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Modeling photosynthetically oxygenated biodegradation processes using artificial neural networks

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Abstract

The complexity of the mechanisms underlying organic matter mineralization and nutrient removal in algal–bacterial photobioreactors during the treatment of residual wastewaters has severely hindered the development of mechanistic models able to accurately describe these processes. Artificial neural networks (ANNs) are capable of inferring the complex relationships existing between input and output process variables without a detailed description of the mechanisms governing the process, and should therefore be more suitable for the modeling of photosynthetically oxygenated systems. Thus, a neural network consisting of a single hidden layer with four neurons accurately predicted the steady-state operation of a continuous stirred tank photobioreactor during salicylate biodegradation by an algal–bacterial consortium. Despite its simplicity and the low number of data sets for ANN training (23), this network topology exhibited a satisfactory fit for both training and testing data with correlation coefficients of 99%. Although the use of ANNs for modeling conventional wastewater treatment systems is not novel, this work constitutes, to the best of our knowledge, the first reported application of ANNs to photosynthetically oxygenated systems and one of the few models for microalgae-based treatment processes. This modeling approach is therefore expected to contribute to improve the understanding of the complex relationships between light, temperature, hydraulic retention time, pollutant concentration and process removal efficiency, which would eventually promote the development of algal–bacterial processes as a cost effective alternative for the treatment of industrial wastewaters.

Keywords: Algal–bacterial systems; Artificial neural networks; Modeling; Photobioreactor; Photosynthetic oxygenation

1. Introduction

In a world simultaneously facing water crisis and global warming, photosynthetically oxygenated biodegradation processes offer an attractive and reliable alternative to conventional energy-demanding and greenhouse gases-emitting wastewater treatment processes [1]. In the presence of sunlight, microalgae consume the CO_2 released during the bacterial degradation of organic pollutants, producing in turn the O_2 required by the latter process [2]. This oxygenation mode is cheaper (no energy need for aeration) and has less environmental impacts (low release of greenhouse gases and volatile organic contaminants) than conventional treatments because sunlight drives the “in situ” photosynthetic O_2 supply [3–5]. Additionally, microalgae-based processes permit to conduct secondary, tertiary and quaternary treatment in a single step due to the ability of algae to remove large amounts of nutrients and heavy metals [6–9]. Recent studies have also shown photosynthetic oxygenation could support the aerobic treatment of toxic wastes containing pollutants such as black oil, phenanthrene, phenol, or acetonitrile [5,10–12].

However, despite the merits of this technology, there are only a few full-scale systems in operation [13,14]. Thus, although more complex, traditional treatment systems often manage to provide a more consistent treatment efficiency than micro-algae based systems, precisely because the poor understanding of the ongoing processes in algal–bacterial systems makes it difficult for a plant operator to adjust system operation. In microalgae based systems, bacterial activity is for instance linked to oxygen supply, which is itself a function of light penetration and microalgae concentration [15]. In addition, microalgae inhibition can occur at high light intensities (photoinhibition), high biomass

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concentrations (mutual shading), and high pollutant concentrations if the process is not properly controlled [9]. Process control is therefore crucial to promote the development of photosynthetically oxygenated processes. Unfortunately, no detailed mechanistic model for describing algal–bacterial process has been developed so far.

