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PREDICTION AND MODELING OF SEASONAL CONCENTRATIONS OF AIR POLLUTANTS IN SEMI-URBAN REGION EMPLOYING ARTIFICIAL NEURAL NETWORK ENSEMBLES

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ABSTRACT: This study utilizes Artificial Neural Network (ANN) ensembles to predict seasonal variation of air pollutants in semi-urban region of Eleme, Rivers state, Nigeria. A ten year monthly concentrations of SO₂, NO₂, CO and CH₄ in the region was obtained for dry and rainy seasons. Air pollutant concentrations in semi urban area of Eleme can be attributed mainly to industrial activities, vehicular emissions and some local background concentrations influenced by meteorological and geographical conditions of the area. Training of the network models was achieved using Neural NetTime Series feature of MATLAB software. Observed concentrations of pollutants and meteorological parameters were used as input variables for the prognostic models. The developed ANN prognostic models accurately captured the dynamic relationships between pollutant concentrations and meteorological predictor variables. The relationships between predicted and observed values were highly significant at 95% of confidence level for all models as dry and rainy seasons models gave R^2 greater than 0.99 (indicating close relationships between observed and predicted values). CH_4 showed R^2 of 0.9946 and 0.9974 for dry and rainy seasons respectively; CO showed R^2 of 0.9918 and 0.9972 for dry and rainy seasons respectively; NO₂ showed R^2 of 0.9998 and 0.9982 for dry and rainy seasons respectively; SO_2 showed R^2 of 0.9921 and 0.9991 for dry and rainy seasons respectively. The trend in predicted pollutants indicated that the study area is a major receptor of air pollutants emanating mainly from industrial activities and vehicular exhaust emissions. Further research study is needed to compare ANN model with other modeling approaches such as with multiple linear regression models for the prediction of air pollutants.

KEYWORDS: Semi-Urban Region, Air Pollutants, Artificial Neural Network, Input layer, Hidden Layer, Output Layer.

INTRODUCTION

In many urban and semi-urban areas concentrations of air pollutants are on the increase (Rao and Rao, 2005) mainly due to burning of fossil fuels for energy production for domestic, industrial, and transportation uses. Thus, air pollution presents a complex issue that is driven by multiple sources ranging from industrial emissions, vehicular emissions, and other emissions from fossil fuels, construction activities to domestic activities. Hence, air pollution is of public health and environmental concern (Davis and Cornwell, 2008), as it impacts widely on the biophysical environment. It is harmful to all forms of life, including plants, animals, and birds.

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LITERATURE REVIEW

Artificial Neural Networks (ANN) offer suitable approach in modeling atmospheric pollutants than conventional deterministic modeling techniques (Elangasinghe et al., 2014). This is because Artificial Neural Networks can capture different kinds of relationships among variables, which otherwise may have been very difficult or impossible with statistical and deterministic models. According to Kukkonen et al., (2003) artificial neural network can be used to model multifactor, nonlinearity and uncertainty. In contrast to stochastic modeling approach, ANN does not make prior assumptions on the pattern of data set (Ming et al., 2009). Artificial neural network has been employed to a greater extent in the prediction of concentrations of air pollutants such as Nitrogen dioxide, Sulphur dioxide (Sudeshana et al., 2013), PM₁₀ (Hooyberghs et al., 2005), Ozone (Elkamel et al., 2001), and Carbon monoxide (Sudhir et al., 2013). Thus, Artificial Neural Network can be regarded as an effective and intelligent modeling approach which has received much attention in the field of environmental engineering (Sudeshana et al., 2013), and has been proven to be a powerful tool in Air Quality Modeling and prediction (Dorling et al., 2003; Primož and Marija, 2011; Amirsasha and Farhad, 2012). Its role is increasing with improving artificial neural networks algorithms that make artificial neural networks applications on real systems even more accurate and reliable (Grivas and Chaloulakou, 2006; Singh et al., , 2012; Elangasinghe et al., 2014). Recent studies have shown that artificial neural networks-based air pollution models have better performances than other deterministic and statistical techniques (Chelani et al., 2002; Grivas and Chaloulakou, 2006; Singh et al., 2012). Dorling et al., (2003) discusses several Air Quality Forecasting using artificial neural networks approaches and concludes that Neural Network models are useful for simulating air quality in an environment.

