

## Development of Models for the Prediction of the Level of Concentration of Gas Pollutants in Utorogu Gas Plant in Delta State, Nigeria

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### Abstract

In adequate modelling of process parameters for the prediction of the level of concentration of gaseous pollutants in gas flaring during the extraction of crude oil poses great challenges to human health. This study focused on the development of models for the prediction of the level of concentration of gas pollutants in Utorogu gas plant in Delta State, Nigeria. Aeroqual multi-parameter environmental monitor (series 500), was employed to monitor the concentrations of volatile organic compounds (VOCs), oxides of nitrogen (NO<sub>2</sub>), oxides of Sulphur (SO<sub>2</sub>), ozone (O<sub>3</sub>) and methane (CH<sub>4</sub>). The concentrations of the particulate matter (PM<sub>2.5</sub>) of these gases were obtained at each monitoring point on daily bases for a period of twelve weeks using Aerocet-531 SPM meter. Sky master thermo anemometer (SM-28) was used to obtain the important climatic variables (wind speed, atmospheric pressure, ambient temperature and relative humidity) which affect the dispersion of gaseous pollutants. The maximum concentration of each monitored gaseous pollutant during the twelve weeks (12) monitoring period was selected and recorded for data processing. In this study, mathematical models were developed for predicting each gaseous pollutant such as volatile organic compounds (VOCs), oxides of nitrogen (NO<sub>2</sub>), oxides of Sulphur (SO<sub>2</sub>), ozone (O<sub>3</sub>) and methane (CH<sub>4</sub>). The curve fitting tool in Matrix Laboratory {MATLAB (2016a)} was employed to select models and to model the exact mathematical relationship between the pollutant concentrations and the flare distance; then the pollutants concentrations were predicted beyond the experimental distance of 500m from the flare point, the models were validated using coefficient of determination (R<sup>2</sup>), and root mean square error (RMSE). Based on the parameters, it was observed that the Fourier function model had the lowest root mean square error value of 0.7694 and coefficient of determination r<sup>2</sup> value of 0.9927. The results obtained satisfy good model predictability.

## 1. Introduction

Global flaring and venting of petroleum associated gas is a significant source of greenhouse gas emissions and airborne contaminants that have proven difficult to mitigate over the years. Douabul et al [1] carried out a study on gaseous pollutants in Basra city, Iraq. Their study was aimed at detecting the present levels and distribution of CO, CO<sub>2</sub>, SO<sub>2</sub>, NO<sub>2</sub> and total hydrocarbons gases (HC<sub>s</sub>) produced from different industrial plants in Basra city, Iraq. Seven stations were chosen in Basra city – Al – Qurna, Al – Deer, Garmatt Ali, Al - Ashar, Abu Al-Khaseeb, Al- Seeba and Al-

Faw. These stations were selected in order to monitor the concentrations of CO, CO<sub>2</sub>, SO<sub>2</sub>, NO<sub>2</sub> and HCs in the ambient air during the winter and summer months of 2011. The products (pollutants) from burning of fossil fuels such as gas, oil, coal and wood affect the earth, buildings, water and air, resulting in fog, smog and global warming, which deteriorate vegetation, forests, and even human health [2, 3, 4, 5].

The increasing population and industrial growth as well as commercial operations in the Niger Delta area due mainly to oil and gas operations and processes brings to the fore the need for air pollution monitoring through assessment of pollutants concentrations, modelling of dispersion and prediction of pollutants spread, to help regulate and manage environmental impacts. Dispersion modelling is undertaken in order to predict the concentration and spread of pollutants [6]. Grigoras et al [7] researched on air pollution dispersion modelling in a polluted industrial area of complex terrain in Romania (the surveyed North-Western part of Romania). They made use of pollutants emitted by non-ferrous metal industrial facilities existing in Baia Mare area and the emissions from other local anthropic activities such as residential heating, traffic and dump heaps. The air pollution modelling was done by using local emissions inventories drafted and validated for 2008 by WESTAGEM and by real-time monitoring results of emissions from lead smelting from lead concentrates and metallurgical residue with lead content. They performed atmospheric pollutants concentrations assessment for SO<sub>2</sub>, particulate matters PM<sub>10</sub> and lead (Pb), referencing to the limits for allowable concentration of pollutants in the ambient air by using 1-hourly and daily maximum concentration values and average concentration values for the air pollutants originated from local sources. The atmospheric emissions assessment was made considering temporal variations of the activities that lead to the time variation of emissions. Gorai et al, [8] carried out the development of Partial Least Squares Path Model (PLS-PM) to understand the role of precursors on ground level ozone concentration in Gulfport, Mississippi, USA. Their model revealed that Photochemical Reaction Catalyst (PRC) had significant direct impact on ground level ozone concentration, but very small overall effect since PRC had significant indirect effect via meteorological factor. They concluded that the direct and indirect effects have made PRC to have the weakest effect on ground level ozone. Yannarwar et al [9] had the opinion that dispersion models are used to predict the fate of pollutants after they are released into the atmosphere. The goal of air quality dispersion modelling is to estimate a pollutant's concentration at a point downwind of one or more emission sources [10]. The first step in the modelling and prediction of ground level concentration of gaseous pollutants is to understand the exact mathematical relationship between the pollutant concentrations and the distance from flow station at normal environmental stability and wind speed.

