.00047	0.998232	10.6775

Table 1 contains a series of MLP with one or two hidden layers trained with experimental data, and their performances registered in the training stage: *MSE*, *r* (the correlation between experimental data and the output of the neural network) and E_p (percent error). Only several examples are presented in Table 1 from many neural networks trained on a different number of epochs (different training time). Taking into account their performance, three neural networks were selected—MLP(4:15:1), MLP(4:25:20:1), and MLP(4:30:25:1).

Stacked Neural Networks

Generally, stacked neural networks provide more accurate results than individual neural networks. In this paper, we compare the predictions of individual and stacked neural networks, especially in the validation phase, in order to select a neural model with a high generalization capability.

For our stack model, we considered the three neural networks previously selected, MLP(4:15:1), MLP(4:25:20:1), and MLP(4:30:25:1), based on their good performances obtained in the training and validation phases. The method used to combine the parallel models was the weighted summation of the individual outputs. Consequently, the performance of the stack is influenced by the aggregated individual models and their corresponding weights. Figure 1 presents the stacked neural networks for our case study.

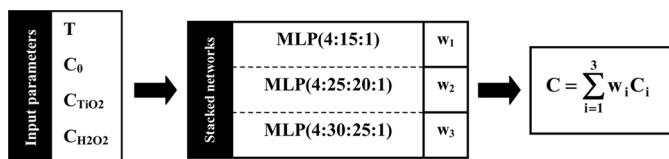


FIG. 1. Stacked neural networks developed for the modeling of photo-catalytic degradation of triclopyr.

RESULTS AND DISCUSSION

Individual and stacked neural networks were applied to the training and validation data sets in order to compare their performance and, finally, to choose the most appropriate model for the studied process. Figures 2 and 3 present some examples of predictions performed with individual networks on training and validation phases.

The performance of individual networks can be improved by stacking them (17,24). Different stacks were developed with the three networks, MLP(4:15:1), MLP(4:25:20:1), and MLP(4:30:25:1), denoted by N_1 , N_2 , and N_3 , respectively, the weight of each being changed. In order to find the optimal weights, the first step was to systematically generate weights between 0% and 100% with a step of 10%, and record the average relative error and correlation on training and validation data sets. Several selected results are presented in Table 2. The first three rows of this table show the performance of the individual networks which compose the stack. Relative errors were calculated using the following formula:

$$E_r \% = \frac{C_{exp} - C_{net}}{C_{exp}} \cdot 100 \quad (1)$$

where *C* represents the concentration of triclopyr, and indexes *exp* and *net* denote experimental and network values.

Table 2 refers to the first case approached in the paper and corresponds to the three of the best neural networks aggregated in a stack.

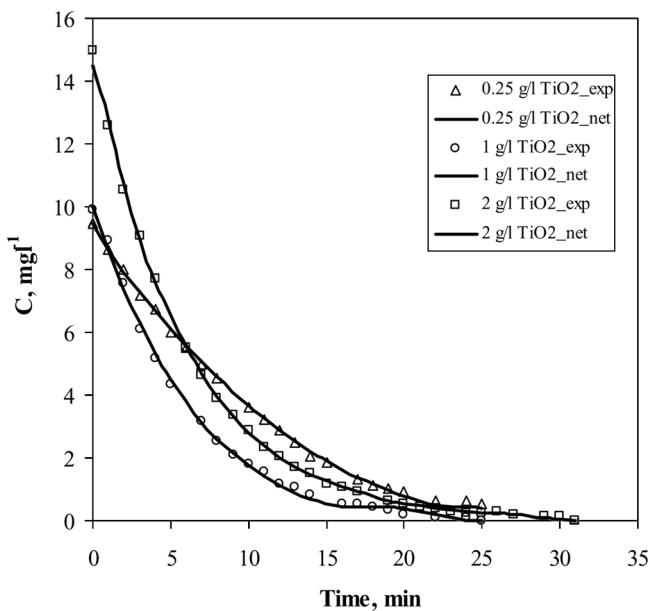


FIG. 2. Predictions of MLP(4:15:1) on training data compared with experimental data for the variation in time of final concentration of triclopyr using different concentration of TiO_2 .