Artificial neural networks (ANNs) represent a valuable instrument in the design and optimization of wastewater treatment processes [16,17]. They are computing systems capable of modeling complex relationships between inputs and outputs that infer a function from observations. A properly trained ANN thus codifies a set of rules within its structure that relate input and output parameters without the need for mechanistic models [18]. This is particularly useful in applications where the complexity of the mechanisms underlying process performance is high, which is the case of biological treatment processes for pollution control. Therefore, ANNs have gained an increasing consideration in wastewater treatment modeling and control [17,19]. Çinar et al., for instance, successfully modeled the performance of a submerged membrane bioreactor treating cheese-whey wastewater using ANNs by using a cascade-forward backpropagation network consisting of a single 3-neurons hidden layer [17]. Likewise, effluent BOD and suspended solids (SS) concentration were accurately predicted in a major WWT plant in Cairo using two ANNs constructed with past operation data [16]. Besides providing a valuable tool for performance prediction, ANN can be used in real-time control during WWT. For instance, Ruey-Fang et al. improved nitrogen removal in a sequential batch reactor by using an ANN-based real-time control strategy which permitted to reduce the retention time of the aerobic and anoxic zones by 45% and 15.5%, respectively, thereby reducing aeration costs by 45% [20]. Similarly, Choi and Park and Aguado et al. employed neural networks as software sensors for inferring wastewater quality parameters such as effluent COD or TKN concentrations [19,21]. This latter application is particularly useful when the on-line measurement of process variables is costly or technically difficult as a software sensor can accurately predict these key variables from other more easily monitored influent or operation parameters.

This study evaluates the ability of ANNs to describe the steady-state operation of a continuous algal–bacterial photobioreactor using salicylate as model contaminant. The potential of the trained ANN as a simulation tool is also investigated. In addition, the merits and limitations of this modeling approach are thoroughly discussed.

2. Materials and methods

2.1. Modeling approach

ANNs are universal approximators for Boolean and continuous functions that are capable of modeling the complex relationships between input and output parameters without requiring a detailed mechanistic description of the phenomena governing the process [22,23]. In ANNs, each neuron receives the information from the surrounding neurons multiplied by a specified weight (w), introduces a constant called bias (b), applies a transfer function (f) to the outcome and sends the result to the surrounding neurons (Fig. 1). The intelligence of ANNs and their capability to solve hard problems derives from the high degree of connectivity, which gives neurons a high computational power [24]. Thus, based on past operation data, ANNs are capable to model existing relationships between inputs and outputs and provide solutions to unforeseen problems.

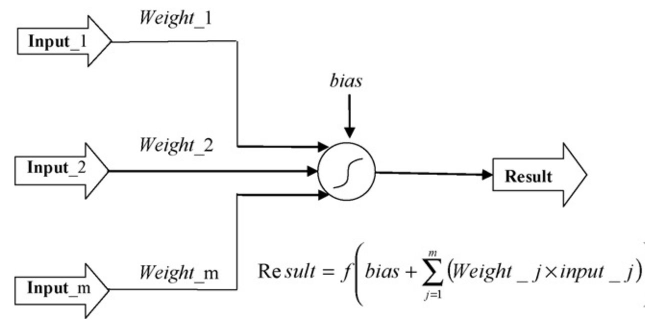

Fig. 1. Basic structure of an artificial neuron.

In this study a feed-forward network consisting of a single hidden neurons layer was selected. With such structure, the information from the input neurons undergoes a transformation in the hidden layer neurons before it is sent to the output neurons (Fig. 2). The number of neurons per layer should be high enough to allow the network reproducing the behavior of the system. However, a too large neuron number can cause data overfitting, a situation that can be encountered when correlating experimental data. This is due to the fact that the large number of parameters to be adjusted when using too many neurons might induce the network to memorize the data used in the training while loosing one of its more functional characteristics: generalization [25].

In the following, a general description of the ANN developed is presented. This network consists of m inputs, n outputs, a single hidden layer of p neurons, and D experimental data sets for network training. X represents the matrix of input variables (dimensions: $m \times D$), Yd ($n \times D$) and Ys the matrices of observed outputs and model outputs, respectively, and S ($p \times D$) the matrix of outputs from the hidden layer. The bias of the hidden layer and output layer are herein represented by A ($n \times D$) and B ($p \times D$), respectively. Finally, the weights matrix of the output layer (Z) and the weights matrix of the hidden layer are illustrated by Z ($n \times p$) and W ($p \times m$), respectively.