This study focused on the development of models for the prediction of the level of concentration of gas pollutants in Utorogu gas plant in Delta State, Nigeria.

## **2. Methodology**

This study focused on the development of models for the prediction of the level of concentration of gas pollutants in Utorogu gas plant in Delta state, Nigeria. OML 34 in the Niger Delta area of Nigeria, was carried out using the following steps: - 1.Data acquisition and processing, 2. Computation of pollution standard index (PSI), 3. Simulation of environmental condition based on the computed PSI, 4. Geo-statistical analysis of the data, 5. Modelling and Data analysis concentration of pollutants, 2. Model validation.

The Utorogu facilities are located at Ughelli South Local Government Area. OML 34 is of utmost strategic importance to Nigeria and the West African sub-region, as a major supplier of gas for electricity generation in Nigeria. It also feeds gas through the West African Gas Pipeline (WAGP) to neighbouring countries (Niger Delta Western Doc., 2014).

The Utorogu facility is very strategic and supplies more than 80percent of gas used in Nigeria. It is the number one gas processing plant in the whole of West Africa (Utorogu HSE department).

Utorogu oil field which is located in OML34 is about 20km South East of Warri and 7km to the south of Ughelli West field. The field was discovered in 1964 and till date a total of 33 wells have been drilled in the field, comprising of 9 Non Associated Gas (NAG) wells, 19 oil wells and 5 abandoned wells (NPDC, 2013). The facility is bounded by three communities namely Otu -Jeremi, Otor – Udu and Iwhreka communities. It produces an average of 205mmscf of gas daily (an equivalent of 786MW of electricity).

## 2.2. Data Acquisition and Processing

In this study, six (6) gaseous pollutants namely; volatile organic compounds (VOCs), methane (CH<sub>4</sub>), nitrogen dioxide (NO<sub>2</sub>), particulate matter (PM<sub>2.5</sub>), ozone (O<sub>3</sub>) and Sulphur dioxide (SO<sub>2</sub>) were monitored on daily bases for a period of twelve (12) weeks and data were transformed into weekly maximum concentration. To select the maximum concentration of the pollutant at each sampling point within the entire period of experimentation for the modelling, extreme value statistics was carried out using the data analysis tool pack of Microsoft Excel 2010. The mandatory frequency of sampling for the gaseous point source emission monitoring shall be weekly but where appropriate, a continuous emission monitoring system approved by the Director of Petroleum Resources (DPR) shall be utilized [11]. According to the descriptive statistics of data stated in Environmental Guidelines and Standards which stated that gaseous point sources emission monitoring shall be at distances of 200m intervals away from the installation along the direction of the prevailing wind [8]. Based on this and to determine the trend, the monitoring locations were established and the range of measurement was 60m to 500m away from the flare point at each station using a spacing distance of 60m, 80m, 100m, 150m, 200m, 250m, 300m, 350m, 400m, 450m and 500m from the flare point. Standard gaseous pollutants monitoring equipment used such as Gas monitor, SPM meter, Anemometer and GPS receiver were calibrated and used as follows. Aeroqual multi-parameter environmental monitor (series 500), having different gas sensors, was employed to monitor the concentration of volatile organic compounds (VOCs), oxides of nitrogen (NO<sub>2</sub>), oxides of sulphur (SO<sub>2</sub>), ozone (O<sub>3</sub>) and methane (CH<sub>4</sub>). The concentrations of these gases were obtained at monitoring location of Ughelli West flow station on daily bases for a period of twelve weeks. Aerocet-531 SPM meter was used to monitor the concentration of particulate matter (PM<sub>2.5</sub>) at the location on daily bases for a period of twelve weeks. Sky master thermo anemometer (SM-28) was used to obtain the important climatic variables (wind speed, atmospheric pressure, ambient temperature and relative humidity) which affect the dispersion of gaseous pollutants. An updated map of the OML 34 was sourced from Shell Petroleum Development Corporation (SPDC), Delta State, Nigeria was used for this study. The Global Positioning System (GPS) receivers and point positioning techniques were used to obtain the geographical coordinates at each monitoring location in the study area. The coordinates were converted to decimal degrees format using the Universal Traverse Mercator (UTM) software version 1.0. The maximum concentration of each monitored pollutant during the twelve weeks monitoring period was selected and recorded for data processing. The data obtained in parts per million (ppm) were processed by converting the pollutants concentrations from ppm to mg/m<sup>3</sup> or µg/m<sup>3</sup>, using the model presented below (Equation 1). This is because the pollutants hourly or daily or annually concentrations are measured in µg/m<sup>3</sup> [14, 15].

