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Prediction of Organic Pollution of Waters from the Déganobo Lake System: A Modeling Study

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Abstract

This work aimed to study the modeling of the organic pollution of the waters of the Déganobo Lake system by three models: Multiple Linear Regression model (MLR model), Mutilayer Perceptron model (MLP model) and Multiple Linear Regression/ Mutilayer Perceptron hybrid model (MLR/MLP hybrid model). In its implementation, the chemical oxygen demand (COD) of these waters, obtained from August 2021 to July 2022, was used. Two approaches were done in the case of the modeling of their COD by the MLP model and the MLR/MLP hybrid model: static modeling and dynamic modeling. The results have highlighted the low predictions of the COD of these waters by the MLR model (36.2 %) and the MLP models (6-8-1 for the static modeling and 7-3-1 for the dynamic modeling, both predicting less than 35% of the experimental values with high error (RMSE upper than 1.30 and relative error upper than 0.750). However, the MLR/MLP hybrid models (MLR/6-3-1 for the static modeling and MLR/7-3-1 for the dynamic modeling) both well predicted the COD of these waters, around 99% with very low errors (RMSE less than 0.0001 and relative error less than 0.006 in both cases). So, the MLR/MLP hybrid model was the most efficient to predict the COD of these waters. The accuracy of this hybrid model for ecological modeling was again provided during this study.

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Introduction

Organic matter has a fundamental role in the aquatic environment for its importance in biogeochemical reactions. However, its strong presence in surface waters contributes to ecological scourges and the consequences are serious health risks [1, 2]. In general, excessive organic matter in aquatic ecosystems generates an important quantity of nitrogenous and phosphorus nutrients, the main cause of eutrophication [3]. Excessive organic matter in these entities could be also an additional source of their metal pollution under some biogeochemical and physical conditions [1]. The presence of non-biodegradable organic matter in the surface waters, such as hydrocarbons and pesticides, could also lead to serious ecological and health risks [4, 5]. The knowledge of organic matter in waters, particularly in the surface waters, has always been important for the assessment of their quality. The assessment of the organic pollution of waters is conducted through several parameters of which the most used are the chemical oxygen demand (COD) and biochemical oxygen demand (BOD). COD and BOD represent approximate measurements of required oxygen quantities for chemical and biochemical degradation of organic matter, respectively. By their experimental implementation, BOD underestimates organic pollution, while COD extrapolates it [6, 7]. Therefore, the use of COD for the modeling of organic pollution would be more advantageous; in as much that is the representation of facts and the theoretical approach from statistics based on their spatial and temporal evolutions [8, 9]. One of the commonly used short-term and long-term methods for ecological monitoring is modeling.

Artificial neuron networks (ANNs), the black box models, are becoming more and more commonly used in the development of prediction models for complex systems as the theory behind them develops and the processing power of computers increases [10, 11]. This is the particular case of the modeling of the COD of the surface waters [12, 13]. The multilayer perceptron (MLP), one of the multiple variants of ANNs, is suitable for this purpose as highlighted by many recent studies, such as those of Ay and Kisi [14], Bachir et al. [15] and Selim et al. [16]. The ability of the multiple linear regression model (MLR model) for the modeling of the COD of the surface waters was also provided by many recent studies [16, 17]. One model, becoming more and more used for ecological modeling, is the multiple linear regression-multilayer perceptron hybrid model (MLR-MLP hybrid model). This hybrid model aims to provide a good approach to experimental data. Any hybrid model based on the MLP model is used when the modeling of experimental data by the MLR model and MLP model could not provide good approaches to experimental values. The use of this model amounts first to adjusting the values of the dependent variable(s) according to the values of the relevant independent variables in their explanation by the MLR model; then to use the values of the dependent variable(s) adjusted by the MLR model as output and the independent variables as input parameters for the MLP model. Many studies have highlighted the accuracy of this hybrid model in ecological modeling. That is the particular case reported by Adnan et al. [18], Kamisan et al. [19], Lola et al. [20], Massouri et al. [21] and Yao et al. [22-24].