A sigmoid transfer function (f) was used in the hidden layer because such neural networks are universal approximators for arbitrary Boolean and continuous functions [22,26]. In addition, sigmoid functions introduce non-linearity into the model, which significantly increases the computational power of these modeling networks.

$$f(\theta) = \frac{1}{1 + e^{-\theta}} - \frac{1}{2} \quad (1)$$

Since the ANN outputs (removal efficiency, RE) in our system were within 0–100%, the same sigmoid transfer function (f) was used in the output layer. Thus, the results from the output neuron

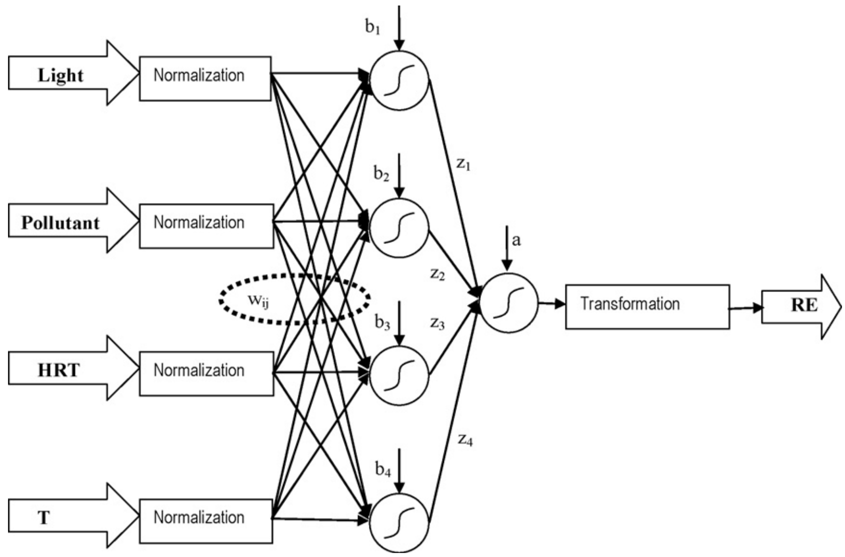

Fig. 2. Basic architecture of the artificial neural network proposed.

obtained using Eq. (1), were linearly transformed into RE:

$$Ys_{id} = f\left(a_i + \sum_{j=1}^{p} z_{ij} \cdot s_{jd}\right) \tag{2}$$

where $$s_{jd} = f\left(b_j + \sum_{k=1}^{m} w_{jk} \cdot x_{kd}\right) \tag{3}$$

Into matrix notation, Eqs. (2) and (3) can be expressed as:

$$Ys = f(A + Z \cdot S) \tag{4}$$

where $$S = f(B + W \cdot X) \tag{5}$$

The optimum values for connecting weights, bias, and number of neurons in the hidden layer were obtained through network training. In this study, a supervised hybrid algorithm combining backpropagation and random methods for searching the minimum of the error function was used as training methodology [27]. The mean squared error (MSE) between the experimental and model outputs was selected as error function:

$$\mathrm{MSE} = \frac{1}{n \cdot D} \sum_{i=1}^{n} \sum_{d=1}^{D} (Yd_{id} - Ys_{id})^2 \tag{6}$$

To model pollutant biodegradation in an algal–bacterial photobioreactor, light intensity, temperature, hydraulic retention time (HRT), and pollutant concentration were selected as the four input variables for being the most important parameters influencing the output variables. Pollutant removal efficiency was selected as the unique output parameter [15]. Pollutant RE in algal–bacterial photobioreactors is often limited by the oxygenation capacity of microalgae, which itself is a function of the temperature, light supply, biomass concentration (X), and inlet pollutant concentration (S) (oxygenation = f(T, light, X, S)) [15,28]. In most of the studies reported in literature process performance was limited by oxygen supply caused by either insufficient light supply, or too high biomass or too high pollutant concentration [5,15,29]. Thus, increasing light intensity or temperature enhanced microalgae activity and with it photosynthetic oxygenation, which improves bacterial salicylate biodegradation (higher RE). Decreasing the HRT however caused an increase in pollutant inlet load and a decrease in process RE, which translated into inhibitory salicylate concentrations in the photobioreactor. Finally, a moderate increase in salicylate inlet concentration increased algal–bacterial concentration when the oxygenation capacity of the reactor was not fully used whereas large increases in pollutant load, at values exceeding the system's oxygenation capacity, caused a decline in RE as a result of the salicylate inhibitory effect on microalgae [29].