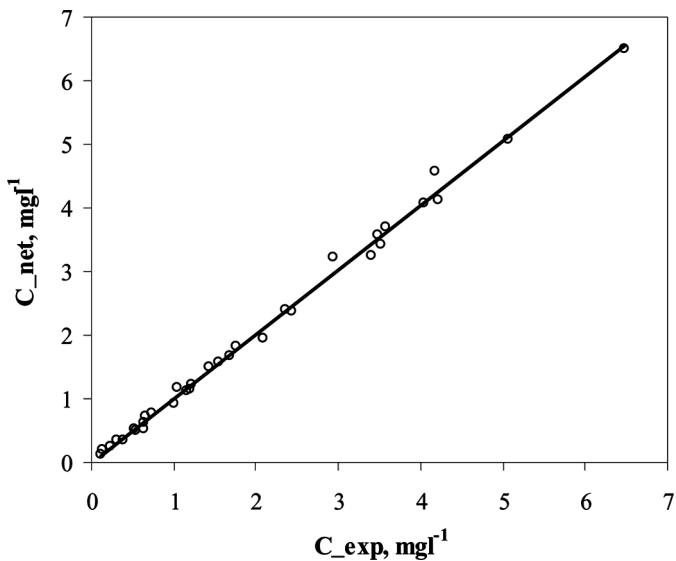


FIG. 3. Predictions of MLP(4:25:20:1) on validation data (C_{net}) compared with experimental data (C_{exp}) for the variation in time of final concentration of triclopyr using different concentration of TiO_2 .

One can see smaller errors and better correlations for the stacked neural networks than for individual networks.

In order to find the optimal stacked neural network, separate neural networks were developed for interpolation. One network was prepared for the interpolation of the training results and another one for the validation results. They had two inputs, the weights for N_1 and N_2 and the correlation, r , as the output. Only two inputs are necessary because the third weight $w_3 = 100 - w_1 - w_2$. The significance of w_1 , w_2 , and w_3 can be seen in Fig. 1. While these networks were admitted to be large enough, several variants were tried: MLP(2:24:8:1) and MLP(2:21:7:1), for training and validation, respectively, because the interpolation capacity here is more important than the generalization capability. The predictions of these models were generated with a step of 1% and the maximum correlation of 0.999045 was obtained with the following contributions of the individual networks N_1 , N_2 , and N_3 : $w_1 = 15\%$, $w_2 = 52\%$, and $w_3 = 33\%$, respectively. Figure 4 shows the variation of the stack performance with the weights of

TABLE 2
Performance of the individual neural networks compared to different types of stacks (case 1)

Weights, %			Training		Validation	
w_1	w_2	w_3	Average relative error, %	Correlation	Average relative error, %	Correlation
100	0	0	11.5402	0.9989	8.3935	0.9954
0	100	0	4.1128	0.9997	6.3715	0.9979
0	0	100	5.5549	0.9995	6.0048	0.9976
0	10	90	3.9941	0.9999	5.2152	0.9989
20	10	70	4.9967	0.9998	4.9750	0.9989
90	10	0	12.0758	0.9991	7.8239	0.9989
20	20	60	4.8894	0.9998	4.7159	0.9989
30	20	50	5.6712	0.9998	4.8335	0.9988
20	30	50	4.8472	0.9998	4.4543	0.9990
30	30	40	5.6193	0.9998	4.6618	0.9989
20	40	40	4.7986	0.9999	4.2697	0.9990
30	40	30	5.5782	0.9998	4.6176	0.9989
40	40	20	6.9750	0.9997	5.0794	0.9987
0	50	50	3.5931	0.9999	4.2809	0.9990
10	50	40	4.0535	0.9999	4.0997	0.9990
20	50	30	4.7449	0.9999	4.2730	0.9990
30	60	10	6.0830	0.9998	4.5913	0.9989
40	60	0	6.9385	0.9998	5.0615	0.9987
20	70	10	4.6821	0.9999	4.3546	0.9990
30	70	0	6.0519	0.9998	4.6191	0.9989
50	0	50	8.1606	0.9996	5.7264	0.9981
60	0	40	9.1060	0.9995	6.1099	0.9978
80	0	20	11.0887	0.9992	7.2274	0.9968
90	0	10	12.1083	0.9991	7.7848	0.9961