The Déganobo lake system, located in the urban center of San-Pedro city, is one of the tourist attractions of this seaside town [25]. It has a remarkable biodiversity [26]. However, it is currently the receptacle of anthropogenic discharges of all kinds without treatment from its watershed. This fact leads to its relatively high pollution. Indeed, Konan and Yao [27] have highlighted the high organic pollution of its waters with serious ecological risks during all seasons. The seasonal mean values of their COD were higher than 220 mg O_2/L, with the annual mean value of their COD of 296.05 mg O_2/L from August 2021 to July 2022. So, it is important to carry out actions and decisions for the protection and sustainable development of this lake system. The knowledge of the static and dynamic evolution of their organic pollution in short or/and long times could contribute to it. This study aimed to study the modeling of the COD of its waters by three models: MLP, MLR and hybrid model MLR/MLP hybrid model.

Materials and Methods

Presentation of the study area

The Déganobo Lake system is geolocated at 6.63775 W and 4.75046 N. It consists of two lakes: Lac Ouest with a currently open water surface area of 49.05 ha and Lac Est with a currently open water surface area of 28.87 ha [27, 28] (Fig 1). It has impressive hydrology, made of the San-Pédro River and the Digboué lagoon, linked between them by a lot of wetlands [26, 27, 29]. Its hydrochemistry is linked to the rainfall in the San-Pédro Department [27].

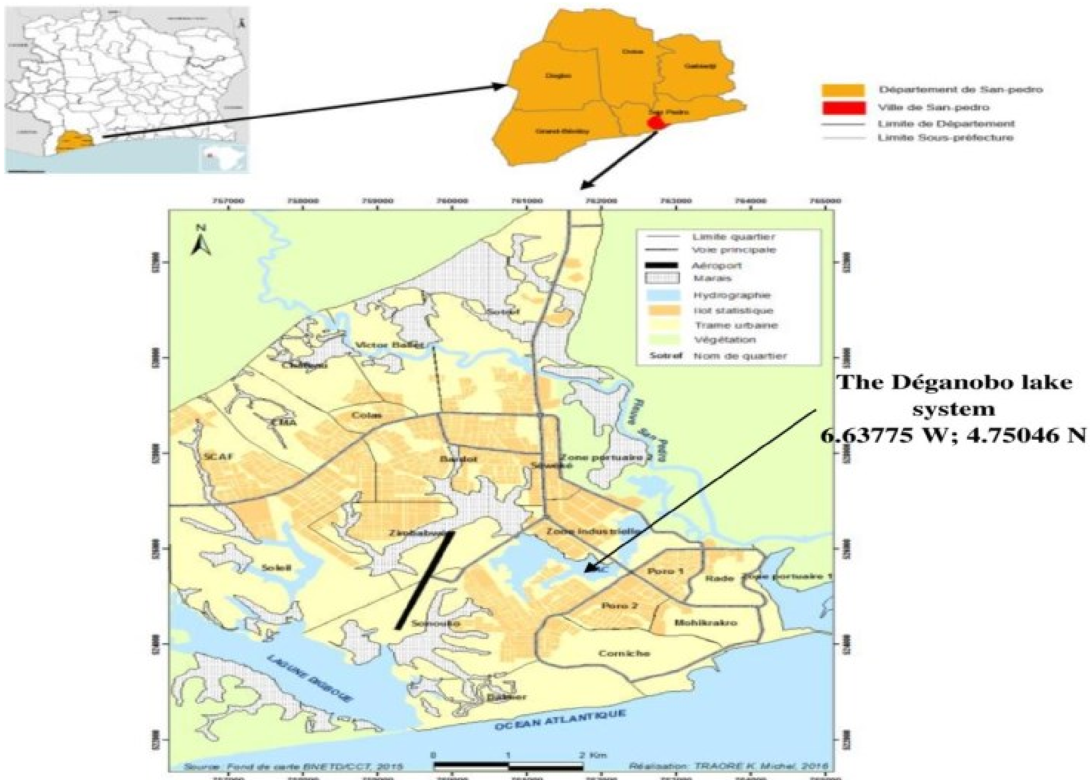

Fig. 1 Geo-localization of the Déganobo Lake system (Map source: Traoré [25], cited by Konan and Yao [27]).

This lake system is under strong anthropogenic pressures, because receives all kinds of discharges from its watershed. Thus, this situation leads to its relatively important pollution as revealed by AIP [26], Konan and Yao [27] and Ogou and Bidi [30].

