

## ORIGINAL ARTICLE

# Modeling Ground Level Ozone (O<sub>3</sub>) of Air Pollution Using Regression Technique

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## ABSTRACT

**Introduction:** Ground-level ozone (O<sub>3</sub>) was a secondary pollutant involving several types of reactions arising from complicated atmospheric chemistry. This research utilized statistical equations to discern the complex influence of meteorological parameters and precursor contaminants influencing O<sub>3</sub> chemistry and concentrations. The goal of this study was to predict ozone (O<sub>3</sub>) concentrations in Nilai, Negeri Sembilan. **Methods:** Data were collected from 1 January 2016 until 31 December 2018 that including ozone (O<sub>3</sub>), nitrogen oxide (NO<sub>x</sub>), nitric oxide (NO), sulphur dioxide (SO<sub>2</sub>), nitrogen dioxide (NO<sub>2</sub>), carbon monoxide (CO), temperature, and relative humidity (RH). The data were analyzed by using Multiple Linear Regression (MLR) in predicting the next hours of O<sub>3</sub> concentration. **Results:** O<sub>3</sub> concentration reached its peak during 15:00 hours and lower at night time (20:00 hours) due to the absence of sunlight and redox reactions. There exists strong significant correlation between O<sub>3</sub> and temperature (r= 0.729, p<0.01), relative humidity (r= -0.732, p<0.01), NO<sub>x</sub> (r= -0.654, p<0.01), NO (r= -0.630, p<0.01) and NO<sub>2</sub> (r= -0.535, p<0.01). Meanwhile, MLR models executed high accuracy for O<sub>3,t+1</sub> (R<sup>2</sup>= 0.5565), O<sub>3,t+2</sub> (R<sup>2</sup>= 0.5326) and O<sub>3,t+3</sub> (R<sup>2</sup>= 0.5197). **Conclusion:** In conclusion, the MLR model is suitable for the next hours O<sub>3</sub> concentration prediction. *Malaysian Journal of Medicine and Health Sciences* (2022) 18(8):97-103. doi:10.47836/mjmhs18.8.14

**Keywords:** Ozone, Regression, Correlation, Ozone Precursor, Prediction

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## INTRODUCTION

In a total of air volume, a trace gas known as ozone (O<sub>3</sub>) comprises of less than 0.001 percent which critically needed for the survival of life on the earth. Two ozone layers are imposed known as stratospheric and tropospheric. The protection from harmful ultraviolet solar rays was protected by stratospheric layer and the latter known as bad ozone formed in the tropospheric

layer (1). Regardless of location, high ozone concentrations might occur especially in the urban area as a result of horizontal transport. Moreover, vertical transport played an important role for the increment of ozone concentrations as investigated in Portugal (2, 3). The detrimental impact of surface ozone on people was determined and documented (4-6). Ozone is created during the photochemical process among the ozone precursors of nitrogen oxides (NO<sub>x</sub>) and volatile organic compound (VOC). In specific, precursors were emitted from anthropogenic sources, and certain VOC has emitted from plant-based biogenic materials. The rise in O<sub>3</sub> was responsible for morbidity and death in humans. In addition, it facilitates short-term effects of ventilation and cardiovascular system issues and breathing death,

and asthmatic problems. Furthermore, high ozone concentration harmed the ecosystem in our environment which including the crop stunting, ecology problem and species threatened. In addition, it also explains why the global atmosphere is adapting to our environment (7).

Machine learning models were developed in a short period of time to improve the accuracy of general environmental prediction models. The ozone concentrations prediction models generally adopted the statistical modeling approach which uses the empirical data. The models combined weather parameters such as wind speed, relative humidity, ambient temperature, and solar radiation, as well as gaseous factors such as methane, carbon monoxide, and nitrogen oxide precursor gases (8). These large number of parameters are suitable to feed into the Multiple Linear Regression (MLR), which very popular statistical model used for the empirical data. MLR was simple and easy to compute, leading to better and commonly used mathematical modelling to explain the underlying influencing factors of O<sub>3</sub> variation (9). Training of models for the prediction of ozone concentrations largely depending on the multivariate statistical performances of the MLR (10). The performance itself depends on the variability of the inserted input. The predictive performance of the developed models are assessed using the performance indicators. The performance indicators comprises of error and accuracy measure such as Mean Square Error (MSE) and Coefficient of Determination (R<sup>2</sup>). A smaller MSE has indicated higher model goodness of fit. A closer R<sup>2</sup> value to 1.0 indicated higher model goodness of fit.