$$\text{Concentration in mg/m}^3 \text{ or } \mu\text{g/m}^3 = \frac{\text{conc. (ppm)} \times \text{MW (g/mole)}}{\text{MV (L)}} \quad (1)$$

where:

Conc. = Concentration of pollutant

mg/m<sup>3</sup> = milligram per cubic meter = 10<sup>-3</sup>g/m<sup>3</sup>

µg/m<sup>3</sup> = microgram per cubic meter = 10<sup>-6</sup>g/m<sup>3</sup>

### 3. Results and Discussion

Table 1 show the input parameter of the flow station presented to the neural network for validation of field data. The input parameters include; the sampling distance from flow station, wind speed, atmospheric pressure, ambient temperature and relative humidity. These parameters were selected because they form the critical climatic variables that affects the dispersion of gaseous pollutants.

**Table 1: Input Parameters for Utorogu Flow Station**

Sampling Distance (m)	Wind Speed (m/s)	Atm. Pressure (mmHg)	Ambient Temperature (deg C)	Relative Humidity (%)
60	1.85	1011	39.8	88.1
80	2.33	1011	37.6	90.2
100	2.56	1011	37.2	87.2
150	2.59	1011	35.7	92.3
200	2.66	1011	34.5	82.7
250	2.67	1011	30.5	87.4
300	2.78	1011	32.5	91.4
350	2.83	1011	31.4	83.6
400	2.91	1011	30.5	81.5
450	2.92	1011	32.1	72.8
500	3.34	1011	29.7	73.9

#### 3.1 Validation of Field Data using Pythia (Neural Net Software)

The field data from the study locations were validated using artificial neural network designer software (Pythia). The field data were validated to evaluate the adequacy of the field data for use in air pollution modelling. The artificial neural network is trained to prevent it from memorizing data presented before it. Using the training data which is the field data collected, Pythia employed the evolutionary optimizer to search the neural network topology that best understand the input and output data presented for training, and the back propagation algorithm to produce the network. The reason for training is for the model to understand the data obtained and the condition under which they were obtained, so as to be able to make accurate correction. The criteria for selecting the best topology are the square of the deviation between the observed output and the predicted output coupled with the fitness accuracy. Topology with the least square deviation having 100% fitness was regarded as the best for the task. Pythia employs the back propagation algorithm to produce the network. During the training phase, the actual output of the network was compared with the experimental output and the error propagated back towards the input of the network. The network parameter which is the input is also called the “weight”.

Based on the conditions of Table 2, the evolutionary optimization was performed to obtain the best neural network topology that best fits the input and output data for Utorogu. The evolutionary optimization is presented in Table 3.

From Table 3, it was observed that a minimum of 12 neurons was needed to obtain an optimum topology of 5, 6, 6 having a fitness of 100% with a square deviation of 0.001055 for Utorogu. Based on these parameters, optimum neural network architecture were produced as shown in Table 3.

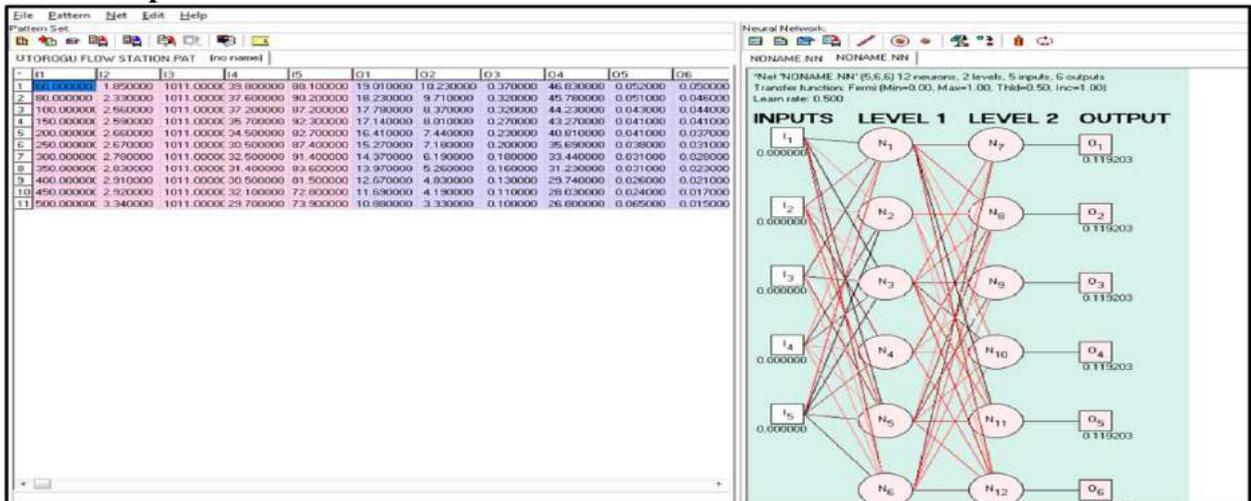
**Table 2: Condition for best performance**