MATERIALS AND METHODS

Study Area

Eleme region (Figure 1) is located within the coastal area of Rivers State in the Niger Delta region between Longitude 706'10"E and Latitude 4047'57"N. The complex coastline and low-lying flat topology of the area result in composite surface wind speed patterns, especially during low wind flows when land and sea breezes dominate the surface wind of the area.



Figure 1: Map of Eleme region

Collection of data

A 10 year data (January 2006 to October 2015) was collected corporate monitoring stations in Eleme area and used in the study. Meteorological data acquired and adopted in the study are monthly ambient temperature, relative humidity, wind speed and direction, while monthly air pollutants parameters are carbon monoxide, CO, sulphur dioxide, SO₂, Nitrogen dioxide, NO₂, and hydrocarbon methane, CH₄. A total of 944 data set was obtained which forms the basis of data analysis and model building presented in this study. In this study, significance importance was placed on using a minimal set of meteorological parameters (predictors) that are readily measured or observed in the area to ensure that the models are of practical use.

Determination of Network Architecture/Topology

A three layer perceptron ANN was used as the base architecture or topology for the designed prediction models. The effectiveness of the multi-layer perceptron (MLP) to accurately predict non-linear systems and its ability to generalize is the main reason for its choice. The prediction models developed are multi-layer perceptron with input layer units, hidden layer units and an output layer unit. The input variables (original data including the target variables) were entered into the input layer of the network. The outputs of the input layer units function as input to the hidden layer units, and the outputs of the hidden layer units function as input of the output layer. The output of the output layer unit was obtained as the final output of the network, which is the pollutant concentration. The number of patterns and features were used to determine the network topology or architecture. The three-layer network architecture model designed for the prediction of pollutants concentrations consists of n neurons in the input layer, m neurons in the hidden layer and q neurons in the output layer. The input features were determined using assembled collected data from 2006 to 2015. Both the input and output data sets form the database of patterns or perceptual structure of the model. The number of neurons in the hidden layer(s) was determined using Akaike's Information Criterion (AIC) rules (Equations 1 to 3) which validate the number of neurons in the hidden layer of the network. The most efficient neural network architectures that accurately predict pollutant concentrations in the area were chosen. The general AIC estimator of Kullback -Leibler information (Gaurang et al., , 2010) is expressed as:

$$AIC = -2(\text{maximum log likelihood of the model}) + 2(\text{number of free parameters of the model})$$
$$AIC = -2\ln(likelihood) + 2k \tag{1}$$

The best ANN model was determined by calculating the difference between lowest AIC model and the others (Gaurang et al., , 2010) as:

$$\Delta i = AICi - AIC_{\min} \tag{2}$$

Equation (2) is used to calculate the likelihood of a model given the set data and to determine the validity of each model being the best approximator (Gaurang et al., , 2010).

$$\sum_{i} i = \frac{Exp(-\frac{1}{2}\Delta i)}{\sum_{i}^{k} Exp(-\frac{1}{2}\Delta i)}$$
(3)

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Model Development Process

In developing the prognostic models, the ten year data was categorized into dry season (November to March) and rainy season (April to October). The data set were further divided into training, validation and testing data sets. The training data set was used to modify and change the synaptic weights of the ANN models. Testing data set was utilized periodically to test the model's generalizing capabilities (Primož and Marija, 2011) during the learning process so as to achieve best optimization during learning. The training and validation sets were organized into the learning set. The testing set was used for model verification to determine its ability to predict accurately and the expected associated error. During ANN models design process original data was randomly separated and arranged into training data set (70%), validation data set (15%) and test data set (15%) by Matlab software capabilities. The training data set used for each model contains the input vector variables and their associated observed targets that constitute one class of the test set. Several numbers of such test classes were fed into the neural network programs. The design ANN models used selected transfer functions for specific algorithms based on their derivability and their non-linearity. Sigmoid (logistic) function was used as the transfer function between the input layer units and the hidden layer units, and the hyperbolic tangent function was used between the hidden layer units and the output layer units. The developed ANN prognostic models (Figures 3 and 5) were trained and genetically optimized on the training data set. Testing data sets were tested on the models to determine their ability to predict from observed data.