**MATERIALS AND METHODS**

**Study area and data acquisition**

Data were collected at one of Air Quality Monitoring Stations (AQMS) at Nilai, Negeri Sembilan. The sources at the study area are mainly came from the domestic fuel burning and motor vehicles which have significant impact to the atmosphere came from human activities. Meteorology and human activity combined to raise pollution levels in the study area. Period of study inclusively taken for three years from 2016 to 2018. The data set was acquired from Malaysian Department of Environment (DOE). The data were available every 1-hour average. Parameters included ozone concentration, nitrogen oxides, nitric oxide (NO), sulfur dioxide (SO<sub>2</sub>), nitrogen dioxide (NO<sub>2</sub>), carbon monoxide (CO), temperature (T), and relative humidity (RH) were plotted by using a line graph to compare the trend with New Ambient Air Quality Standard (NAAQS.) The value in the dataset may be missing for a variety of reasons. All the missing records were omitted from this study in order to reduce the risk of bias. The dataset was used to develop models 70% and the remaining 30% for validation.

**Data analysis**

The data are used for the development of statistical model utilizing the MLR. The data collected were used to calculate the descriptive statistics for mean, median, mode, sample variance, standard deviation, maximum, minimum, skewness, and kurtosis value to determine the trend of ozone by using a line graph to compare with NAAQS. MLR research leads to a deeper and commonly used interpretation of the underlying driving factors of O<sub>3</sub> heterogeneity by statistical simulation through quick and fast computation. Future concentrations of O<sub>3</sub> were important for prediction, since effective steps may be suggested by the local authority for any suitable preventive measures and increase the quality of the air (9). The model of with multiple parameters MLR is shown in Equation (1).

$$Y = \beta_0 + \sum_i \beta_i x_i + \varepsilon_i \tag{1}$$

Where,

- x<sub>i</sub> = the explanatory variable of i (or independent variable)
- y = the dependent variable
- β<sub>i</sub> = the regression coefficient
- ε<sub>i</sub> = the residual

The decision on selection of best-fitted MLR models were used the concept of error and accuracy. Error measures used are Root Mean Square Error (RMSE) and Normalized Absolute Error (NAE), while the accuracy measures used are R<sup>2</sup> and Prediction Accuracy (PA). The error values near to zero were considered as the best model, and for the accuracy must near to one. The specification of performance metrics used in this analysis was illustrated in Equations (2) – Equation (5) (11).

- (a) Root Mean Square Error

$$RMSE = \left( \frac{1}{n} \sum_{i=1}^n [P_i - O_i]^2 \right)^{1/2} \tag{2}$$

- (b) Normalized Absolute Error

$$NAE = \frac{\sum_{i=1}^n |P_i - O_i|}{\sum_{i=1}^n O_i} \tag{3}$$

- (c) Prediction of Accuracy

$$PA = \sum_{i=1}^n \frac{[P_i - \bar{P}]}{(n-1) S_{pred} S_{Obs}} \tag{4}$$

- (d) Coefficient of Determination

$$R^2 = \left( \frac{\sum_i (P_i - \bar{P})(O_i - \bar{O})}{n \cdot S_{pred} S_{Obs}} \right)^2 \tag{5}$$