**Table 3: Evolutionary Optimization for Selecting Best Network Topology**

No	Topology	Neurons	$\emptyset$ dev <sup>2</sup>	* dev <sup>2</sup>	Fitness
31	5,6,7,6,6,6,6	31	0.000305	0.000868	100.00000
32	5,6,6,6,6,6,6	30	0.000524	0.001431	100.00000
33	5,6,6,6,6,6,6	30	0.000479	0.000941	100.00000
34	5,6,6,6,6,6	24	0.000588	0.002221	100.00000
35	5,6,6,6,6	18	0.000765	0.002121	100.00000
36	5,6,5,5,6	17	0.001469	0.004796	89.36437
37	5,7,6	13	0.000805	0.001918	100.00000
38	5,6,6	12	0.002072	0.007394	82.75606
39	5,6,5,5,6	17	0.000609	0.001953	100.00000
40	5,6,6	12	0.001338	0.005047	91.58726
41	5,6,5,5,6	17	0.001399	0.004289	90.48680
42	5,5,5,5,5,6	21	0.000546	0.001897	100.00000
43	5,5,5,4,6	20	0.001216	0.004123	94.07202
44	5,5,5,4,4,6	24	0.000751	0.002169	100.00000
45	5,5,5,4,4,6	24	0.014059	0.141193	59.31273
46	5,5,4,3,6	18	0.001790	0.004660	85.29146
47	5,5,4,3,6	18	0.003841	0.011044	75.34487
48	5,4,3,6	13	0.003315	0.015837	76.72220
49	5,4,4,6	14	0.003555	0.015841	76.04195

**Table 4: Optimum Neural Network Architecture**



Using the network of Table 4, the Repro Pattern Set function of the Pythia program was then activated to predict the pollutants concentrations based on the input and output data from Ughelli West flow stations. Reliability plots of the field data and the ANN predicted data were obtained to test the correlation between the field data and the ANN predicted data.

### 3.2 Sensitivity analysis of ANN

A sensitivity analysis was performed to allow the network assign weight to each input variable on the bases of their significant contribution so as to determine the input parameter that contributes mostly to variation in the pollutant concentrations around the study locations.

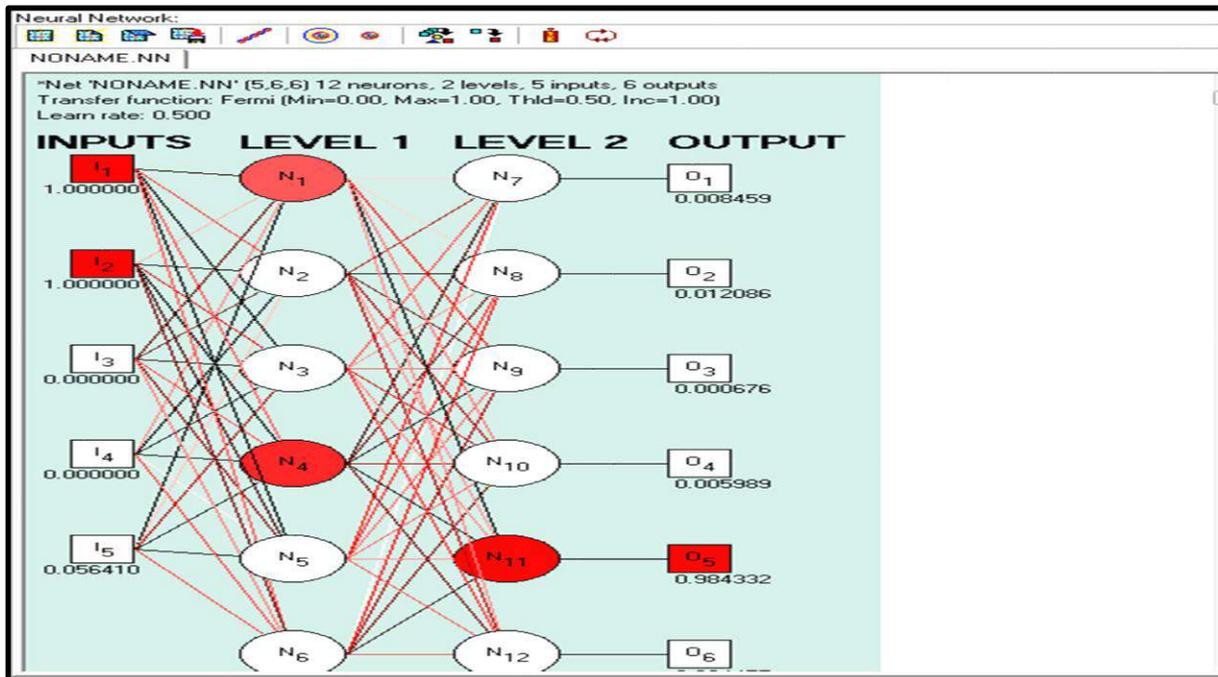


Figure 3: Sensitivity Analysis of ANN (Utorogu)

