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Comparison between traditional methods and artificial neural networks for ammonia concentration forecasting in an eel (*Anguilla anguilla* L.) intensive rearing system

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Abstract

One of the main problems in the management of fishfarms with water recirculating system is the forecasting and control of ammonia concentration in order to minimise the fish stress status. This paper examines methodologies of prediction in a real-time environment for an eel intensive rearing system. Approaches based on linear multiple regression, univariate time series models (exponential smoothing and autoregressive integrated moving average (ARIMA) models) and computational neural networks (ANNs) are developed to predict the daily average ammonia concentration in rearing tanks with water recirculating. The models are established using actual data from an eel fishfarm in southern Spain. The input variables used in the models (multiple regression, Holt smoothing model, ARIMA models and ANN models) are the ammonia concentration of previous days. In ANN models, the training method used is a standard back-propagation variation known as extended-delta-bar-delta (EDBD). Different neural architectures, whose learning is carried out by crossvalidation and controlling several threshold determination coefficients, are compared. Globally, the nonlinear ANN model approach is shown to provide a better prediction of daily average ammonia concentration than linear multiple regression and univariate time series analysis when the correlation between data series is low and when the

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models were obligated to predict in a situation for which specifically had not been calibrated. The best results were obtained by 5:10*s*:15*s*:1*l* ANN model in the pre-growth series.

Keywords: Ammonia; Time series forecast; Multiple regression; ARIMA model; Artificial neural network

1. Introduction

One of the main problems in the fish intensive culture systems is the rapid ammonia, nitrite and nitrate accumulation in the water. The problem is caused primarily by the fish metabolism, decomposition of unconsumed fish foods and disturbances in the nitrifying bacteria population (Alcaraz and Espina, 1995; Twarowska et al., 1997). Ammonia (in the unionised form) and nitrite are toxic to fishes and the tolerable concentration levels of those compounds for an intensive rearing system are quite low, usually being much less than $1\,mg\,l^{-1}$ (Lin and Wu, 1996). Generally, ammonia and nitrite concentrations above $1\,mg\,l^{-1}$ unchains for the short-term in the fishes physiological (i.e. the secretion of hepatic hormones) and behavioural changes. This stress status changes the blood composition and increase the breathing and the heart beat frequency, causing a decrease of the immune system effectiveness and an increase of the susceptibility to diseases and the attack of parasites (Palackova et al., 1990). Therefore, some possible consequences of increase of the ammonia and nitrite concentration levels are the unfavourable effects on growth rates, mortality rates and final yield.

In many fishfarms, the ammonia and nitrite levels are easily reduced and controlled by adjusting the water supply rate (Abeysinghe et al., 1996). However, in most cases this strategy supposes a low economic benefit/productivity relationship. Usually, in most European eel farms the ammonia and nitrite concentrations control (removal/conversion) is carried out by application of recirculation technology and biological filtration (Kamstra et al., 1998). This is because the recirculating systems provide several advantages: minimise water use, allow greater control of the rearing environment (especially water temperature), allow fishfarms to locate in better market areas and significantly reduce the waste volume discharged in the out effluent. This way, higher economic benefit is obtained. But on the other hand, recirculating systems have disadvantages due to their requirements for additional equipment to treat the water for reuse. This additional equipment expands the risk of catastrophic loss due to the use of a more complex operating system. Therefore a higher forecast capacity of important variables for the system (i.e. ammonia, nitrites, pH, temperature, etc.) can provide higher control ability and can attenuate the risk of high loss.

Because of the risk that supposes the accumulation of these compounds for the yield, some authors like Kochba et al. (1994) and Avnimelech et al. (1994) developed models to predict concentrations of these pollutants in rearing tanks. In this way, Gujer and Boller (1986), Nijhof (1994a,b) and Kamstra et al. (1998) developed complex physic models with the capacity to predict the behaviour of the biologic filtration units for water reuse. These models join variables like the hydraulic load of the filter, the filter medium type, the filter size and the bacterial stratification in the column of water, allowing to estimate the

ammonia load in the biofilter, its removal rate and ammonia concentration in rearing tanks. However Heinsbroek and Kamstra (1990) and Kamstra et al. (1998) report the intricacies involved in the application of this kind of modeling to full-scale system. The fluctuations in the utilisation of feed by fishes and therefore of waste production over time, the fish feeding method, the influence of others water physical-chemical properties (for example: pH and temperature) in the nitrification process and the apparent nonlinearity of data series are some of the main reasons causing application difficulty. An alternative to this kind of models is trying to predict the future value of one variable (i.e.: ammonia concentration) based on its own past values (stochastic analysis of time series). It is supposed therefore, that the influence of the physical-chemical-biological variables that may affect at ammonia concentration (i.e.: stock, density in rearing tanks, feed rate, pH, temperature, waste load, etc.) is contained in the variability of past values of the ammonia concentration. This way, the Box-Jenkins form of time series models and linear regression have been most commonly used in such situation because they are relatively easy to develop and implement (Stergiou et al., 1997; Park, 1998; Becerra-Muñoz et al., 1999).

Significant progress in the fields of nonlinear pattern recognition and system control theory has recently been made possible through advances in a branch of nonlinear system theoretic modelling called artificial neural networks (ANNs). An ANN is a nonlinear mathematical structure capable of representing complex nonlinear processes that relate the inputs to the outputs of any system. ANN models are increasingly being applied in many fields of science and engineering and usually provide highly satisfactory results (Rizzo and Dougherty, 1994; Chen and Ware, 1999; Laë et al., 1999; Gutiérrez-Estrada et al., 2000; Pulido-Calvo et al., 2003). In this paper, the performances of traditional prediction methods (linear multiple regression and univariate time series models: exponential smoothing and autoregressive integrated moving average (ARIMA) models) and ANNs models are used in predicting ammonia concentration in eel rearing tanks.

2. Material and methods

2.1. Fishfarm description

The methods discussed here were applied to Hidrorecursos S.A., an intensive eel fishfarm located in the province of Córdoba (southern Spain). In this fishfarm, the water is drawn from two primary sources: (1) the Puente Nuevo reservoir (cold water) and (2) the cooling water of Puente Nuevo power station (heat water) (Fig. 1). Under these conditions the water temperature was maintained to $23.4 \pm 3.5\,^{\circ}C$ between July of 1997 and March of 2001. In this period the average density was $53.6 \pm 16\,kg/m^3$ and the feed rate fluctuated between 0.9 and 2% of fish biomass per day.