Where,

$n$  = total number of data

$P_i$  = predicted values

$O_i$  = observed values

$P$  = mean of predicted

$\bar{O}$  = mean of observed values

$S_{pred}$  = standard deviation of predicted values

$S_{obs}$  = standard deviation of observed values

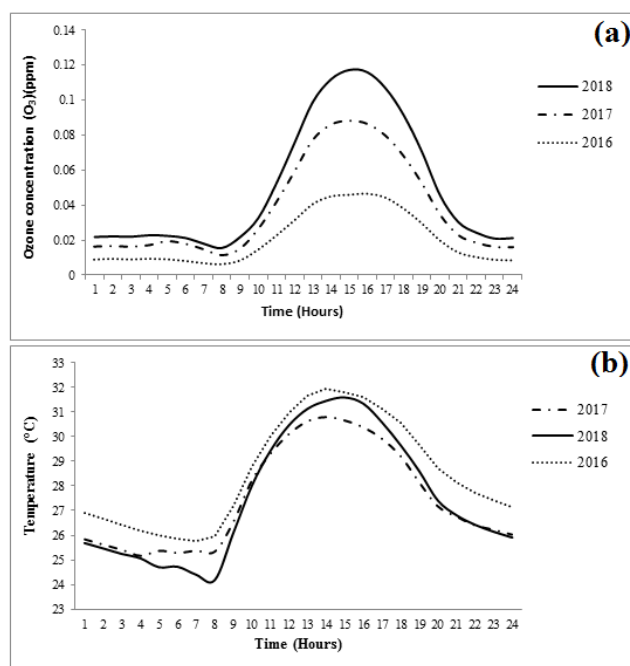
## RESULT

Descriptive statistics is used for describing the trend of selected parameters which including the gaseous pollutants and meteorological factors such as  $O_3$  concentration,  $NO_x$ ,  $NO$ ,  $SO_2$ ,  $NO_2$ ,  $CO$ ,  $T$  and  $RH$  as tabulated in Table I. The mean for  $O_3$  concentration is

Parameter	Ozone ( $O_3$ ) (ppm)	Temperature ( $^{\circ}C$ )	Relative Humidity (%)	Nitrogen Oxide ( $NO_x$ ) (ppm)	Nitric Oxide ( $NO$ ) (ppm)	Sulfur Dioxide ( $SO_2$ ) (ppm)	Nitrogen Dioxide ( $NO_2$ ) (ppm)	Carbon Monoxide ( $CO$ ) (ppm)
Mean	0.0170	28.1	73.5	0.0248	0.0098	0.0025	0.0151	0.5908
Median	0.0113	27.6	74.0	0.0196	0.0050	0.0014	0.0140	0.5400
Mode	0.0030	26.1	85.0	0.0100	0.0010	0.0020	0.0070	0.4500
Variance	0.0003	8.0	183.5	0.0003	0.0002	0	0.0001	0.0549
Standard Deviation	0.0170	2.8	13.5	0.0179	0.0131	0.0024	0.0080	0.2343
Minimum	0	20.7	39.0	0	0.0007	0	0	0
Maximum	0.1350	36.1	98.0	0.1510	0.1290	0.0170	0.0530	2.4560
Skewness	1.6577	0.4	-0.2	1.6041	2.8036	1.7846	0.7309	0.8677
Kurtosis	3.2773	-0.8	-0.9	3.6368	10.6577	3.3914	0.4606	1.5817

0.0170 ppm,  $NO_x$  (0.0248 ppm),  $NO$  (0.0098 ppm),  $SO_2$  (0.0025),  $NO_2$  (0.0151 ppm),  $CO$  (0.5908 ppm),  $T$  (28.1  $^{\circ}C$ ) and  $RH$  (73.5%). The minimum value for  $O_3$  concentration,  $NO_x$ ,  $SO_2$ ,  $NO_2$ , and  $CO$  is 0 while the minimum value for  $NO$  is 0.0007 ppm,  $T$  (20.7  $^{\circ}C$ ), and  $RH$  (39.0%). The maximum value for  $O_3$  concentration is 0.1350 ppm,  $NO_x$  (0.1510 ppm),  $NO$  (0.1290 ppm),  $SO_2$  (0.0170 ppm),  $NO_2$  (0.0530 ppm),  $CO$  (2.4560 ppm),  $T$  (36.1  $^{\circ}C$ ) and  $RH$  (98.0%). The median for  $O_3$

concentration is 0.0113 ppm,  $NO_x$  (0.0196 ppm),  $NO$  (0.0050 ppm),  $SO_2$  (0.0014 ppm),  $NO_2$  (0.0140 ppm),  $CO$  (0.5400 ppm),  $T$  (27.6  $^{\circ}C$ ) and  $RH$  (73.6%). The mode for  $O_3$  concentration is 0.0030 ppm,  $NO_x$  (0.0100 ppm),  $NO$  (0.0010 ppm),  $SO_2$  (0.0020 ppm),  $NO_2$  (0.0070 ppm),  $CO$  (0.4500 ppm),  $T$  (26.1  $^{\circ}C$ ) and  $RH$  (85.0%). The sample variance for  $O_3$  concentration and  $NO_x$  is 0.0003 ppm,  $NO$  (0.0002 ppm),  $SO_2$  (0 ppm),  $NO_2$  (0.0001 ppm),  $CO$  (0.0549 ppm),  $T$  (8.0  $^{\circ}C$ ) and  $RH$  (183.5%). The standard deviation for  $O_3$  concentration is 0.0170 ppm,  $NO_x$  (0.0179 ppm),  $NO$  (0.0131 ppm),  $SO_2$  (0.0024 ppm),  $NO_2$  (0.0080 ppm),  $CO$  (0.2343),  $T$  (2.8  $^{\circ}C$ ) and  $RH$  (13.5 %). Fig. 1(a) shows the average ground level  $O_3$  concentration.