Table 5: Calculated model parameters for VOC (Utorogu)

Model	R-Square	Adj. R-Square	SSE	RMSE
Linear polynomial	0.9951	0.9946	0.3674	0.223
Quadratic Polynomial	0.9952	0.9946	0.3606	0.2123
Exponential	0.9892	0.9880	0.814	0.3007
Gaussian	0.9948	0.9931	0.3606	0.227
Fourier	0.9952	0.9931	0.3606	0.227

Based on the parameters of Table 5, it was observed that the Quadratic polynomial model had the lowest root mean square error value of 0.2123 and coefficient of determination  $R^2$  value of 0.9952.

**Table 6: Quadratic polynomial function for VOCs versus sampling distance**

```

Linear model Poly2:
  f(x) = p1*x^2 + p2*x + p3
Coefficients (with 95% confidence bounds):
  p1 = -1.421e-006 (-9.909e-006, 7.067e-006)
  p2 =      -0.017 (-0.02171, -0.0123)
  p3 =      19.74 (19.2, 20.27)
    
```

where;

f(x): VOCs concentration ( $\mu\text{g}/\text{m}^3$ )

x: Sampling distance (m)

Using the quadratic polynomial function of Table 6, the concentration of VOCs was projected to a sampling distance of 1500m at 95% confidence level.

**Table 7: Calculated Model Parameters for PM<sub>2.5</sub> (Utorogu)**

Model	R-Square	Adj. R-Square	SSE	RMSE
Linear polynomial	0.9792	0.9769	11.74	1.142
Quadratic Polynomial	0.9870	0.9837	7.347	0.9583
Exponential	0.9863	0.9848	7.745	0.9276
Gaussian	0.9863	0.9829	7.743	0.9838
Fourier	0.9927	0.9895	4.144	0.7694

Based on the parameters of Table 7, it was observed that the Fourier function model had the lowest root mean square error value of 0.7694 and coefficient of determination  $r^2$  value of 0.9927.

**Table 8: Fourier function model for PM<sub>2.5</sub> versus sampling distance**

```

General model Fourier1:
  f(x) = a0 + a1*cos(x*w) + b1*sin(x*w)
Coefficients (with 95% confidence bounds):
  a0 =      37.75 (35.1, 40.41)
  a1 =      10.3 (9.049, 11.56)
  b1 =      -2.663 (-12.4, 7.071)
  w =      0.005637 (0.003057, 0.008217)
    
```

where;

f(x): particulate matter concentration ( $\mu\text{g}/\text{m}^3$ )

x: Sampling distance (m)

Using the Fourier function model of Table 8, the concentration of particulate matter was projected to a sampling distance of 1500m at 95% confidence level

### 3.3 Selection of Trend Analysis Model using Normality Test

In order to check the distribution of the field data, normality test was also employed to select the most appropriate model for trend detection and estimation. If data are linearly distributed then parametric model (linear regression model) such as least square linear regression will be most appropriate for trend detection and estimation otherwise non-parametric model such as Mann-Kendall and Thiel Sen's slope estimation will be employed for detection and estimation of trend in the data. To test if the field data followed a normal distribution, histogram plot and normal Q-Q plot

was employed. For normality, the histogram must be assumed to have a bell shape configuration and the data points on the normal Q-Q plot must follow the 45° center line else it will be concluded that the data are not normally distributed. Consequently, non-parametric analysis will be needed to determine the occurrence of trend in the data [6]. The practical implication of trend detection is to know exactly what is happening around the study location.

### 3.4 Analysis of Seasonal Variability using Autocorrelation Function

Accurate analysis of data collected over time requires that seasonality analysis to check for the presence of seasonal variability be performed [6]. To estimate the degree of seasonality present in the field data collected from the three flow stations, autocorrelation plot was employed. A statistical software EViews version 9.0 was employed to generate the correlogram.

### 3.5 Trend Estimation using Non-Parametric Analysis

Since it was established that the field data collected from Ughelli West flow station are not normally distributed by exhibiting some characteristics that is occasioned by the presence of trend and seasonal variability, then non parametric analysis became the most suitable method to estimate the presence of trend in the data. Mann- Kendall trend test was therefore carried out by plotting the pollutants concentration against generated index.