The fishfarm has three biological filtration units (trickling filters) for water reuse. The first biological filter treats the water from the first nursery tanks (eel weight: 0.3–40 g). This tank series has $12 \times 3.2\,m^3$ circular tanks ('A' series). The second biological filter decreases the ammonia concentration of the second series of tanks. In this tank series there are also $12 \times 3.2\,m^3$ circular tanks ('B' series). The third purifies the water of pre-grow tanks (eel weight: 40–110 g). In this case, the number of tanks are $16 \times 16\,m^3$ rectangular tanks and

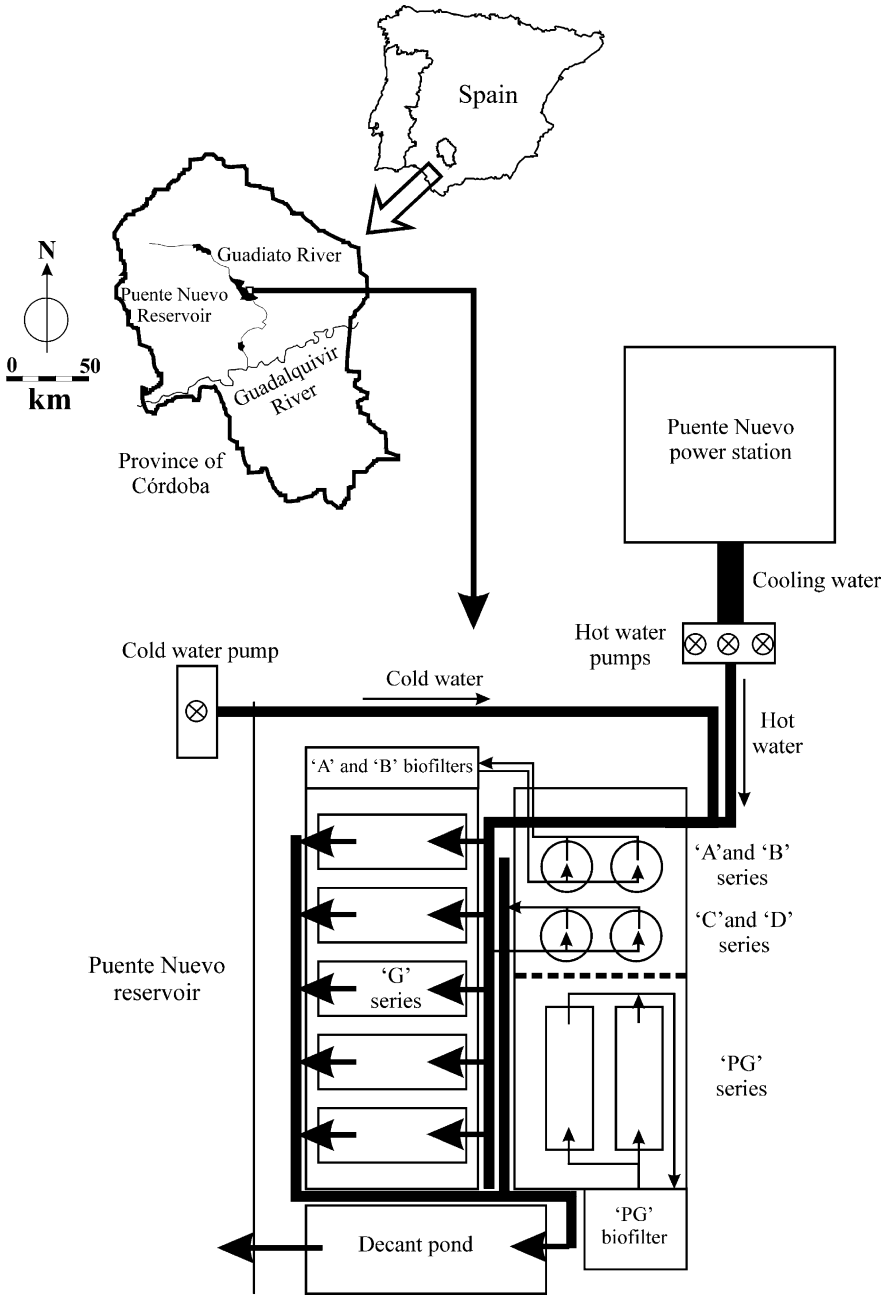

Fig. 1. Geographical location of Hidrorecursos S.A. and schematic representation of the fishfarm.

$4 \times 32\,m^3$ rectangular tanks ('PG' series). In the three cases, the filter medium used is a vertical flow medium (Bionet®, NSW Umwelttechnik, SSA $160\,m^2/m^3$). Two more series of twelve circular tanks each one ('C' and 'D' series) are present in the fishfarm, none of which have water recirculating systems. In the last tank series ($14 \times 110\,m^3$ rectangular tanks, 'G' series), the eels grow to commercial weight (150 g). This series also has no water recirculation capacity (Fig. 1). Globally, the average flow through the system was $3185 \pm 1634.2\,m^3$ per day and the exchange rate in the biological filters were 10% per day.

2.2. Linear multiple regression models

Multiple regression procedure will estimate $b_0, b_1, \ldots, b_q$ parameters of the linear equation:

$$e = b_0 + b_1 x_1 + \cdots + b_q x_q \tag{1}$$

where the regression coefficients b_0, b_1, ..., b_q represent the independent contributions of each independent variable x_1, ..., x_q to the prediction of the dependent variable e. The global statistical significance of the relationship between e with the independent variables is analysed by means of an analysis of variance to ensure the validity of the model in a quantified manner.

2.3. Univariate time series models

In general, there are two categories of univariate time series models which can be used for forecasting: exponential smoothing and autoregressive integrated moving average models. Smoothing model forecasts are based on the future projection of the basic pattern after eliminating randomness with smoothing. Exponential smoothing models apply unequal exponentially decreasing weights for averaging past observations. In this study, we used simple exponential smoothing and linear exponential smoothing (Holt's two-parameter method). Although ARIMA models are similar to smoothing in that forecasts are developed from historical time series analysis, they are based on well-articulated statistical theory. ARIMA models capture the historic autocorrelations of the data and extrapolate them into the future.

In simple exponential smoothing, the future values e_{t+1} of a variable d for each instant of time $t+1$ are computed as the weighted average of their past values d_t in instant t. This way, the smoothed variable S_t for each instant of time t is obtained (forecast):

$$S_t = \eta_d d_t + (1 - \eta_d) S_{t-1} \tag{2}$$

$$e_{t+1} = S_t \tag{3}$$

Thus, in effect, each smoothed value is the weighted average of the previous observations, where the weights decrease exponentially depending on the value of parameter η_d ($0 < \eta_d < 1$).

Holt's two-parameter method is also an exponential smoothing method that uses two exponential factors: η_d and β_d. Two smoothed variables, S_t and T_t, are also calculated for each instant of time t. The prediction is obtained with Eq. (6):

$$S_t = \eta_d d_t + (1 - \eta_d)(S_{t-1} + T_{t-1}) \tag{4}$$

$$T_t = \beta_d (S_t - S_{t-1}) + (1 - \beta_d) T_{t-1} \tag{5}$$

$$e_{t+1} = S_t + T_t \tag{6}$$

ARIMA(P, D, Q) models assume that a time series is a linear combination of its own past values and current and past values of an error term. The formulation considered to simulate the behaviour of the ammonia concentration is:

$$(1 - \Phi_1 B - \cdots - \Phi_P B^P)(1 - B^D) d_t = (1 - \Theta_1 B - \cdots - \Theta_Q B^Q) A_t \tag{7}$$

where d_t is the observed value of the daily ammonia concentration in instant t; A_t the difference between the observed and estimated concentrations in instant t in absolute value; B the backshift operator that assigns a value to a variable in the previous instant: $Bd_t = d_{t-1}$ and $B^m d_t = d_{t-m}$; Φ_i ($i = 1, \ldots, P$) the stationary autoregressive operator; Θ_j ($j = 1, \ldots, Q$) the invertible moving average operator; P the number of autoregressive parameters; D the degree of the differencing factor and Q the number of moving average parameters.