Data collection

The monthly values of pH, conductivity, temperature, redox potential and COD of these waters used in this study were obtained from the works of Konan and Yao [27] during the period from August 2021 to July 2022. Those of the monthly rainfall in the same period were downloaded from the website "historiqueméteo.net" [31, 32].

Implementation of the MLR model, MLP model and MLR/MLP hybrid model

The implementation of these different models was done as same as done by Yao et al. [23, 24]. In the development of these models, pH, redox potential, conductivity and temperature of the waters from the Déganobo lake system, as well as the rainfall in the San-Pédro Department were taken into account, because playing important roles in the dynamics of the COD of these waters from August 2021 to July 2022 as highlighted by Konan and Yao [27].

Multiple linear regression model (MLR model)

In this study, the development of the MLR model was done considering the monthly COD (COD) of these waters as the dependent variable; the monthly pH (pH), conductivity (Cond), temperature (T) and redox potential (U) of these waters, as well as the monthly rainfall in the San-Pédro Department, as independent variables. The MLR model was performed in this study using the IBM SPSS statistics V20 software. A dataset of 1048 data was used for this purpose. All calculations were performed in double precision. The model obtained in this study was validated if these two conditions are simultaneously observed: the determination coefficient of the MLR model (R^2_{MLR}) obtained is greater than 0.5, *i.e.*, the MLR model expresses more than 50% of the experimental values of the COD of these waters and the *p*-value is less than 0.05 (5%).

Multilayer perceptron model (MLP model)

Two approaches were considered in the implementation of the MLP models: the static modeling and the dynamic modeling of the COD of

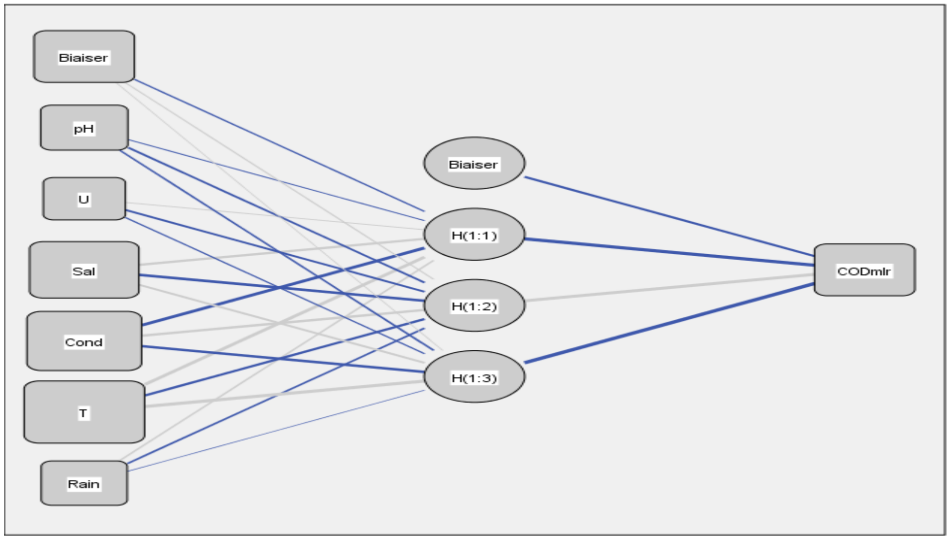

Fig. 2 Architecture of the MLR/6-3-1 hybrid model obtained in the case of the static modeling of the chemical oxygen demand of the waters from the Déganobo Lake system.
Biaser, biais; Month, time; pH, pH of these waters; U, redox potential of these waters; Sal, salinity of these waters; Cond, conductivity of these waters; T, temperature of these waters; Rain, monthly rainfall; CODmlr, chemical oxygen demand of lake waters obtained with MLR model; blue lines show positive synaptic weight and grey lines show negative synaptic weight.