Data Normalization

Before use, the input data was initially normalized and made uniform to avoid overflows of the network due to variations in synaptic weights. Normalization also eliminates errors and missing data (which was 3% of the data set). In order to improve network sensitivity, the data set was normalized into the range (-1, 1) using Equation (4). After prediction the output of the network was transformed and de-normalized back to the original values.

$$\overline{X}_{norm} = 1 - \frac{2(X_{\max} - X_i)}{(X_{\max} - X_{\min})}$$

$$\tag{4}$$

Where: \overline{X}_{norm} = normalized value, X_i = original value, X_{max} = maximum value of X_i and X_{min} = minimum value of X_i

The output of the network must be de-normalized or transformed back to the original values after prediction by making X_i the subject of the above Equation.

Network Training and testing process

Training of the network models was achieved using a Nonlinear Autoregressive with External (Exogenous) Input (NARX) of Neural NetTime Series feature of MATLAB. Alyuda Forecaster software (Alyuda NeuroIntelligence 2.2, http://www.aluyada.com) was used as control software to establish the reliability of MATLAB software in training the network models. Training and testing of the network models were conducted after the network topology was determined and the patterns prepared. The goal of the training process was to obtain a desired output given a set of inputs vectors and synaptic weights. MATLAB Conjugate Gradient

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Descent backpropagation algorithm training algorithm was used to train, validate and test the ANN models for dry and rain seasons prediction. The goal of the learning process was to find the minimum of the mean square error function. Care was taken during the training process to ensure that the network reach the minimum error function and avoid local minima. The learning rate and momentum coefficient parameters were chosen to optimally control the speed of the network during learning and weight updates so as to achieve best convergence. The network was periodically tested on the testing data set in order to prevent overtraining. The network that produced the best optimization results was selected as the best model.

Neural Network Model Building Process

Consider the three-layer network of Figure 2 with input, hidden and output layers denoted as i, j, and k, where i is the input units index, j is the hidden unit index, and k is the output unit index. The McCulloch-Pitts model or activation function (Sengupta, 2009) was adopted as given in Equation (5).

$$A_k = \sum_{j=1}^n x_j w_{kj} \tag{5}$$

Applying bias to the network, Equation (5) becomes:

$$V_{k} = A_{k} + b_{k} = \sum_{j=1}^{n} x_{j} w_{kj} + b_{k}$$
(6)

A general nonlinear sigmoid or logistic transfer function is adopted and applied:

$$Y_k = f(V_k) = \frac{1}{(1 + Exp(-\beta V_k))}$$
(7)

Where A_k is the activation function of the output unit, bk is the bias, x_j is the input of the output unit, w_{kj} is the weight between the hidden units and the output unit, Y_k is the output, V_k is the activation of output unit k (including weighted bias input, b_k) and β is the slope of the activation function (assumed to be 1).



Figure 2: Information Processing in ANN models design process

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$$E = \sum_{k} E^{p} = \frac{1}{2} \sum \left(T_{kq}^{p} - Y_{kq}^{p} \right)^{2}$$
(8)

Where E is the total network error, E^p is the error of the p pattern for the qth neuron, T_{kq}^p is the target (observed) value of the p pattern of the qth neuron, and Y_{kq}^p is the output of the output layer for the p pattern in the qth neuron. Y_{kq}^p is determined by state of the output neuron in the kth unit and the weight, w_{kj} between the mth neuron in the hidden layer units and the qth neuron of the output layer unit. Equation (8) was used to compute the total network error, which is the sum of all the errors of the output layer neurons.

The synaptic weights of the hidden layer units on the output unit are computed by applying the Delta rule as follows:

$$\Delta w_{kj} = \eta \sum_{p} \sum_{k} \left(T_{kq}^{p} - Y_{kq}^{p} \right) \frac{dY_{k}^{p}}{dV_{k}} Y_{jm}$$
⁽⁹⁾

Where Y_{jm} is the output of the hidden layer units, p is the patterns index.