2.4. Artificial neural network models

Artificial neural networks are mathematical models inspired by the neural architecture of the human brain. The ANNs can recognise patterns and learn from their interactions with the environment. The most widely researched and used structures are multilayer feed forward networks (Rumelhart et al., 1986). These networks have been found to have the best performance with regard to input–output function approximation. A typical four-layer feed forward ANN is shown in Fig. 2. The first layer connects with the input variables and is called the input layer. The last layer connects to the output variables and is called the output layer. Layers in-between the input and output layers are called hidden layers. The processing elements in each layer are called nodes or neurons. In Fig. 2, there are q, n, m and s nodes in the input, first hidden, second hidden and output layers, respectively [the notation of the neural network is (q, n, m, s)]. Each of the nodes is connected to the nodes of neighbouring layers. The parameters associated with each of these connections are called weights. All connections are 'feed forward'; that is, they allow information transfer only from an earlier layer to the next consecutive layers. Nodes within a layer are not interconnected, and nodes in nonadjacent layers are not connected.

The architecture of a typical node is also shown in Fig. 2. Each node j receives incoming signals from every node i in the previous layer. Associated with each incoming signal (x_i) is a weight (W_{ji}). The effective incoming signal (I_j) to node j is the weighted sum of all the incoming signals:

$$I_j = \sum_{i=1}^{q} x_i W_{ji} \tag{8}$$

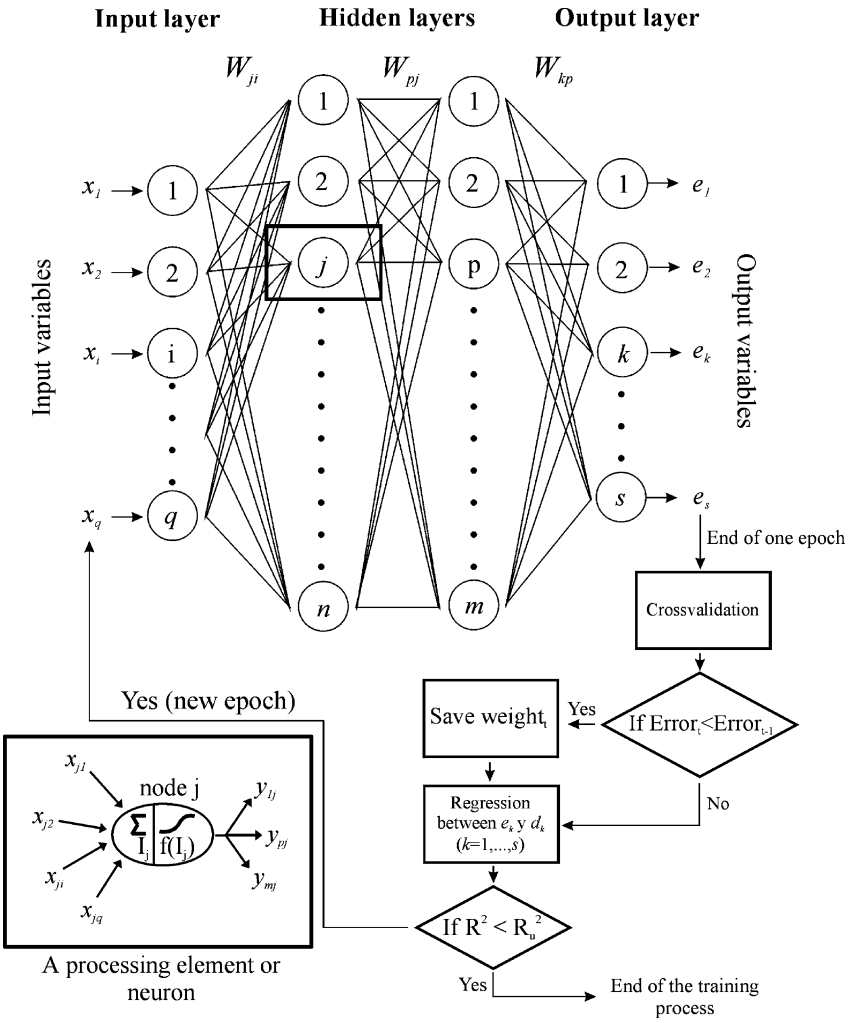

Fig. 2. Four-layer feed forward artificial neural network (q, n, m, s). Input variables: $x_1, \ldots, x_q$. Estimated output variables: $e_1, \ldots, e_s$. Observed output variables: $d_1, \ldots, d_s$.

The effective incoming signal, I_j, is passed through an activation function (sometimes called a transfer function) to produce the outgoing signal (y_j) of the node j. In this study, the linear (l) function ($y_j = I_j$) is used in the output layer and the sigmoid (s) nonlinear function is used in the hidden layers:

$$y_j = f(I_j) = \frac{1}{1 + \exp(-I_j)} \tag{9}$$

in which I_j can vary on the range $(-\infty,\infty)$, but y_j is bounded between 0 and 1. Because of the use of sigmoid functions in the ANN model, the values of the data variables must

be normalised onto range [0, 1] before applying the ANN methodology. This problem was solved through the following scaling (Griñó, 1992):

$$V_b^* = \frac{V_b - V_{\min,b}}{V_{\max,b} - V_{\min,b}} \tag{10}$$

where V_b are the values of the data variables; V_b^* is the scaled value of variable V_b; $V_{\min,b}$ is the minimum value of variable V_b minus 15%; and $V_{\max,b}$ is the maximum value of variable V_b plus 15%. Hence, the scaled series are in the range [0, 1]. This scaling has the advantage of mapping the desired range of a variable to the full 'working' range of the network input and, moreover, the scaled series lies in the central zone of the sigmoid function, where the function is approximately linear. Therefore during the validation model, the problem of output signal saturation that can sometimes be encountered in ANN applications is avoided (Tsoukalas and Uhrig, 1997).

To determine the set of weights a corrective-repetitive process called 'learning' or 'training' is performed. This training forms the interconnections between neurons, and is accomplished using known inputs and outputs (training sets or patterns), and presenting these to the ANN in some ordered manner, adjusting the interconnection weights until the desired outputs are reached. The strength of these interconnections is adjusted using an error convergence technique so that a desired output will be produced for a given input. The training method used is a standard back-propagation variation proposed by Rumelhart et al. (1986) and known as extended-delta-bar-delta (EDBD) (Minai and Williams, 1990). This method improves the convergence speed of the standard back-propagation algorithm and includes modifications through learning and momentum rate adaptation. The parameter values used to ensure optimal learning by the neural network, which proved to be good enough in most instances (Ventura et al., 1995), were: $\kappa_\alpha = 0.095$, $\kappa_\mu = 1$ (κ_α and κ_μ are scaling factors for the learning rate increment and momentum coefficient, respectively); $\gamma_\alpha = 0.1$, $\gamma_\mu = 0.05$ (γ_α and γ_μ are exponential factors for the increment of these coefficients, respectively); $\varphi_\alpha = 0.1$, $\varphi_\mu = 0.01$ (φ_α and φ_μ are decrement factors); and $\theta = 0.7$ (θ is a weighting factor).