Input variables were normalized by setting the mean to 0 and the standard deviation to 1 before feeding the network. Among the 26 steady-state experimental data sets available to build the ANN, 23 were used for network training and 3 for validation. Due to the low number of experimental data available, the number of point for validations was low. All simulations were carried out using MATLAB™ (The Mathworks Inc., USA).

2.2. Experimental

Data for network training and validation was taken from Muñoz et al. [15]. The algal–bacterial process was set up in a magnetically stirred, 600-ml conical glass vessel. The photobioreactor was inoculated with a mixed culture formed by the bacteria *Ralstonia basilensis* (GenBank accession number AY047217) and the microalgae *Chlorella sorokiniana* 211/8k (CAAP Collection, UK). Light was provided by three fluorescent lamps (Gelia E27, 15 W) in a triangular configuration. The photobioreactor was operated at illuminances ranging from 2000 to 15000 lux, salicylate inlet concentrations from 0.75 to 2 g l^{-1}, temperatures from 25 to 31 °C, and HRT from 0.5 to 4.5 days. After each change in one of the process parameters the reactor was allowed to equilibrate (i.e. reach a steady-state), and once the salicylate outlet concentration was stable (for a period of 1 HRT) the reactor was monitored for a period of at least 2 HRT. During that period of time, 3–7 samples (depending on the duration of the HRT) were withdrawn, and each sample was considered as a replicate for this specific steady-state. Salicylate inlet and outlet concentrations were monitored to assess process performance (evaluated as salicylate RE) and the mean values of RE within each steady-state used for both model training and validation. Apart from the steady-state presented in Muñoz et al. [15], two extra data sets corresponding to process operation in the absence of light supply (no photosynthetic oxygenation leading to bioreactor washout) were included within the training and data sets [15]. The influence of the tested parameters (light, temperature, HRT, and salicylate inlet concentration) on process performance (RE) was analyzed using a one-way ANOVA with significance at $P \leq 0.05$. For a more detailed description of the statistical treatment refer to [15].

3. Results and discussion

Wastewater treatment (WWT) in activated sludge processes is usually described by mechanistic models such as the ASM2D or ASM3 models [30]. Unfortunately, the application of these models is often limited by the availability of certain microbiological model parameters or by the mathematical complexity to describe certain inhibitory mechanisms when dealing with toxic effluents [30–32]. Likewise, the complexity of the mechanisms underlying BOD and N removal in algal–bacterial processes has seriously limited the development of mathematical models capable to accurately describe and predict these systems.

In this study a network topology using four input neurons (light, HRT, temperature, and pollutant concentration), one output neuron (RE), and one hidden layer of neurons was used to describe the steady-state salicylate removal in an algal–bacterial chemostat. It must be stressed that a single layer of hidden sigmoid neurons constitutes the simplest structure capable to simulate any function with a finite number of discontinuities. During network training, the MSE rapidly decreased when increasing the number of neurons in the hidden layer up to four neurons (Fig. 3a). Further increases did not cause a significant decrease in MSE values. The number of neurons composing the hidden layer of the ANN was thus selected as the maximum number of neurons providing a significant decrease in the MSE between the experimental and model predicted RE in the training data sets. Similarly, during process validation, the MSE reached a minimum when the ANN was trained with four neurons in the hidden layer (Fig. 3b) and increased when increasing the number of neurons, which was likely due to data overfitting. Therefore, four neurons provided the best fit of the experimental data while minimizing at the same time data overfitting. The fact that four neurons decreased the MSE between experimental and predicted RE in the validation data only confirmed the good data fit obtained during ANN training, and was not selected as the main criterion to establish the optimum number of neurons.