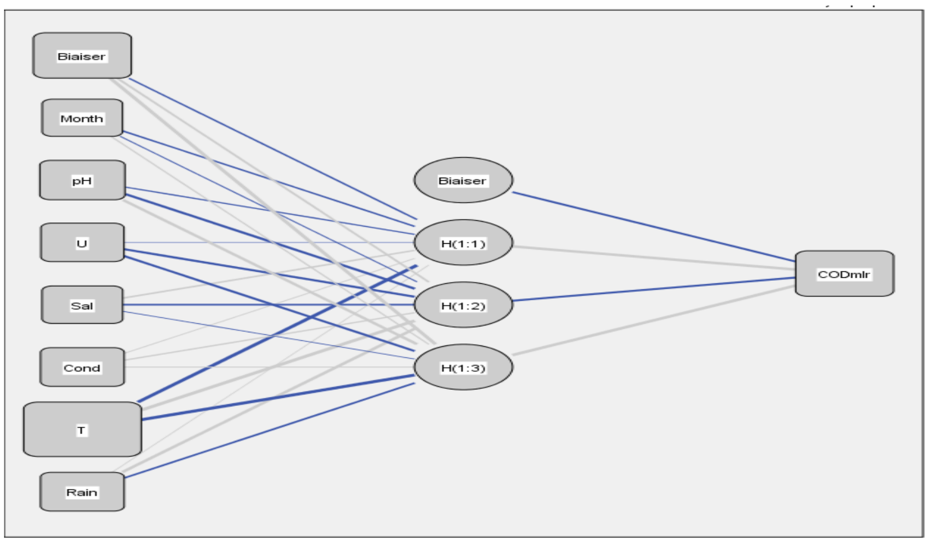

Fig. 3 Architecture of the MLR/7-3-1 hybrid model obtained in the case of the dynamic modeling of the chemical oxygen demand of the waters from the Déganobo Lake system.
Biaser, biais; Month, time; pH, monthly pH of these waters; U, monthly redox potential of these waters; Sal, monthly salinity of these waters; Cond, monthly conductivity of these waters; T, monthly temperature of these waters; Rain, monthly rainfall; CODmlr, monthly chemical oxygen demand of lake waters obtained with MLR model; blue lines shows positive synaptic weight and grey lines show negative synaptic weight.

these waters. For the static modeling of the COD of these waters: the monthly COD of these waters was the output parameter and the monthly pH (pH), conductivity (Cond), temperature (T) and redox potential (U) of these waters, as well as the monthly rainfall in the San-Pédro Department, were the input parameters. For the dynamic modelling of the COD of these waters, the time (month) was added to the input parameters considering the case of the static modeling. The different MLP models were performed using the IBM SPSS statistics V20 software. A dataset of 1048 data was used for the static modeling of the COD of these waters and that of 1060 data was for the dynamic modeling of their COD. In the development of the MLP models, the different datasets were partitioned into three: 40% for the learning phase, 30% for the validation phase and 30% for the test phase. The number of hidden layers was 1. The transfer function used on the hidden layer neurons is sigmoid (Tanh) and the function used on the output layer neuron is the identity function (y = x). Before processing, the different values of the input and output parameters were normalized according to equation (1) and coded in a range between 0 and n (n is an entire number).

$$x_{ni} = \frac{2(x_i - x_{min})}{(x_{max} - x_{min})} - 1 \qquad (1)$$

The weights of the network are initialized before their variation in the learning phase to obtain a low error. The Levenberg-Marquardt algorithm was used to speed up the learning phase. The learning rate was initially set to 0.4 and gradually decreased to 0.001 at ± 0.5 steps. The network architecture was optimized by the trial-and-error method. The number of hidden layers varied from 1 to 10. For each value of the hidden layer, the simulations were performed 2000 times and the best result (simultaneous highest values of the determination coefficients in the learning phase ($R^2_{learning}$) and in the test phase (R^2_{test}) of the corresponding network architecture was recorded. The best model for each case of the COD modeling of these waters was the model that presented the highest value of the determination coefficient (R^2), which was the mean of the determination coefficient obtained in the learning phase ($R^2_{learning}$) and that determined in the test phase (R^2_{test}) equation (2):

$$R^2 = \frac{R^2_{learning} + R^2_{test}}{2} \qquad (2)$$

This model is validated if these two following conditions are observed: R^2_{test} is higher than 0.5, *i.e.*, the model expresses more than 50% of the experimental values of the COD of these waters in the test phase, and $RMSE_{test}$ (root mean square error in the test phase) and RE_{test} (relative error in test phase) are very low, the lowest of all of the different MLP models established.