Epoch is the time period that encompasses all the iterations performed after all the patterns are displayed. The weights are updated at the end of each epoch. An important aspect of the ANN is its capacity to generalise from examples. Generalisation refers to the capacity of the ANN to provide a correct response with patterns that have not been employed in its training. Thus, a neural network will learn until reaching the optimum point at which the generalisation error is minimum for the neural network architecture. In this study, learning is controlled by two methods: (1) cross validation (Ventura et al., 1997) and (2) an arbitrary threshold determination coefficient (R_t^2) (Gutiérrez-Estrada et al., 2000) (Fig. 2).

A ANN with a single hidden layer can implement any continuous and bounded multivariate function mapping. In this paper, ANNs with two hidden layers (universal approximators of any function) have been used because the type of relationship among the variables a priori is unknown or poorly defined form and complexity. Also, it may occur that with a single hidden layer the number of necessary intermediate nodes to reach a certain error is so high that its application is unapproachable in practice (Cybenco, 1989). Diverse values of the number of hidden nodes are compared, and the one with the smallest error in the generalisation is chosen.

2.5. Data series and identification models

The ammonia concentration was measured each three hours (eight data per day and series) in the inlet pipe of filters from July of 1997 to March of 2001. The ammonia concentration value (in its unionised form) was obtained by a Merck-Microquant® colorimetric test. For each day and series an average value was obtained and later on, a convolution process on data series was carried out. This way, the noise of data series due to changes in amplitude is reduced (Cabrera and Vela, 1994).

The stochastic analysis of time series need the selection of a number of previous days as input data. This selection was made based on autocorrelation and partial autocorrelation functions of the ammonia concentration series (Wilson and Keating, 1996).

The data of 'A' series from 1997 to 1999 were used for the model calibration (training in the ANN). The independent variable was the ammonia concentration in t day and the dependent variables were the ammonia concentrations in previous days ($t-1$, $t-2$, etc.). To check the generalisation capacity of the models, data of 'A' series from 2000 to 2001 were used (generalisation phase). Additionally, two type of tests were carried out: (a) the extend of the validation process to 'B' and 'PG' series (years 2000 and 2001) and (b) the analysis of the forecasting for $t+2$ and $t+3$ days using the best models of the generalisation phase (years 2000 and 2001).

To estimate ammonia concentration with the ANNs the REDGEN® neural network simulation software (Gutierrez-Estrada and Pulido-Calvo, 2002) for Windows developed in MS Visual Basic® language was used.

In univariate time series models, ammonia data from 1997 to 1999 were used to identify model structure and estimate the associated parameters. In exponential smoothing methods, the exponential factors η_d and β_d were selected by a trial and error scheme to minimise mean square errors in one-step-ahead prediction. In ARIMA models, the values of P, D and Q were each varied over range 0–5. To identify P, D and Q, each was increased by a unit. Those that were most approximate were chosen. The parameters Φ_i and Θ_j were estimated using function minimisation procedures, so that the sum of squared residuals is minimised. The level of significance of these parameters should be evaluated (acceptable if $P_\alpha < 0.05$). A good way to evaluate these models is to examine the autocorrelogram of residuals (there should be no serial dependency between residuals).

2.6. Measures of accuracy

A measure of correlation between the observations and predictions is the coefficient of determination (R^2). Measures of variances are the percent standard error of prediction (% SEP) (Ventura et al., 1995), the coefficient of efficiency (E) (Kitanidis and Bras, 1980) and the average relative variance (ARV) (Griñó, 1992). These estimators are not biased by the range of variation of its elements. These are employed to see how far the model is able to explain the total variance of the data. The percent standard error of prediction is defined as:

$$\%\,\mathrm{SEP}_k = \frac{100}{\bar{d}_{kg}}\sqrt{\frac{\sum_{g=1}^{N}(d_{kg}-e_{kg})^2}{N}} \tag{11}$$

where d_{kg} is the observed output k of pattern g; e_{kg} is the estimated output for pattern g; N is the total number of generalisation patterns and $\bar{d}_{kg}$ is the mean value of the observed outputs of the prediction set.

The coefficient of efficiency (E) and the average relative variance (ARV) are expressed by:

$$E_k = \frac{M_{\text{obs}} - M}{M_{\text{obs}}}; \quad \text{ARV}_k = \frac{M}{M_{\text{obs}}} \tag{12}$$

$$M_{\text{obs}} = \sum_{g=1}^{N} (d_{kg} - \bar{d}_{kg})^2; \quad M = \sum_{g=1}^{N} (d_{kg} - e_{kg})^2 \tag{13}$$

where M_{obs} is the measure of variability of the observed values from their means and M is the measure of association between predicted and observed values. For a perfect match, the R^2 and E values should be close to 1.0 and the values of % SEP and ARV close to 0.

3. Results

3.1. Multiple regression analysis ('A' series)

The daily average ammonia concentration model using multiple regression with ammonia concentration of the 5 previous days as independent variables, achieved good results in the calibration and validation periods (Calibration: $R = 0.9891$, $R^2 = 0.9783$, $F(5, 866) = 3031.6$, $p_\alpha < 0.001$, $N = 872$. Validation: $R = 0.9782$, $R^2 = 0.9568$, $F(1, 376) = 8335.1$, $p_\alpha < 0.001$, $N = 378$, % SEP = 21.3099, $E = 0.9545$, ARV = 0.0455). The coefficients b_i for only two independent variables, average ammonia concentration of the 2 previous days, were both statistically significant ($P_\alpha < 0.05$). Therefore, another multiple regression analysis was performed with concentrations of the 2 previous days as independent variables. Almost equivalent results were obtained in the correlation coefficient (R) and in the statistical estimators (% SEP, E and ARV) in validation (Table 1). The simple regression between observed and estimated ammonia concentration values showed a slope very close to one and a low dispersion around the regression line. On the other hand, estimated ammonia concentrations versus residues (observed values minus estimated values) showed a slope very close to zero and homogeneous deviations around this value (Fig. 3).

3.2. Smoothing and ARIMA models ('A' series)

Table 2 shows the results of simple and linear exponential smoothings and the results of the ARIMA(P, D, Q) model with parameters with a level of acceptable statistical significance ($p_\alpha < 0.05$). Similar behaviour was seen for the both smoothing models but the best error magnitudes was obtained by Holt model. In this case, the % SEP was two points minor to calculated for simple exponential smoothing (Table 2). The same as in the multiple regression, the Holt model provided low deviations around the regression line and homogeneous dispersions of residues versus estimated ammonia concentration values (Fig. 4).