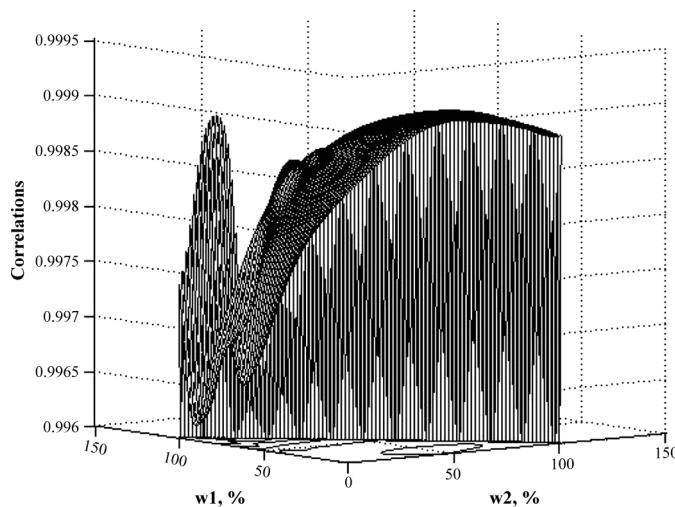


FIG. 4. The variation of the stack performance in the validation stage with the weights of the component neural networks for stack 1.

the component neural networks, for the validation stage in case 1.

Because of the interpolation errors, the above result (the maximum) is not precise. Additional experiments were performed in the neighborhood of the potential maximum in order to improve the solution. The value 0.999048 for correlation corresponds to a stack with 12%, 50%, and 38% (stack 1).

In another trial, three neural networks with one single layer (the simplest networks with acceptable performances), MLP(4:5:1), MLP(4:10:1), and MLP(4:15:1) were considered for the stack. The entire procedure described above was repeated to obtain the weights of the individual networks in the stack which leads to the best correlation in the validation phase. Table 3 presents comparatively some of the results provided by individual and stacked neural networks. Here, N_1 , N_2 , and N_3 refer to the neural networks with one hidden layer and 5, 10, and 15 hidden neurons, respectively, and w_1 , w_2 , and w_3 are the contributions of the networks to the stack output.

An optimization procedure based on a separate neural network for all training and validation results, MLP(2:15:5:1), with the weights as inputs and the correlation as the output, gives the weights 9%, 55%, and 36% with a correlation of 0.996071. Figure 5 presents the variation of the correlation values with the weights of the stack, emphasizing the optimum (maximum). Additional simulations around this optimum point found a correlation of 0.996087 for the following weights: 11%, 53%, and 36% (stack 2).

Certainly, the results of the stacks are better than those of the individual models as it can be seen in Tables 2 and 3. Both stacks, with optimum values for the weights, were tested with validation experimental data; a part of these results are presented in Table 4. It is evident that the results

TABLE 3
Performance of the individual neural networks compared to different types of stacks (case 2)

Weights, %			Training		Validation	
w_1	w_2	w_3	Average relative error, %	Correlation	Average relative error, %	Correlation
100	0	0	17.4134	0.9979	14.9485	0.9925
0	100	0	12.7506	0.9986	9.7000	0.9948
0	0	100	11.5402	0.9989	8.3935	0.9954
30	10	60	12.2974	0.9988	8.7145	0.9958
10	20	70	11.8047	0.9989	7.6877	0.9959
20	20	60	11.9118	0.9989	8.0733	0.9959
10	30	60	11.6393	0.9989	7.5663	0.9960
30	30	40	11.9454	0.9988	8.7902	0.9959
40	30	30	21.0089	0.9987	9.6016	0.9957
10	40	50	11.5215	0.9989	7.6186	0.9961
20	40	40	11.6410	0.9988	8.2003	0.9960
30	40	30	11.8988	0.9988	8.8925	0.9959
40	40	20	12.4304	0.9987	9.7276	0.9957
20	50	30	11.5937	0.9988	8.4065	0.9960
10	60	30	11.4386	0.9988	8.2020	0.9961
20	60	20	11.6012	0.9988	8.6493	0.9960
10	70	20	11.4941	0.9988	8.6330	0.9960