**Fig 1:** Average ground-level ozone ( $O_3$ ) concentration and temperature ( $^{\circ}C$ ). Ozone reached highest concentration in the middle of the day due to presence of solar radiation (a). The incoming solar radiation comprising high temperature is in line with the high concentration of ozone due to the photochemical reactions (b).

Correlation analysis was introduced to correlate the two variables among the interested parameters utilizing the Statistical Packages for Social Sciences (SPSS®) as shown in Table II. Two variables were correlated using Spearman's correlation coefficient. Analyses of correlations between  $O_3$  and selected pollutants are carried out in this study in order to determine if there is a correlation between  $O_3$  and other pollutants. Emissions, the height of the planetary boundary layer, and long-distance transport all have an effect on pollutant concentrations, including  $O_3$  (12). More than 0.50 is considered strong, 0.40-0.49 is considered moderate, and less than 0.30 is regarded as weak (13).  $O_3$  and  $T$  ( $r = 0.729$ ,  $p < 0.01$ ),  $RH$  ( $r = -0.732$ ,  $p < 0.01$ ),  $NO_x$  ( $r = -0.654$ ,  $p < 0.01$ ),  $NO$  ( $r = -0.630$ ,  $p < 0.01$ ), and  $NO_2$  ( $r = -0.535$ ,  $p < 0.01$ ) have a strong significant correlation.  $RH$  a significant impact on the  $O_3$  variability, and the lower  $O_3$  associated with increasing relative humidity

was a surprise (14). When it comes to T and RH, there is an extremely strong negative correlation ( $r=-0.894$ ,  $p<0.01$ ). Because the study area is temperature-sensitive, these findings indicate the photochemical reaction of  $O_3$  formation is a major contributor to this phenomenon (9). A strong correlation between  $NO_x$  and NO ( $r=0.834$ ,  $p<0.01$ ) and  $NO_2$  ( $r=0.863$ ,  $p<0.01$ ) was found. NO and  $NO_2$  were found to have a strong correlation ( $r=0.521$ ,  $p<0.01$ ). The correlation between  $O_3$  and CO ( $r=-0.423$ ,  $p<0.01$ ) is moderately significant. T is expected to influence  $O_3$  variability, but CO emissions associated with biomass on the  $O_3$  surface have been shown to be of significant importance (14). T has a moderately significant correlation with  $NO_x$  ( $r=-0.442$ ,  $p<0.01$ ), NO ( $r=-0.427$ ,  $p<0.01$ ), and  $NO_2$  ( $r=-0.346$ ,  $p<0.01$ ). There is a correlation between the presence of sunlight and high temperatures and nitrogen's value decreasing (9). Another significant correlation was found between  $NO_x$  ( $r=0.484$ ;  $p<0.01$ ) and NO ( $r=0.362$ ;  $p<0.01$ ) as well as  $NO_2$  ( $r=0.454$ ;  $p<0.01$ ) and CO with RH ( $r=0.365$ ;  $p<0.01$ ). This study found that there was a moderately significant correlation between  $NO_x$  ( $r=0.472$ ), NO ( $r=0.343$ ), and CO ( $r=0.494$ ). T ( $r=0.143$ ;  $p<0.01$ ), RH ( $r=-0.299$ ;  $p<0.01$ ),  $NO_x$  ( $r=0.084$ ;  $p<0.01$ ) and  $NO_2$  ( $r=-0.023$ ;  $p<0.05$ ) were all found to have weak significant correlations with  $SO_2$  and  $O_3$  ( $r=$

**Table II Summary of spearman correlation analysis (r-value) between  $O_3$  concentration, meteorological factors, and gaseous pollutants**

Parameter	$O_3$	T	RH	$NO_x$	NO	$SO_2$	$NO_2$	CO
$O_3$	1							
T	0.729**	1						
RH	-0.732**	-0.894**	1					
$NO_x$	-0.654**	-0.442**	0.484**	1				
NO	-0.630**	-0.427**	0.362**	0.834**	1			
$SO_2$	0.140**	0.143**	-0.299**	0.084**	0.206**	1		
$NO_2$	-0.535**	-0.346**	0.454**	0.863**	0.521**	-0.023**	1	
CO	-0.423**	-0.280**	0.365**	0.472**	0.343**	-0.066**	0.494**	1

\*\*Correlation is significant at the 0.01 level (2-tailed)

0.140;  $p<0.01$ ).