Multiple linear regression-multilayer perceptron hybrid model (MLR/MLP hybrid model)

Two approaches were also made with this hybrid model: the static modeling and the dynamic modeling of the COD of these waters. In the implementation of this model, the COD of these waters was before modeling by the MLR model in the same conditions as II-2-3. This step was followed by the static modeling and the dynamic modeling of the calculated values of the DCO of these waters (obtained by the equation established by the MLR model) by the MLP model with the same input parameters as done in the case of the implementation of the MLP models. The choice of the best MLR/MLP hybrid model in each case of the modeling of the COD of these waters and their validation conditions were the same as in the case of MLP models.

Results

Multiple linear regression model (MLR model)

The MLR model predicts 36.2% of the experimental values of the COD of these waters (Table 1). Considering its R^2_{MLR} less than 0.9 and its *p*-value superior to 0.05 (Table 2), this model is not accurate for this purpose in this study. So, there is no good linearity between the COD of these waters and the independent variables used in this case.

Table 1 Some statistical parameters of the MLR model obtained in this study.

R_{MLR}	R^2_{MLR}	$R^2_{MLR\ adjusted}$	*p*-value
0.190	0.362	-	0.907

Table 2 Coefficient and p-value of each parameter obtained with the MLR model.

Parameters	Coefficient	*p*-value
Ordinate origin	784.4773	0.112085
pH	6.7442	0.894993
Potential redox	-0.0415	0.957740
Salinity	-44.3410	0.835169
Conductivity	0.1078	0.803677
Temperature	-18.1034	0.246282
Rainfall	-0.0615	0.773322

Table 3: Statistical parameters for MLP models obtained in the case of the static modeling of the chemical oxygen demand of the waters from the Déganobo Lake system.

MLP model	$R^2_{learning}$	R^2_{test}	R^2	$RMSE_{test}$	RE_{test}
6-1-1	0.0013	0.016	0.0087	1.5192	1.1430
6-2-1	0.1502	0.0093	0.0798	2.5132	0.9330
6-3-1	0.0074	0.0106	0.0090	1.2124	1.8380
6-4-1	0.0267	0.0192	0.0230	2.1610	1.0120
6-5-1	0.031	0.001	0.0160	2.8609	0.8630
6-6-1	0.0875	0.1670	0.1273	0.9644	0.9740
6-7-1	0.1152	0.3975	0.2564	2.2338	0.8650
6-8-1	0.3824	0.3088	0.3456	1.8942	0.7590
6-9-1	0.0294	0.0000	0.0147	2.5558	1.0570
6-10-1	0.3681	0.0633	0.2157	0.6595	0.7040

Table 4 Statistical parameters for MLP models obtained in the case of the dynamic modeling of the chemical oxygen demand of the waters from the Déganobo lake system.

MLP model	$R^2_{learning}$	R^2_{test}	R^2	$RMSE_{test}$	RE_{test}
7-1-1	0.0666	0.0349	0.0508	0.9648	1.0367
7-2-1	0.0008	0.0017	0.0013	3.2334	1.0470
7-3-1	0.3363	0.0612	0.1988	1.3038	0.8990
7-4-1	0.0030	0.0877	0.0454	2.0030	0.9100
7-5-1	0.0900	0.0207	0.0554	1.1100	1.3760
7-6-1	0.0631	0.0039	0.0335	0.4806	1.0110
7-8-1	0.5336	0.0508	0.2922	2.3994	1.0620
7-8-1	0.0000	0.0190	0.0095	0.8803	1.3610
7-9-1	0.1390	0.1559	0.1475	1.6559	0.9050
7-10-1	0.0451	0.0004	0.0223	2.6216	1.1830

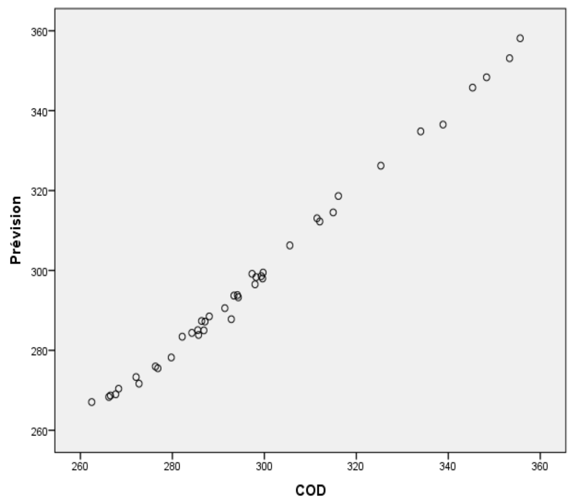

Fig. 4 Representation of experimental values of the chemical oxygen demand of lake waters as a function of their predicted values by the MLR/6-3-1 in the test phase.