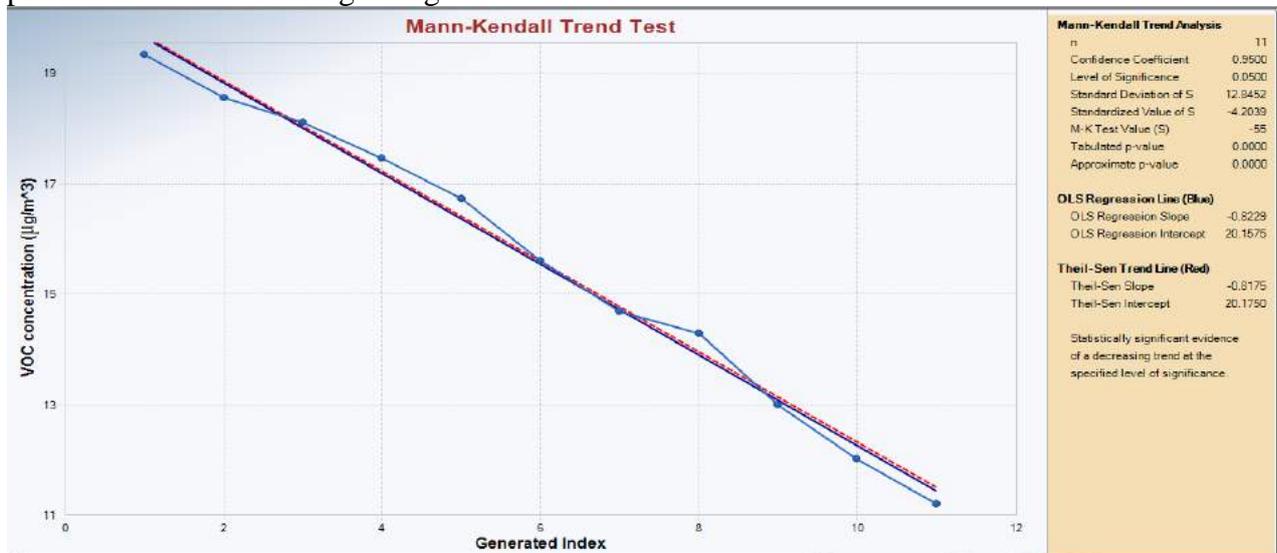


Figure 4: Mann-Kendall Trend Test of VOCs Data from Utorogu Flow Station

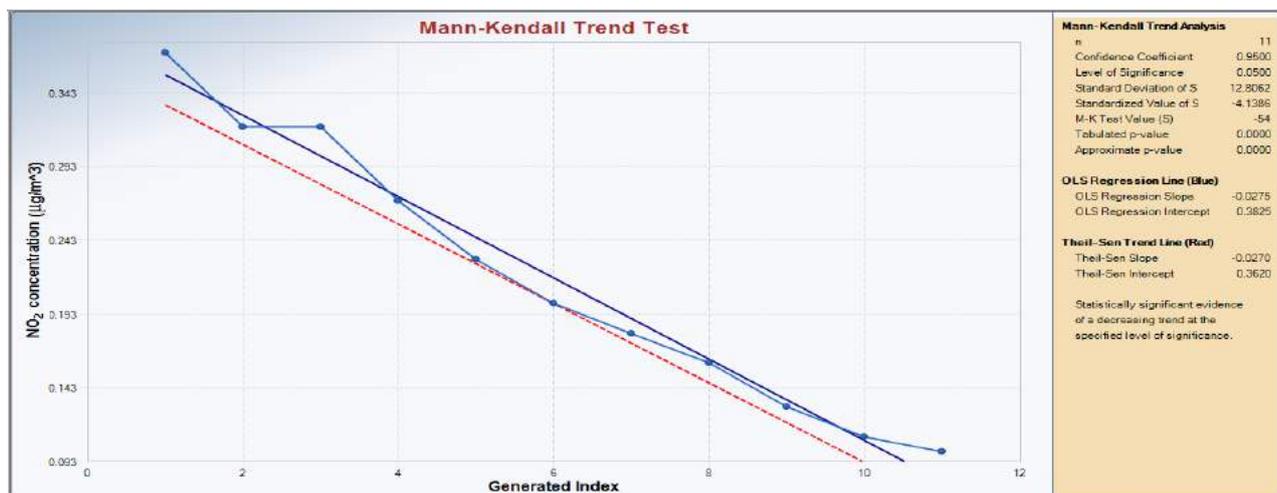


Figure 5: Mann-Kendall trend Test of NO<sub>2</sub> Data from Utorogu Flow Station