The synaptic weight on the output unit was computed from Equation (9). The weights were thus adjusted in order to minimize the mean square error of the network. The weights adjustment is done using the method of gradient descent (Sengupta, 2009). How much error depends on the change in synaptic weights is computed as:

$$\frac{dE}{dw_{kj}} = \frac{dE}{dY_{kq}^{p}} \frac{dY_{kq}^{p}}{dw_{kj}} = \left(T_{kq}^{p} - Y_{kq}^{p}\right)Y_{k}^{p}(1 - Y_{kq}^{p})Y_{jm}$$
(10)

The weight Δw_{kj} is adjusted and updated using Equation (11) given as:

$$\Delta w_{kj} = \eta \frac{dE}{dw_{kj}} = \frac{dE}{dY_{kq}^{p}} \frac{dY_{kq}^{p}}{dw_{kj}} = \eta \left(T_{kq}^{p} - Y_{kq}^{p}\right) Y_{kq}^{p} (1 - Y_{kq}^{p}) Y_{jm}$$
(11)

The increment in weight update Δw_{ki} for the three layer networks is given as:

. n

$$\Delta w_{kj} = \eta \frac{dE^{p}}{dw_{kj}} = \frac{dE^{p}}{dY_{kq}^{p}} \frac{dY_{kq}}{dV_{kq}} \frac{dV_{kq}}{dY_{jm}} \frac{dY_{jm}}{dV_{jm}} \frac{dV_{jm}}{dw_{kj}} = \eta \left(T_{kq}^{p} - Y_{kq}^{p}\right) Y_{kq}^{p} (1 - Y_{kq}^{p}) . w_{j} \left(1 - Y_{jm}\right) Y_{jm} . Y_{in} + \tau \Delta w_{kj}$$

(12)

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Published by European Centre for Research Training and Development UK (www.eajournals.org) Where Y_{jm} is the output of the mth neuron in the hidden layer, Y_{in} is the output of the nth neuron in the input layer; V_{jm} and V_{kq} are the activation signals of the hidden layer and output layer units respectively; $\tau \Delta w_{kj}$ is the momentum term, τ is the momentum coefficient introduced to reduce rapid fluctuations in weights adjustments and avert oscillation during network training process. η is the training control parameter called learning rate that speeds up convergence while reducing network errors.

Equations (9), (10) and (11) were used to update the synaptic weights of the ANN models. Equation (12) was used to train the ANN predictive models. The developed ANN prognostic models (Figures 3 and 5) were trained and genetically optimized on the training data set. Testing data sets were tested on the models to determine their ability to predict from observed data. The training mean square error is shown in Figure 4.

Model Verification

In order to determine the models' ability to accurately predict future values with minimum network error, the models were trained, validated and tested on the test data. To obtain a good judgment of the model's ability to predict accurately, a new data set was queried on the models.

Sensitivity Analysis

To achieve the aim of building simple forecasting models for the prediction of seasonal atmospheric pollutants, the best subset of input predictor variables were selected in the ANN model building process. Forward Stepwise, backward stepwise elimination and genetic optimization standard input optimization techniques (Elangasinghe et al., 2014) were applied for the optimization of input vectors. Year and Month were considered negligible inputs by Forward Stepwise, while backward stepwise eliminated only RH to give the best network. All the input variables were considered as significant by genetic optimization in making the best predations. Sensitivity analysis was performed to determine the response of the ANN prognostic models to each input vector. Each predictor variable was varied while keeping others constant. This analysis was performed to test the sensitivity of the ANN predicted models to each predictor parameter and to determine the non-linear relationship between each predictor variable and the modeled pollutant concentrations.

RESULTS AND DISCUSSIONS

Results and Findings

Dry season predictive model was found to perform best with Conjugate Gradient Descent algorithm and architecture of **7-5-1** (Figure 3) with learning control parameter η of 0.1 and momentum coefficient of 0.75. While rainy season predictive model performed best with Conjugate Gradient Descent algorithm and architecture of **7-9-1** (Figure 5) with learning control parameter η of 0.2 and momentum coefficient of 0.8. For most of the time, the predicted values were very close to the observed pollutant concentrations both in trend and pattern. It was found that all the developed ANN prognostic models perform absolutely well with prediction accuracy of more than 95%.