Table 1
Multiple regression model and validation

Dependent variable	Independent variables	b_i ($i = 0, 1, \ldots, q$)	p_α
(A) Regression summary in the calibration model[a]			
Ammonia (t)	Intercept (b_0)	0.0616	0.0709
	Ammonia ($t-1$)	1.5733	0
	Ammonia ($t-2$)	−0.6030	0
(B) Regression summary in the validation model[b]			
Ammonia estimated (t)	Intercept (b_0)	0.5531	0.0725
	Ammonia observed (t)	1.0186	0

(A) Multiple regression model between several independent variables (ammonia concentration of 2 previous days) and the average ammonia concentration of 1 day in advance, as the dependent variable. (B) Validation of the model, after the regression between estimated and observed ammonia concentrations.

[a] $R = 0.9890$; $R^2 = 0.9782$; $F(2, 880) = 7626.6$; $p_\alpha < 0.001$; $N = 882$.

[b] $R = 0.9785$; $R^2 = 0.9574$; $F(1, 376) = 8450.9$; $p_\alpha < 0.001$; $N = 378$; % SEP = 20.7449; Coefficient $E = 0.9569$; ARV = 0.0431.

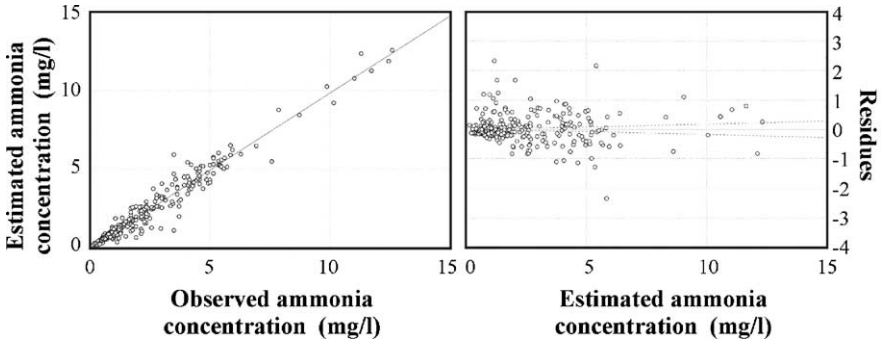

Fig. 3. Scatterplot comparing observed and estimated ammonia concentration for the multiple regression model and scatterplot comparing estimated ammonia concentration and residues (observed minus estimated values) in the validation process of 'A' series.

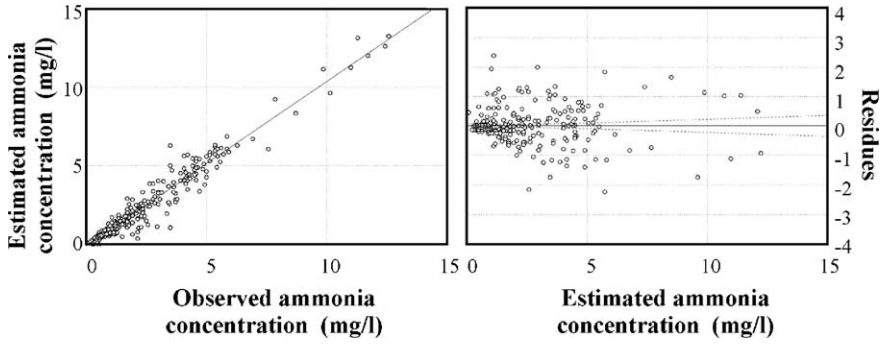

Fig. 4. Scatterplot comparing observed and estimated ammonia concentration for the Holt smoothing model and scatterplot comparing estimated ammonia concentration and residues (observed minus estimated values) in the validation process of 'A' series.

Table 2
Goodness-of-fit of univariate time series analysis (exponential smoothing and ARIMA models)

Model	Parameters	Validation			
		R^2	% SEP	E	ARV
Simple exponential smoothing	$S_0 = 2.5940$; $\alpha_d = 1$	0.9328	26.1196	0.9316	0.0684
Holt smoothing	$S_0 = 0.6437$; $T_0 = -0.0020$; $\alpha_d = 1$; $\beta_d = 0.3800$	0.9512[a]	24.1336[a]	0.9416[a]	0.0584[a]
ARIMA(0,0,1)	$\Theta_1 = -0.9254$**	0.8363	76.5036	0.4134	0.5866
ARIMA(1,0,0)	$\Phi_1 = 0.9849$**	0.9358	25.4364	0.9352	0.0648
ARIMA(0,1,1)	$\Theta_1 = -0.4725$**	0.9527	21.9946	0.9515	0.0485
ARIMA(1,0,1)	$\Phi_1 = 0.9751$**; $\Theta_1 = -0.4766$**	0.9527	21.8918	0.9520	0.0480
ARIMA(1,1,0)	$\Phi_1 = 0.5539$**	0.9572	21.2352	0.9548	0.0452
ARIMA(1,2,1)	$\Phi_1 = 0.2906$**; $\Theta_1 = -0.9946$**	0.7986	48.7636	0.7617	0.2383
ARIMA(2,2,1)	$\Phi_1 = 0.4357$**; $\Theta_1 = -0.9904$**; $\Phi_2 = -0.4927$**	0.9444	25.8011	0.9333	0.0667
ARIMA(2,1,1)	$\Phi_1 = 1.5282$**; $\Theta_1 = 0.9903$**; $\Phi_2 = -0.5785$**	0.9571[a]	20.7257[a]	0.9569[a]	0.0431[a]
ARIMA(1,2,2)	$\Phi_1 = -0.1454$**; $\Theta_1 = -1.8701$**; $\Theta_2 = -0.8769$**	0.9469	24.8852	0.9379	0.0621
ARIMA(2,2,2)	$\Phi_1 = -0.1084$*; $\Theta_1 = -1.7963$**; $\Phi_2 = -0.2925$**; $\Theta_2 = -0.8047$**	0.9510	24.0028	0.9423	0.0577

* $p_\alpha < 0.05$.
** $p_\alpha < 0.01$.
[a] Best value.

Also all ARIMA models (except ARIMA(0, 0, 1) and ARIMA(1, 2, 1)) have provided acceptable statistical results. Globally, different behaviour is observed in function of the differentiation degree (order D). In this way, the ARIMA models with order $D = 0$ provided the worst estimates for the validation data series (Table 2). The ARIMA models with order $D = 2$ provided results like to smoothing models and the best results were obtained for ARIMA models with order $D = 1$. Individually, the best estimates in the validation process was obtained with the ARIMA(2, 1, 1). This model had the smallest error magnitudes and decreased in 3.4 points the best result obtained for smoothing models (Table 2). On the other hand, the autocorrelation function shows a significant correlation at least for the seventh lag (Wilson and Keating, 1996) (Fig. 5). In spite of it, the regression between observed and estimated ammonia concentrations provided the lowest deviations around the regression line and the lowest residues versus estimated ammonia concentrations values (Fig. 5).