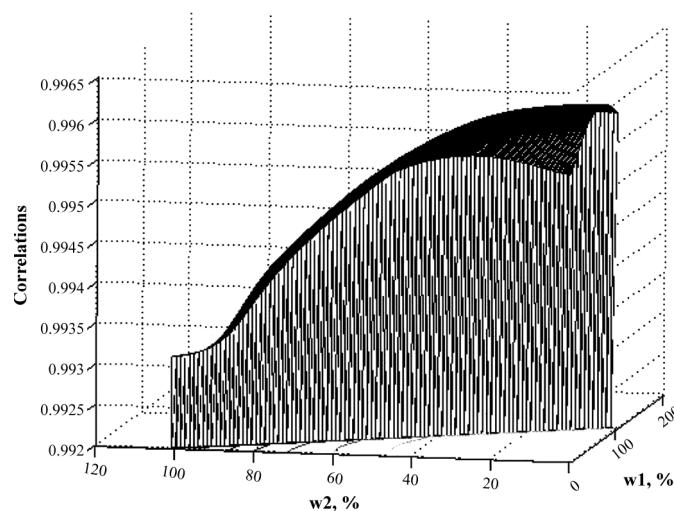


FIG. 5. The variation of the stack performance in the validation phase with the weights of the component neural networks for stack 2.

of the two stacks are similar. Consequently, the simpler stack, with only one hidden layer, can be chosen to model the decomposition process of triclopyr.

CONCLUSIONS

In this paper, we compare the predictions of individual and stacked neural networks, especially in the validation phase, in order to select a neural model with a high generalization capability. The procedure is applied to the photocatalytic decomposition of triclopyr and the process is evaluated by the final concentration of triclopyr as a function of the reaction conditions—initial concentration, time, pH, and catalyst concentration.

The stack was constructed from three feed-forward neural networks with one or two hidden layers whose outputs were weighted. Different stacks were developed by changing the component networks and the weights with which each individual network contributes to the total (stack) output. An optimization method based on an interpolation neural network with individual neural network weights as inputs and the correlation between experimental and predicted data as the output leads to the finding of the decision surface of the values for the three weights, and to the discovery of the optimum set of weights.

The results of the stacks were better than those of the individual models. Good predictions were obtained in the validation phase, so these models give a very good

TABLE 4
Results obtained with the two stacks in the validation phase

Time	Reaction conditions (input parameters)			Output parameter C exp	Stack 1 12%, 50%, 38%		Stack 2 11%, 53%, 36%	
	C ₀	TiO ₂	H ₂ O ₂		C _{net}	Error, %	C _{net}	Error, %
11	10	0.1	0	3.47	3.577	2.974367	3.577	2.974367
19	10	0.1	0	1.15	1.157	0.076864	1.158	0.0095
16	10	0.25	0	1.54	1.581	2.568428	1.580	2.503552
19	10	0.5	0	0.52	0.502	4.620038	0.500	5.000038
6	10	1	0	3.57	3.738	4.444041	3.735	4.360217
15	10	1	0	0.63	0.654	3.549991	0.656	3.866658
6	10	2	2	2.44	2.440	0.181637	2.441	0.140728
4	10	2	10	3.40	3.516	3.211716	3.525	3.47591
8	10	2	15	1.04	1.108	5.813032	1.103	5.335536
9	10	2	50	0.65	0.607	7.938381	0.609	7.635048
7	10	2	100	1.01	0.887	12.4089	0.885	12.6064
14	10	2	100	0.63	0.545	13.88995	0.539	14.83795
3	10	2	150	5.07	5.031	0.794277	5.033	0.754839
18	15	2	0	0.72	0.766	5.385821	0.766	5.385821
4	5	2	0	1.67	1.633	2.514447	1.633	2.514447
17	7.5	2	0	0.10	0.106	2.203196	0.109	0.564638
5	15	2	0	6.48	6.501	0.270999	6.502	0.286422
28	15	2	0	0.14	0.166	14.93935	0.167	15.63175
6	10	3	0	2.94	3.172	7.621371	3.171	7.587442
18	10	3	0	0.31	0.320	1.333485	0.320	1.333485
Average Error					4.139456		4.101125	

representation of the photocatalytic oxidation of triclopyr, and they could be capable of providing useful information for experimental practice.

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