The model herein developed provided a satisfactory correlation of the training data sets with a correlation factor between

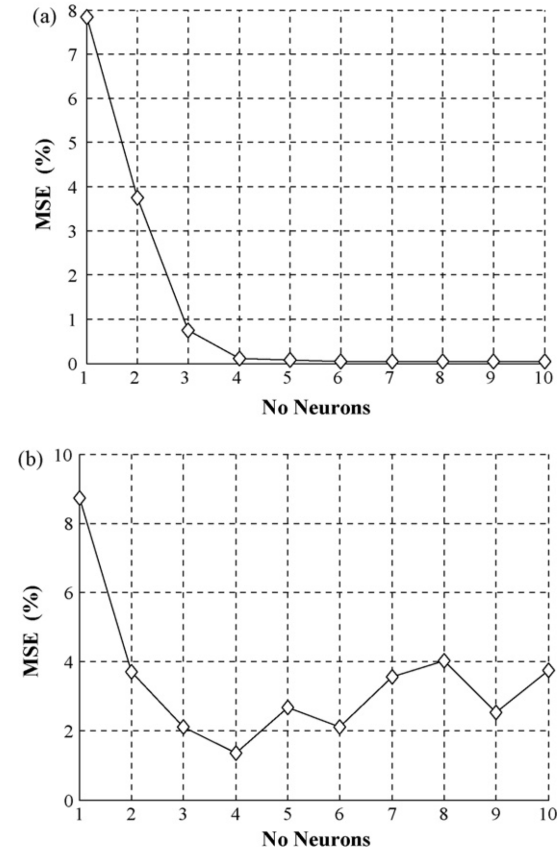

Fig. 3. Influence of the number of neurons in the hidden layer on the mean square error during network training (a) and testing (b).

observed and model outputs higher than 99% and a MSE of 0.11% (Fig. 3a and 4a). Model testing with the three steady-states, evenly distributed in the range of experimental RE and not used during training, exhibited a satisfactory correlation factor of 99% and a MSE of 1.35% (Fig. 3b and 4b). In addition, paired t-test analyses showed no significant differences (at $P \leq 0.05$) between experimental and model generated RE for all data set used in model training and validation. The correlation achieved in the present study was however remarkable, taking into account the relatively low number of steady-states used for training and testing. The availability of a high number of experimental points for ANN training would have certainly improved the predictive capability of the network [16]. This demonstrates the high correlating capacity of this type of black box models. Each steady was maintained for at least 2 HRT, which limited the number of steady-states attained during 1 year of experimentation to 26. The work herein presented is intended to illustrate the merits of ANNs for modeling and prediction of the performance of microalgae based processes, and constitutes, to the best of our knowledge, the first attempt to model the treatment of industrial wastewaters using algal–bacterial systems.

Despite their merits, ANNs present several drawbacks such as the great deal of computational efforts needed to adjust the network parameters or the fact that the individual relationships between input and output variables are not based on engineering or mechanistic judgments. In addition, ANNs are only capable to