3.3. ANNs models ('A' series)

The same cases of multiple regression were considered with the ANNs. Different architectures and different trainings have been tested. That is, different node numbers in the hidden layers and threshold determination coefficients for each ANN model have been tested. Table 3 shows the goodness of fit of the ANNs that gave the best results. The best estimates were obtained when the ammonia concentration of the 5 previous days were used

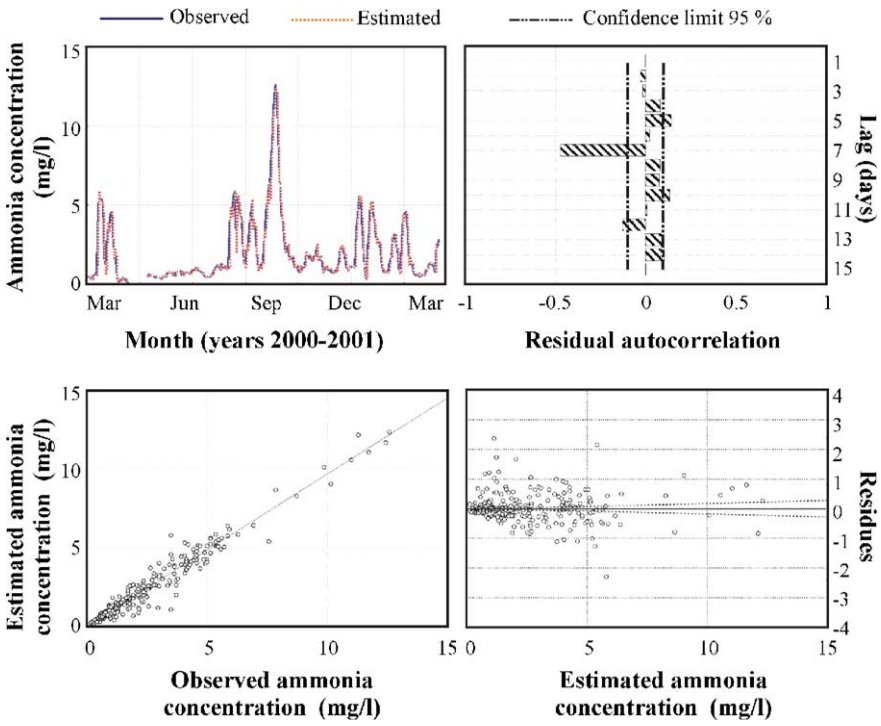

Fig. 5. One-step-ahead prediction ammonia concentration with univariate time series model and autocorrelation function of residuals for the validation period. Scatterplot comparing observed and estimated ammonia concentration for the ARIMA(2, 1, 1) model and scatterplot comparing estimated ammonia concentration and residues (observed minus estimated values) in the validation process of 'A' series.

as inputs, with 10 nodes in the first hidden layer and 15 nodes in the second hidden layer, and a threshold determination coefficient of 95%. In this case, the error magnitudes were lightly worst in the validation process ($R^2 = 0.9508$, % SEP $= 22.1665$, $E = 0.9508$, ARV $= 0.0492$). Compared with the best multiple regression, smoothing and ARIMA

Table 3
Results of training and validation of ANNs with average ammonia concentration of the 5 previous days as inputs

Calibration			Validation			
ANN	Weights	Epochs	R^2	% SEP	E	ARV
5:5s:5s:1l	55	55	0.9402	25.8434	0.9331	0.0669
5:10s:10s:1l	160	6836	0.9409	25.2448	0.9361	0.0639
5:10s:15s:1l	215	1975	0.9508	22.1665[a]	0.9508[a]	0.0492[a]
5:15s:10s:1l	235	976	0.9511[a]	22.5176	0.9492	0.0508
5:15s:15s:1l	315	1286	0.9488	24.0225	0.9422	0.0578
5:15s:20s:1l	395	756	0.9466	24.8347	0.9382	0.0618
5:20s:20s:1l	520	713	0.9385	25.8179	0.9332	0.0668

[a] Best value.

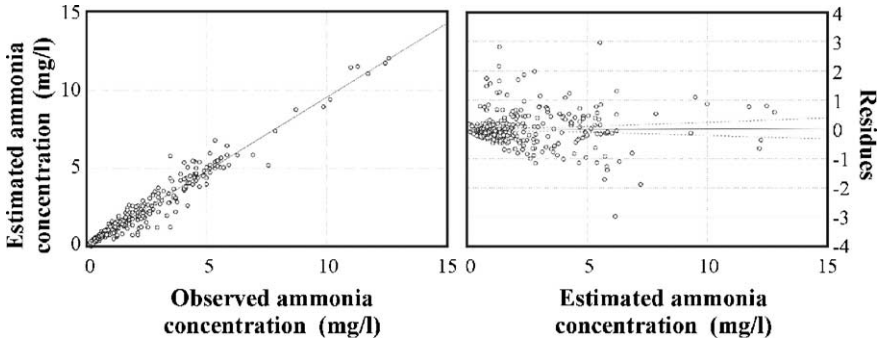

Fig. 6. Scatterplot comparing observed and estimated ammonia concentration for the 5:10*s*:15*s*:1*l* ANN model and scatterplot comparing estimated ammonia concentration and residues (observed minus estimated values) in the validation process of 'A' series.

model, the best ANN model obtain valid statistical results (Fig. 6) but globally only obtain better results than smoothing models.

3.4. Test a: extent of validation process to 'B' and 'PG' series

To check the generalisation capacity of the best models calibrated in 'A' series, the validation process was extended to 'B' and 'PG' series. Table 4 shows the results of this generalisation process. In 'B' series the absolute best result was obtained by the multiple regression model (% SEP = 18.1548, $E = 0.9681$, ARV = 0.0319) although the determination coefficient of ARIMA model was slightly higher ($R^2 = 0.9716$). The simple regression between observed and estimated ammonia concentrations showed the best fit of the multiple regression and ANN model because the Holt smoothing and ARIMA(2, 1, 1) model provided negative estimations (Fig. 7).

In 'PG' series, the absolute best results were obtained by the ANN model (% SEP = 17.4983, $E = 0.9660$, ARV = 0.0339) (Table 4). In this case, the explained variance of ARIMA model was higher again ($R^2 = 0.9618$). Substantially, in both ('B' and 'PG') series the most important decrease of error magnitudes was produced by ANN model. This way, the ANN model validation decreases 3.6 points in 'B' series and 4.7 points in 'PG' series in relation to the error in 'A' series (ANN model: % SEP = 22.1664). A similar behaviour was observed in the R^2, E and ARV coefficients. This effect was magnified when the relative improvements were compared (Table 4). Estimated versus observed ammonia concentration for the multiple regression, the Holt smoothing, ARIMA(2, 1, 1) and ANN model for validation data are given in Fig. 8. Again, the Holt smoothing model provide negative estimations.