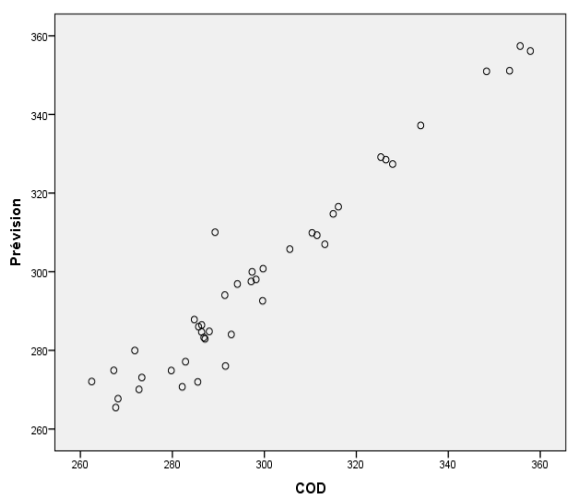

Fig. 5 Representation of experimental values of the chemical oxygen demand of lake waters as a function of their predicted values by the MLR/7-3-1 in the test phase.

Multilayer perceptron model (MLP model)

The statistical parameters ($R^2_{learning}$, R^2_{test}, $RMSE_{test}$ and RE_{test}) of the MLP models obtained in this study for the static modeling and the dynamic modeling of the COD of these waters are presented in Tables 3 and 4. The best MLP model for the static modeling of the COD of these waters is 6-8-1. This model expresses at 30.88 % the experimental values of COD in the test phase, less than 50%, with the relatively high $RMSE_{test}$ and RE_{test}. The best model for the dynamic modeling of their COD is 7-3-1. This model expresses at 6.12 % the experimental values of their COD in the test phase, less than 50%, again with the relatively high $RMSE_{test}$ and RE_{test}. So, these two models are not suitable for the prediction of the static and dynamic evolutions of the COD of the waters of this lake system in this study, according to the conditions defined.

Multiple linear regression-multilayer perceptron hybrid model (MLR/MLP hybrid model)

The best MLR/MLP hybrid models for the static modeling and the dynamic modeling of the COD of these waters are respectively MLR/6-3-1 and MLR/7-3-1. The MLR/6-3-1 expresses 99.50% of the experimental values of the COD of these waters during the test phase, while the MLR/7-3-1 does it at 99.85 %. These two hybrid models have relatively very low $RMCE_{test}$ and RE_{test}, the lowest of all of the different hybrid models (Table 5 and 6). So, the two models, validated according to the conditions defined, are more accurate for the prediction of the COD of these waters. The architectures of these two models are given in the Fig. 2 and 3, respectively. The representations of the experimental values of the COD of these waters in function to those predicted by these models are presented in Fig. 4 and 5, respectively.

Discussion

In this study, the poor predictions of the COD of the waters of this lake system by the MLR model and MLP model according to their salinity, redox potential, pH, conductivity, as well as the rainfall in its watershed, would highlight the complexity of the biogeochemical reactions within this lake system. Indeed, these physical, chemical and hydrological parameters play important roles in the fate of organic matter in surface waters and, consequently, in the dynamic of their organic pollution [33-36]. This seems to be particularly shown for the waters of this aquatic ecosystem during the long dry season, where

Konan and Yao [27] noted significant correlations between their COD and their pH, salinity and rainfall in its watershed with the Principal Components Analysis (PCA). The strong anthropogenic pressures on the watershed of this aquatic ecosystem, leading to its serious ecological degradation [26, 27, 30], would therefore have qualified the relevance of these parameters on the dynamic of the COD of its waters over the entire study period of Konan and Yao [27]. This fact is common in natural waters, especially polluted ones, where the direct interactions between the different forms of pollution with all the biogeochemical and physical parameters playing important roles in them are difficult to highlight in most cases [37, 38].