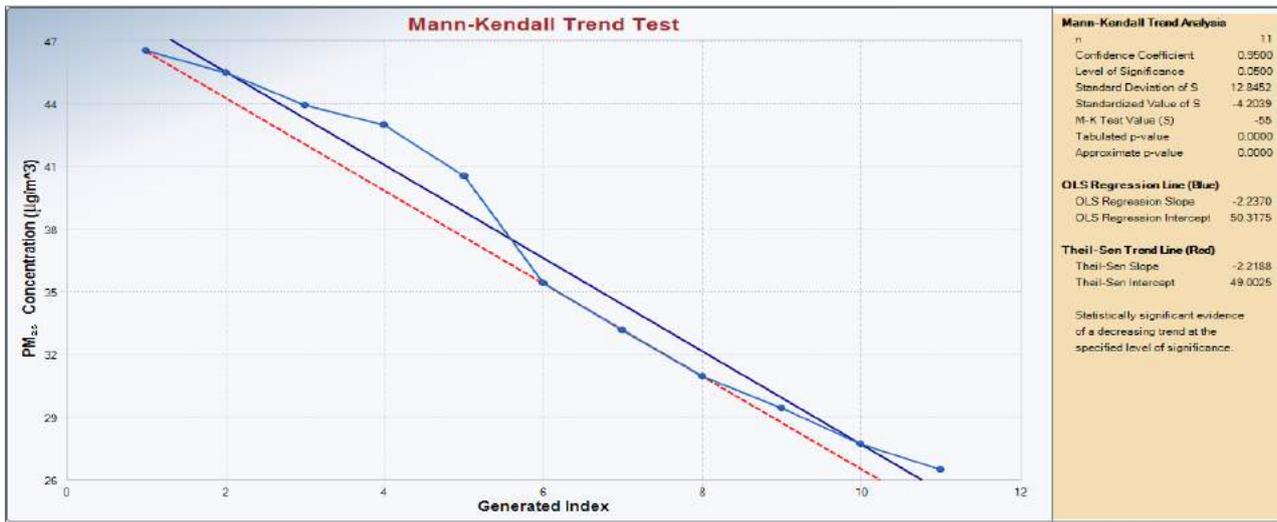


Figure 6: Mann-Kendall Trend Test of PM<sub>2.5</sub> Data from Utorogu Flow Station



Figure 7: Mann-Kendall Trend Test of Ozone Data from Utorogu Flow Station

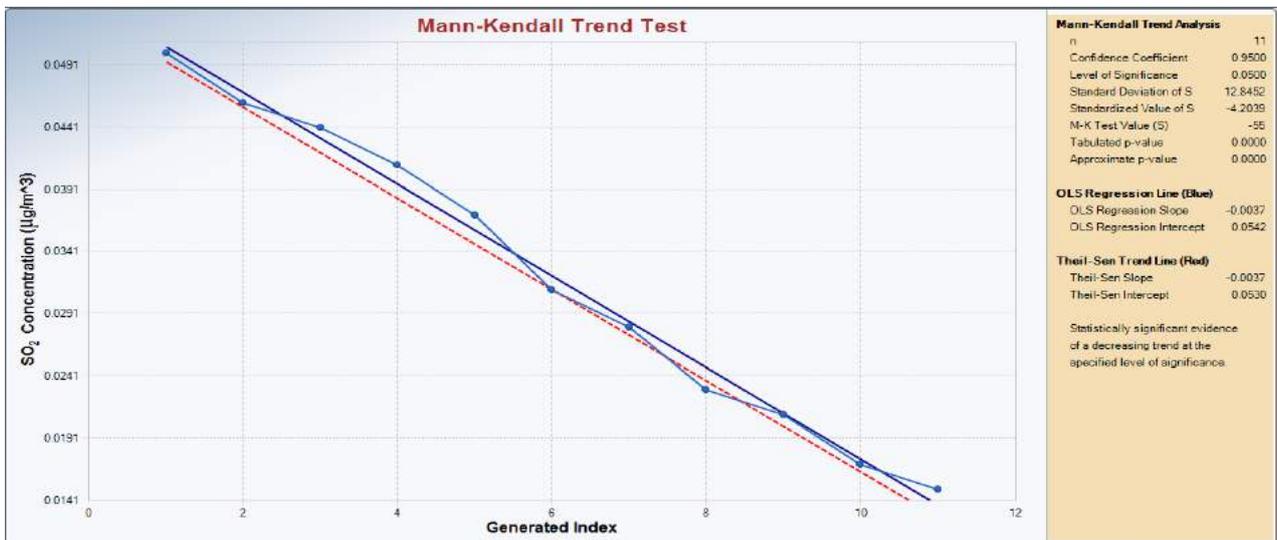


Figure 8: Mann-Kendall Trend Test of SO<sub>2</sub> Data from Utorogu Flow Station