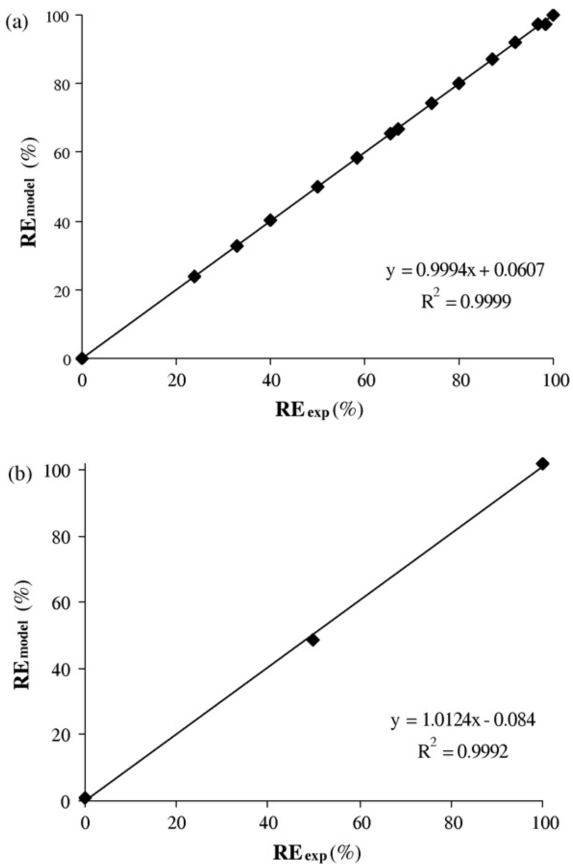

Fig. 4. Model predicted vs. experimental removal efficiencies during network training (a) and testing (b).

predict process performance within the range of environmental and operational conditions used during network training, which can seriously limit their applicability.

In order to illustrate the capacity of the ANN constructed herein to provide reasonable predictions of process performance, the influence of light intensity, HRT, and temperature on salicylate removal efficiency was evaluated and compared to empirical results previously reported in literature.

Steady-state simulations showed that operation under high HRT resulted in high RE (Figs. 5 and 6). The RE of the contaminant in the photobioreactor raised due to the inherent decrease of the pollutant loading rate at higher HRT and due to the fact that the oxygenation capacity of the system increased supported by the increasing biomass concentration with increasing HRT. The negative impact of mutual shading, caused by the increasing biomass concentration (due to the increasing substrate consumption), was negligible compared to the RE enhancement derived from the longer HRT. Operation at high retention times (HRT > 3 days in this photobioreactor configuration) is therefore recommended to provide an oxygenation capacity higher than the influent BOD load. This is in accordance to the experimental observations of Muñoz et al. who reported complete removal of acetonitrile when a tubular photobioreactor was operated at high HRT (2.5 days) [5]. Simulation results confirmed thus the superior performance of enclosed photobioreactors compared to conventional stabilisation ponds, where retention times ranging from 10 to 30 days are required for complete WWT under similar BOD concentrations [3,9].

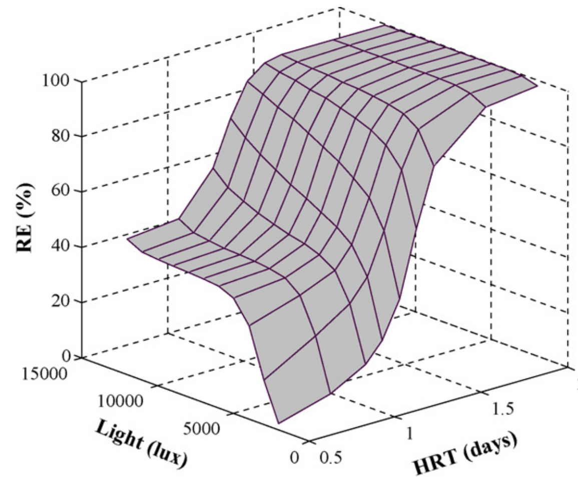

Fig. 5. ANN prediction of the influence of the HRT and light intensity on the removal efficiency of an enclosed algal–bacterial photobioreactor treating 1 g salicylate l^{-1} at 30 °C.

The influence of light input on process efficiency was only significant at low light intensities (2000–5000 lux) (Fig. 5). This is explained because algal activity increases with light intensity up to a certain level where the photosynthetic apparatus becomes saturated [33,34]. This relationship is, however, only valid at low cellular densities where all the cells received the same amount of energy. At high cell densities mutual shading is likely to occur and light intensity within the reactor becomes a function of the biomass concentration, which itself is a function of the HRT [35]. Thus, the fact that RE, and therefore the concentration of the algal–bacterial biomass, was influenced by the HRT might explain the different rates of increase of RE with increasing light intensities (Fig. 5). In addition, high HRT supported total pollutant removal and consequently the influence of light intensity under these particular conditions was negligible.