3.5. Test b: analysis of the forecasting for $t + 2$ and $t + 3$ days using the best multiple regression and ANN models of the generalisation phase

Table 5 shows the analysis results of the forecasting for $t + 2$ and $t + 3$ days using the best multiple regression and ANN models of the generalisation phase. In the $t + 2$ case,

Table 4
Test a results

	R^2	% SEP	E	ARV	Differences in R^2	Differences in % SEP	Differences in E	Differences in ARV
Extended validation to 'B' series								
Multiple regression	0.9682	18.1548[a]	0.9681[a]	0.0319[a]	0.0108 (1.1%)	−2.5901 (12.5%)	0.0112 (1.2%)	−0.0112 (26.0%)
Holt smoothing	0.9547	23.9283	0.9446	0.0554	0.0035 (0.4%)	−0.2053 (0.9%)	0.0030 (0.3%)	−0.0030 (5.1%)
ARIMA(2, 1, 1)	0.9716[a]	18.6563	0.9663	0.0337	0.0145 (1.5%)	−2.0694 (10.0%)	0.0094 (1.0%)	−0.0094 (21.8%)
5:10*s*:15*s*:1*l* ANN	0.9664	18.5569	0.9667	0.0333	0.0156[a] (1.6%)	−3.6095[a] (16.3%)	0.0159[a] (1.6%)	−0.0159[a] (32.3%)
Extended validation to 'PG' series								
Multiple regression	0.9610	18.7714	0.9609	0.0391	0.0036 (0.4%)	−1.9735 (9.5%)	0.0040 (0.4%)	−0.0040 (9.3%)
Holt smoothing	0.9555	22.1086	0.9458	0.0542	0.0043 (0.5%)	−2.0250 (8.4%)	0.0042 (0.4%)	−0.0042 (7.2%)
ARIMA(2, 1, 1)	0.9618[a]	18.5212	0.9620	0.0380	0.0047 (0.5%)	−2.2045 (10.6%)	0.0051 (0.5%)	−0.0051 (11.8%)
5:10*s*:15*s*:1*l* ANN	0.9580	17.4983[a]	0.9660[a]	0.0339[a]	0.0072[a] (0.6%)	−4.6681[a] (21.1%)	0.0152[a] (1.6%)	−0.0153[a] (31.1%)

Extended validation to 'B' and 'PG' series of the best models (multiple regression [2 days], Holt smoothing, ARIMA(2, 1, 1) and 5:10*s*:15*s*:1*l* ANN model) calibrated in 'A' series and differences (absolute and relative values) between the coefficient values of validation in 'A' series and 'B' and 'PG' series

[a] Best value.

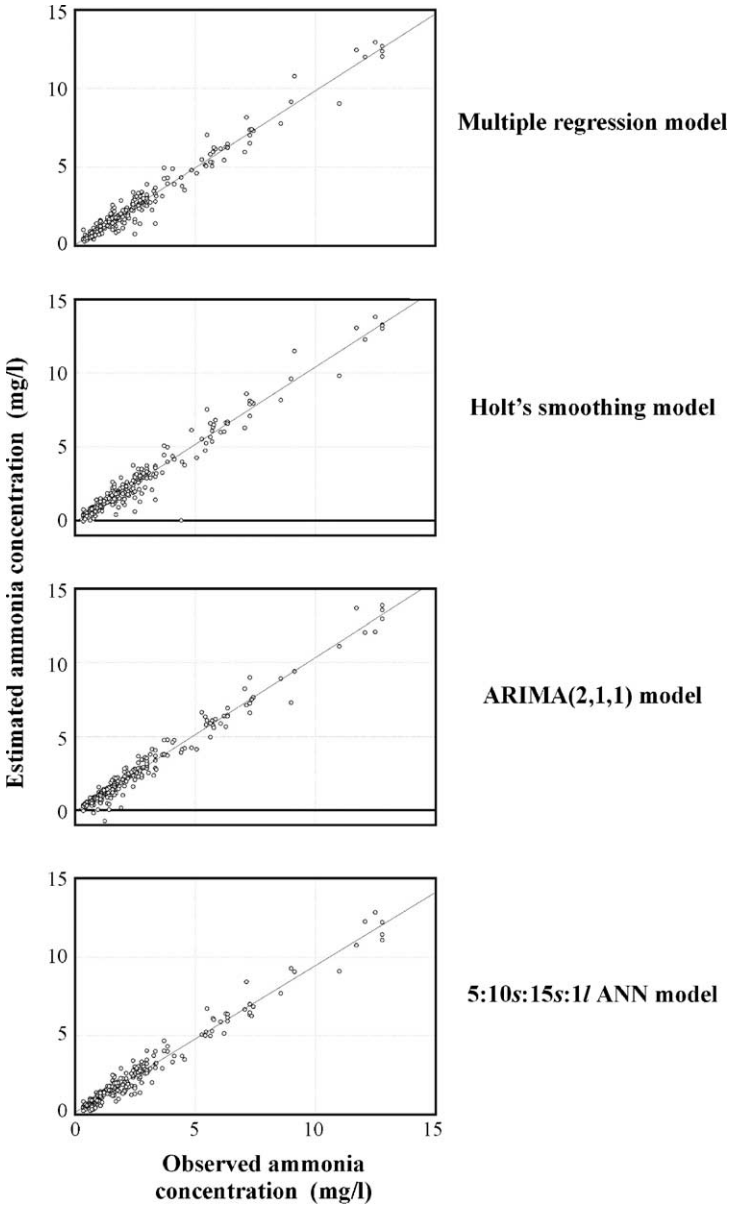

Fig. 7. Scatterplots comparing observed and estimated ammonia concentrations for multiple regression, Holt smoothing, ARIMA(2, 1, 1) and 5:10*s*:15*s*:1*l* ANN models in the validation of 'B' series.

the multiple regression provides worst results than ANN model. In spite of it, the explained variance in the multiple regression was higher than ANN model (multiple regression $R^2 = 0.81$; ANN $R^2 = 0.72$). However, this value was a consequence of the high negative relationship between observed and estimates data. This negative correlation is not observed