### 3.6 Geo-statistical Analysis of the Data

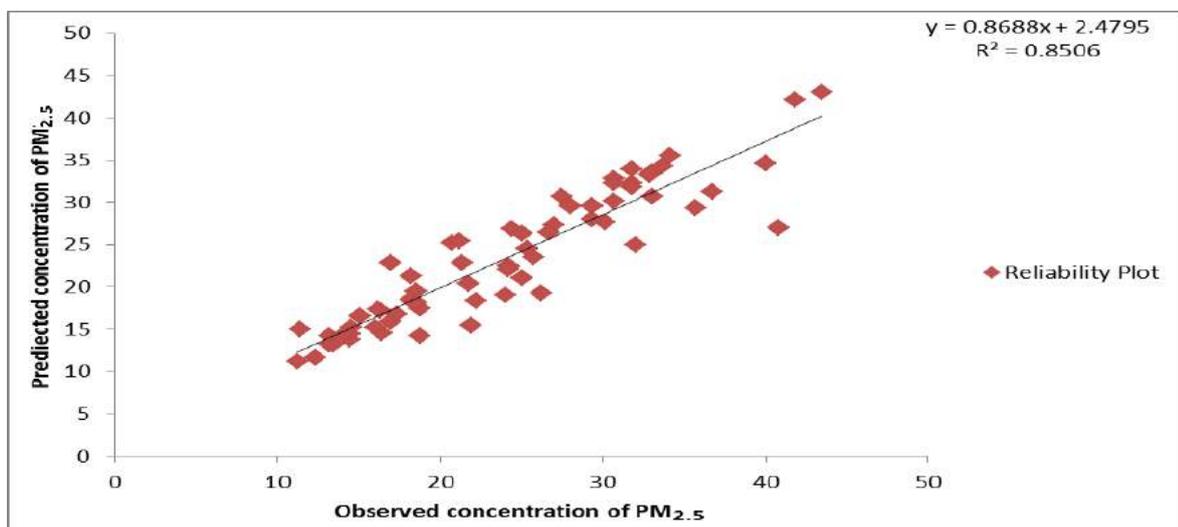
Detailed geo-statistical analysis of the data acquired from the three locations was carried out using ArcGIS 10.4.1. Geospatial modelling was employed to generate the prediction maps which show the distribution of the pollutants around the study locations. The prediction map is a pictorial presentation of the pollutant concentrations in space. The input parameters for the modelling were the rectangular coordinates of each sampling point and the concentration of the different pollutants measured, namely: volatile organic compounds (VOCs), methane (CH<sub>4</sub>), nitrogen dioxide (NO<sub>2</sub>), particulate matter (PM<sub>2.5</sub>), ozone (O<sub>3</sub>) and Sulphur dioxide (SO<sub>2</sub>). Several geostatistical methods exist for geospatial modelling but the kriging method for point source pollution was employed.

### 3.7 Network Testing/Validation

Cross validation data representing 25% of the total input data was introduced to monitor the training process and to prevent the network from memorizing the input data while the remaining 15% was employed to test the performance of the trained network [4].

**Table 10: Utorogu Network Testing using Different Sets of Input Parameters**

Sampling Distance (m)	Wind Speed (m/s)	Atm. Pressure (mmHg)	Ambient Temperature (deg C)	Relative Humidity (%)	Predicted PM <sub>2.5</sub>
600	3.44	1255	31.4	89.6	23.42117115
650	3.76	1023	32.3	87.3	33.69709548
700	4.89	1015	33.8	99.2	10.62684594
750	5.6	1116	28.2	94.2	14.12509455
800	4.33	1222	29.7	83.8	17.87388326
850	6.43	1033	34.8	90.1	15.67482703
900	5.89	1035	36.3	75.4	33.55783796
950	2.33	1010	31.8	78.8	16.36324347
1000	4.44	1056	30.9	88.2	18.72096977



**Figure 9: Regression plot of observed versus predicted concentration of PM<sub>2.5</sub>**

Based on the calculated coefficient of determination ( $R^2$ ) as observed in Figure 9, the trained network was then employed to predict the concentration of  $PM_{2.5}$  around **Utorogu** flow station as presented in Table 7.

### 3.8 Computation of Pollution Standard Index (PSI)

The PSI values for PM,  $O_3$  and  $SO_2$  were computed and checked against the units in the standard Table. Computation of Pollution standard index (PSI) was done to determine the status of the environment within and around the study location. PSI gives reliable information on whether the environment is good, moderate, healthy, unhealthy, very unhealthy or hazardous [10]. The computed PSI values of the gaseous pollutants were compared and the pollutant with the highest PSI value was used to describe the air quality and environmental status as shown in Figure 4-8.

### 2.9 Results of ANN prediction

Table 11 shows ANN Predicted values of  $PM_{2.5}$  in the study locations

**Table 11: ANN Predicted values of  $PM_{2.5}$  in the study locations**

Sampling Distance (m)	Utorogu predicted
600	23.42117
650	33.69710
700	10.62685
750	14.12509
800	17.87388
850	15.67482
900	33.55783
950	16.36324
1000	18.72097

The results of the ANN predicted  $PM_{2.5}$  concentrations in all the study locations showed that wind speed is a critical factor to the concentration of particulate matter at each sampling distance. This is responsible for the variation in the concentration at the various sampling distance. This is a confirmation that air pollution is not boundary restricted and hence it is a critical global problem. Despite the wind effect in the variability in particulate matter concentration, it is still below the DPR/FMENV permissive limit (Table 11).

### 4. Conclusion

The development of models for the prediction of the level of concentration of gas pollutants in Utorogu gas plant in Delta state has been achieved. The models developed were validated using coefficient of determination and mean square error. The values obtained from the validation show that good predictability of the model terms. Based on the parameters, it was observed that the Fourier

function model had the lowest root mean square error value of 0.7694 and coefficient of determination  $r^2$  value of 0.9927.

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