Figure 3: Dry Season Design Architecture (7-5-1)





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Figure 5: Rainv Season Design Architecture (7-9-1)

DISCUSSION

Details of ANN design (training/learning) parameters, architectures and network output reports for forecasting of pollutant concentrations in the study area are shown in Table 1. Mean Absolute Errors (MAE), Mean Absolute Related Errors (MARE) and Mean Square Errors (MSE) for each forecasted pollutant are given in Table 1. Time series of predicted versus observed pollutant concentrations for both dry and rainy seasons are shown Figures 6, 7, 9, 10, 12, 13, 15 and 16. The predicted pollutant levels were compared with the measured values to determine the accuracy of the prognostic models in predicting concentrations of air pollutants in the study area. Predicted results compared considerably with observed values with high degree of accuracy. The best fit lines (Figures 8, 11, 14, 17 and 18,) generated between

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observed and predicted values give correlation coefficients and R^2 very close to 1 for both dry and rainy seasons (Table 1). These coefficients of determinations are acceptable as values close to 1.0 are considered to be best fits. Statistically, modeling results further indicated that the relationships between observed and predicted values are highly significant at 95% of confidence level. Hence, the ANN models properly trained with past pollutants data accurately predict air pollutant concentrations in the area. The trend in predicted pollutants indicated that the study area is a major receptor of air pollutants emanating mainly from industrial activities and vehicular exhaust emissions.



Figure 6: Dry Season Observed versus Predicted CH4



Figure 7: Rainy Season Observed versus Predicted CH4

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Figure 8: Dry and Rainy Seasons Best fits of Observed and Predicted CH4



Figure 9: Dry Season Observed versus Predicted CO

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Figure 10: Rainy Season Observed versus Predicted CO



Figure 11: Dry and Rainy seasons Best fits of Observed and Predicted CO

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Figure 12: Dry Season Observed versus Predicted NO₂



Figure 13: Rainy Season Observed versus Predicted NO2



Figure 14: Dry and Rainy Seasons Best fits of Observed and Predicted NO2

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Figure 15: Dry Season Observed versus Predicted SO₂



Figure 16: Rainy Season Observed versus Predicted SO₂



Figure 17: Dry and Rainy Seasons Best fits of Observed and Predicted SO2

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Figure 18: Goodness of fits of seasonal pollutants during network testing

 Table 1: Coefficient of Determination and Correlation Coefficient for observed and predicted pollutant concentrations

DRY SEASON					
	ANN Topology	7 - 5 - 1			
Pollutant	Correlation	Coefficient of	MAE	MARE	MSE
	Coefficient, R	Determination, R ²	$(\mu g/m^3)$	$(\mu g/m^3)$	$(\mu g/m^3)$
CH ₄	0.9973	0.9946	2.754056	0.025226	8.9x10 ⁻⁸ .
CO	0.9959	0.9918	1.100008	0.019322	8.92x10 ⁻¹⁰
NO ₂	0.9999	0.9998	0.257015	0.004476	1.6x10 ⁻⁸
SO ₂	0.9961	0.9921			
RAINY SEASON					
	ANN Topology	7 - 9 - 1			
CH ₄	0.9987	0.9974	2.994053	0.030234	5.75x10 ⁻⁸

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Figure 19: Network error output response during network

CONCLUSION

The relationships between observed and predicted values are highly significant at 95% of confidence level for all models. The best fit lines generated between observed and predicted values give correlation coefficient of determination very close to 1 (R^2 greater than 0.99) for dry season and rainy season models. Results indicated that the developed ANN prognostic models accurately captured the non-linear relationships between pollutant concentrations and meteorological predictor variables that exist in the area. Study indicated that air pollutant concentrations in Eleme region have nonlinear composite relationship with industrial, vehicular exhaust emissions, and meteorological factors. All of which were used as input variables to the neural networks to predict seasonal concentrations of air pollutants in the region. Prediction results also showed that wind speeds and directions are the parameters that mostly influence pollutants concentrations in the ambient air of the study area.

Significance of the study to research and practice (contribution to knowledge)

The study which was mainly empirical in nature revealed that ANN model when properly trained with historical air quality and meteorological data can accurately forecast air pollutant concentrations in an area.

In addition, the study explored the application of Artificial Neural Networks as a predictive tool to effectively model the dynamic nonlinear relationships between air pollutants and meteorological variables in an area.

The study further provided effective techniques for the prediction of air pollutants concentrations in the area, thus serves as useful tools in environmental impact assessment (EIA) studies for the prediction of air quality impacts of a new development in the study area.

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RECOMMENDATION

Further research study is needed to compare ANN model with other modeling approaches such as with multiple regression models for the prediction of air pollutants in the study area.

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