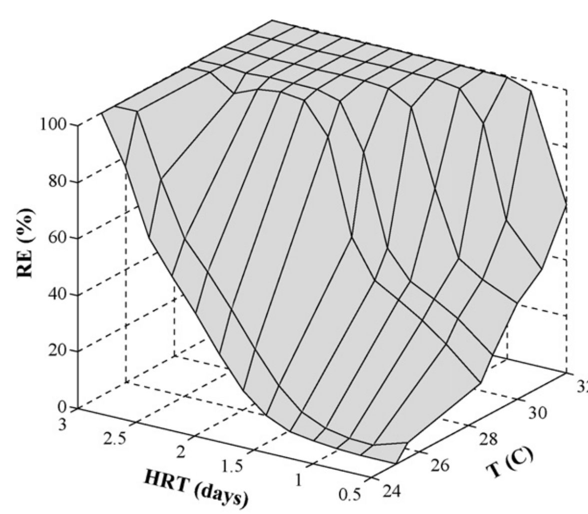

Fig. 6. ANN prediction of the influence of the HRT and temperature on the removal efficiency of an enclosed algal–bacterial photobioreactor treating 1 g salicylate l^{-1} under continuous lighting at 4000 lux.

Process efficiency significantly increased at high temperatures as RE approached 100% at 32 °C even at 0.5 days of HRT. Complete pollutant removal was achieved at a HRT higher than 2 days when the process was operated at 30 °C (Fig. 6). This result is not surprising considering the fact that the process was limited by microalgal activity (i.e. oxygen supply, [5]) and taking into account that *C. sorokiniana* is a thermophilic microalgae capable to support good photosynthetic productivity even at 46.5 °C [36]. This is also in agreement with the results of Muñoz et al. who observed an increase in phenanthrene removal rates when process temperature increased from 25 to 29 °C [29]. Therefore, the good correlation coefficients for both training and validation data sets, together with the results of the paired *t*-test and the realistic descriptions of process performance illustrated in Figs. 5 and 6 provide a satisfactory evidence of model robustness and prediction potential. In addition, the fact that the ANN was capable to successfully simulate the influence of HRT, *T* and light intensity on process RE producing a smooth surface function confirmed the absence of overfitting in the model herein proposed despite the low number of experimental data set available for training. Indeed, overfitting would have generated random peaks or valleys within the surface functions generated in Figs. 5 and 6. However, these phenomena were not observed in the model simulations carried out.

Finally, the sensitivity of the predicted removal efficiency (RE) to the input parameters in the model was investigated. This analysis was performed using the ratio between the relative variation of the removal efficiency and the relative variation of the target parameter as response variable. Thus, the sensitivity ratio (SR) for a generic parameter *P* was defined as follows:

$$\mathrm{SR} = 100\frac{\Delta \mathrm{RE}/\mathrm{RE}}{\Delta P/P} \tag{7}$$

In our particular case, the study was performed during operation at illuminances of 7500 lux, salicylate inlet concentrations of $1\,\mathrm{g\,l^{-1}}$, HRT of 1.5 days, and temperatures of 29 °C. SR of 56, −186, 122 and 127% were obtained when increasing lighting, salicylate inlet concentration, HRT and *T* by 20%, respectively. These results predict a decreasing process performance at increasing salicylate concentrations and point out the HRT and temperature as the main operation parameters enhancing process efficiency.

4. Conclusions

Despite its simplicity, the ANN herein proposed was capable to accurately describe the steady-state operation of a photosynthetically oxygenated biodegradation process. The network provided a satisfactory fit of both training and testing data, being to the best of our knowledge, the first reported application of ANNs to microalgae-based processes, and one of the few modeling approaches available in literature in the field of applied phycology. This good performance should be however validated with a greater amount of data, since in this particular case, the long time required to achieve each steady-state limited the number of experimental data available for network training and validation. The use of ANNs represents thus a robust modeling approach which is expected to contribute to improve the understanding and control of the complex relationships between environmental and operational variables, and treatment performance in photosynthetically oxygenated processes.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.jhazmat.2007.11.027.

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