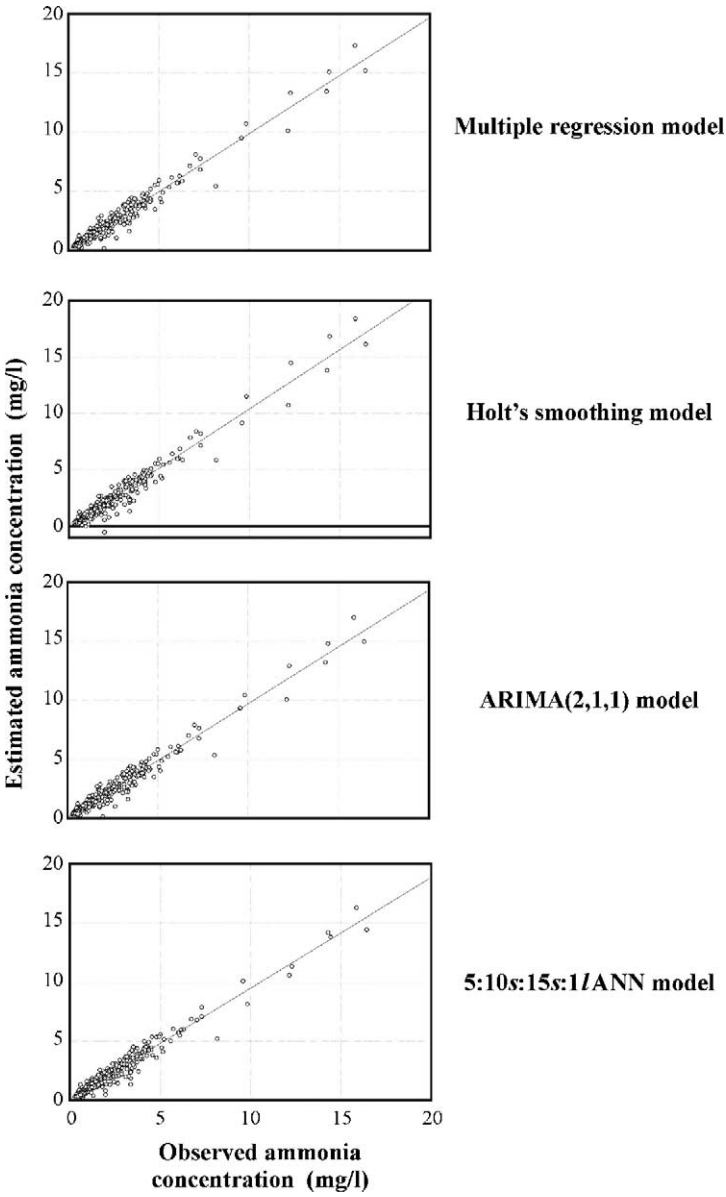

Fig. 8. Scatterplots comparing observed and estimated ammonia concentrations for multiple regression, Holt smoothing, ARIMA(2, 1, 1) and 5:10*s*:15*s*:1*l* ANN models in the validation of 'PG' series.

in the ANN model. The rest of the error magnitudes are significantly better in the ANN model.

Similar results are obtained in the $t + 3$ forecasting, that is to say, the error of the ANN prediction was significantly lower to multiple regression error (Table 5). In this case, the

Table 5
Test b results

	Multiple regression	ANN
$t + 2$ days forecasting		
Pearson correlation coefficient (R)	−0.9004	0.8536
Determination coefficient (R^2)	0.8108	0.7286
% SEP	223.0196	62.1857
E	−3.9847	0.6124
ARV	4.9847	0.3876
$t + 3$ days forecasting		
Pearson correlation coefficient (R)	0.8534	0.9678
Determination coefficient (R^2)	0.7283	0.9366
% SEP	133.0962	39.2753
E	−0.7754	0.9082
ARV	1.7754	0.0918

Extended validation to $t + 2$ and $t + 3$ days forecasting.

Pearson correlation coefficient of the multiple regression was closed to one. On the other hand, the percent standard error of prediction was approximately a 50% lower than the $t+2$ forecasting. Globally, the results indicate that error magnitudes are better than the $t + 2$ forecasting. Also, in this particular situation, the ANN predictions are more approximate than the multiple regression forecasting.

4. Discussion

The potential of multiple regression, smoothing models, ARIMA models and artificial neural network for daily ammonia concentration forecasting in an eel intensive rearing system have been presented in this paper. In estimating daily average ammonia concentration, explained variance upper 95% and error magnitudes lower 25% (% SEP) and 0.06 (ARV) have been obtained in the validation process. These results are significantly better to those obtained by Kamstra et al. (1998) ($42 > \%\,\mathrm{SEP}_{\mathrm{estimated}} > 31$, $\%\,\mathrm{SEP}_{\mathrm{estimated}}$ = estimated starting from graph data) using physic models in prediction of ammonium removal rate in one tricking filter, although Kamstra et al. (1998) used a more accurate temporal scale. This may be a consequence of that the relative importance of the variables used in the physic models, and others don't used, are included in the ammonia concentration values. This way, the use of temporal series models may provide smaller error than the physic models. Also, statistical models avoid the difficult implementation on the physical models reported by Heinsbroek and Kamstra (1990) and Kamstra et al. (1998) by only depending on the same variable that they try to predict.

Globally, all estimations obtained are very similar with small differences in the four coefficients (R^2, % SEP, E and ARV) very low. However, the complementary use of measures (standard and relatives) recommended by other authors (Stergiou et al., 1997) indicate that the best behaviours are showed by the artificial neural networks. This can be concluded although the best result in 'A' series is obtained by ARIMA(2, 1, 1) model and the best result in 'B' series is obtained by the multiple regression. It is necessary to keep in mind that

the more linearity behaviour and the smaller extreme values of ammonia concentrations are due in 'A' and 'B' series. This way, it's coherent that linear models obtain better results than the ANN models because in the last ones to reach the absolute minimum of the error function to minimise during the calibration process is not guarantied (Tsoukalas and Uhrig, 1997). In spite of it, the more important improvements in 'B' series of the accuracy measures respect to those obtained in 'A' series are observed in ANN model (absolute and relative values). On the other hand, the good results obtained in 'B' series by multiple regression model are favoured by the significant correlation ($R = 0.5429$, $p_\alpha < 0.05$) between the data of 'A' and 'B' series. In the 'PG' case, the best coefficients (except determination coefficient) are obtained by the ANN model. This may be a consequence of the correlation between the data of 'A' and 'PG' series was significant but very low ($R = 0.2649$, $p_\alpha < 0.05$). These results are similar to those obtained by Gutiérrez-Estrada et al. (2000).

This effect is more significant in the test b. In this case, the ANN model showed a great generalisation power in relation to exceptional situations. For the manager of the fishfarm is very important to dispose of a generalist character model because it may facilitates the ammonia concentration forecasting process and avoid the model recalibration in a short time. This way, the ANN provided very good approximations compared with the multiple regression when the models were obligated to predict in a situation for which specifically had not been calibrated.

On the other hand, the multiple regression and the ANN model detected the data series periodicity. This phenomena propitiated better estimations in the more distant predictions ($t + 3$). This may be related with three principal factors: the filter system, the biofilters management and the feed system. The trickling filters are generally used for nitrification in fishfarm. The design of this type of filter are based on laboratory research which can result in over-estimation of predicted biofilter performance when the design is translated directly into commercial systems (Kamstra et al., 1998). This factor together with an incorrect operation of the filter and a wrong feed distribution could change the variation frequency of the daily fluctuations in ammonia concentration.

The standard backpropagation procedure of ANN gave very high correlation coefficients, especially for the training calculation, but a disadvantage of the standard backpropagation model is that it can overfit the examples during the training process. However, the training method proposed here, developed by the authors and based on threshold determination coefficients combined with a crossvalidation process, was very efficient during generalisation, as the ANNs provided correct responses with data not used during the learning, as Gutiérrez-Estrada et al. (2000) also conclude.

On the other hand, the number of epochs employed during the training process was clearly lower than those obtained by other authors (Ranjithan et al., 1993; Rizzo and Dougherty, 1994). These differences can be explained by the type of parameters estimated, but also by the use in this study of a modified standard backpropagation model (EDBD) as the learning algorithm, which accelerates the effective learning process in certain directions.

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