Table 5 Statistical parameters for MLR/MLP hybrid models obtained in the case of the static modeling of the chemical oxygen demand of the waters from the Déganobo lake system.

Hybrid model	$R^2_{learning}$	R^2_{test}	R^2	$RMSE_{test}$	RE_{test}
6-1-1	0.9885	0.9827	0.9856	0.1225	0.005
6-2-1	0.9748	0.9649	0.9699	0.2588	0.038
6-3-1	0.9970	0.9930	0.9950	0.0949	0.006
6-4-1	0.9946	0.9943	0.9945	0.1581	0.009
6-5-1	0.9498	0.9121	0.9310	0.4733	0.123
6-6-1	0.9859	0.9440	0.9650	0.4025	0.043
6-7-1	0.9925	0.9696	0.9811	0.4025	0.042
6-8-1	0.9850	0.9735	0.9793	0.4231	0.060
6-9-1	0.9933	0.9635	0.9784	0.1342	0.008
6-10-1	0.9842	0.9807	0.9825	0.2898	0.048

Table 6 Statistical parameters for MLR/MLP hybrid models obtained in the case of the dynamic modeling of the chemical oxygen demand of the waters from the Déganobo lake system.

Hybrid model	$R^2_{learning}$	R^2_{test}	R^2	$RMSE_{test}$	RE_{test}
7-1-1	0.9936	0.9933	0.9935	0.1304	0.007
7-2-1	0.9881	0.9907	0.9894	0.1049	0.007
7-3-1	0.9979	0.9985	0.9982	0.1000	0.002
7-4-1	0.9989	0.9921	0.9955	0.2214	0.013
7-5-1	0.9831	0.9893	0.9862	0.1949	0.016
7-6-1	0.9755	0.9720	0.9738	0.3131	0.027
7-7-1	0.9762	0.9603	0.9683	0.3661	0.044
7-8-1	0.9666	0.9436	0.9551	0.1789	0.082
7-9-1	0.9769	0.9687	0.9728	0.4324	0.059
7-10-1	0.9918	0.9848	0.9883	0.3507	0.045

The acuity of the MLR/MLP hybrid model in predicting ecological phenomena [18-24] is once again highlighted in this study, where this model predicts more than 99% of the COD of the waters of this lake system, and that with very low errors. This fact could be explained by the partial linearity previously introduced by the MLR model between the COD of these waters and the independent variables used for this purpose. This has the effect of further revealing the relevance of these independent variables used as input parameters for the MLP model on the one hand, and the better prediction of the independent variable through that predicted by the MLR model, used as parameter output, on the other. Indeed, more there are high correlations between the input parameters and the output parameter(s), the better the results obtained with the MLP model [22]. That could explain the high accuracy of the MLR/MLP hybrid model for the prediction of the COD of these waters relatively of the MLR model and the MLP model in this study. This was also noticed by Yao et al. [24] in the case of the modeling of the COD of the waters from the Tiagba Lagoon Bay. The ability of the “MLR/MLP” hybrid model more than the MLR model and the MLP model was reported by many studies in other cases, such as those of Kamisan et al. [19] in the modeling of the load forecasting of Malaysian City, Lola et al. [20] in the modeling of the chlorophyll-a of the waters from the Offshore Kuala Terengganu, Manssouri et al. [21] in the modeling of the water quality indicators of groundwater and, Yao et al. [22] in the modeling of the eutrophication of the waters from the Tiagba lagoon bay. On the whole, the hybrid models based on the MLP model have very good accuracy, as reported by many recent studies, including those of Li et al. [39], He et al. [40] and Zhu et al. [41].

Conclusion

The use of different models in this context has once again highlighted the acuity of the MLR-MLP hybrid model in translating environmental phenomena, especially those related to the pollution of surface waters. The MLR-MLP hybrid models obtained in this study could serve as a basis for any decision concerning the rehabilitation and protection of this aquatic ecosystem. Other studies concerning the modeling of chemical pollution of the waters of this lake system by this hybrid model, especially those related to their pollution pesticides and aromatic polycyclic aromatic, should be explored for the same purposes.

Conflict of interest

The authors have declared that no competing interests exist.

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