All data ( $n=5451$ ) from the MLR models were analysed and summarised in Table III. Durbin Watson statistics show that the models can handle autocorrelation, as the value was in the range of (0.413-1.333). MLR is used to determine which variables are most important in predicting the concentration of  $O_3$ . The predicted  $R^2$  for  $O_{3,t+1}$  ( $R^2=0.5565$ ),  $O_{3,t+2}$  ( $R^2=0.5326$ ) and  $O_{3,t+3}$  ( $R^2=0.5197$ ). The significant predictors were  $O_{3,t+1}$  ( $O_3$ , T,  $NO_2$ , CO, NO,  $NO_x$  and  $SO_2$ ),  $O_{3,t+2}$  ( $O_3$ , T,  $NO_2$ , CO, NO,  $NO_x$ ,  $SO_2$  and RH), and  $O_{3,t+3}$  (T,  $O_3$ ,  $NO_2$ , NO, CO,  $NO_x$ ,  $SO_2$  and RH).

**Table III Summary of the Multiple Linear Regression (MLR) models for  $O_3$  forecasting at the study area**

Model	$R^2$	D-W Statistics
$O_{3,t+1} = 0.751(O_3) + 0.139(T) + 0.155(NO_2) + 0.077(CO) + 0.593(NO) - 0.631(NO_x) - 0.014(SO_2) - 0.036$	0.5565	1.333
$O_{3,t+2} = 0.475(O_3) + 0.197(T) + 0.144(NO_2) + 0.129(CO) + 0.746(NO) - 0.735(NO_x) - 0.031(SO_2) - 0.030(RH) - 0.009$	0.5326	0.636
$O_{3,t+3} = 0.043 + 0.185(T) + 0.250(O_3) + 0.134(NO_2) + 0.871(NO) + 0.148(CO) - 0.803(NO_x) - 0.038(SO_2) - 0.054(RH)$	0.5197	0.413

D-W: Durbin-Watson;  $R^2$ : Correlation Coefficient

**DISCUSSION**

The  $O_3$  concentration in the study area rises from 08:00 hours to 15:00 hours due to the emissions of  $NO_x$ , mainly from automobiles, which could cause the  $O_3$  concentration to rise (9). The diurnal pattern shows that the  $O_3$  concentration was increasing towards noon. It is due to the increasing of solar radiation, emission from vehicles, and high population growth notified through human activities such as construction activities, open burning, and mobile resources (7). In meeting the economic expansion, industrial activities as well as traffic have become the culprit for the increases of ozone sources (15). Starting from 09:00 to 13:00-15:00 hours, an increase of  $O_3$  concentration and temperature shows that the  $O_3$  concentration is highly correlated with temperature (16). A high level of  $O_3$  concentration during the afternoon around 13:00 hours to 15:00 hours is due to the maximum temperature and the high intensity of solar radiation occurred during this time (17). Based on Fig. 1(a) and Fig. 1(b), the average ground level  $O_3$  concentration and the average temperature have the same form of the line graph. The sensitivity of ozone concentration decreases along with temperature as a results of the declination of  $NO_x$  and VOCs (18). According to (16), maximum ozone concentration can be found in the mid of the day which is around 14:00 hours until 15:00 hours while there was starting slower  $O_3$  concentration during night time around 20:00 hours due to the photochemical reaction of  $O_3$  precursors, such as VOC with ambient air from the natural

resources and the long-distance transport of  $\text{NO}_x$  react to sunlight. The higher solar radiation intensity during day time may lead to favorable conditions for powering photochemical reactions (13).  $\text{NO}_x$  accumulated during night time as a result of reaction of  $\text{NO}$  and  $\text{NO}_2$  during the daytime, which clarified as the main reason on the existence of ozone concentration during night time with the help of inversion layer (9). The  $\text{O}_3$  concentration was decreasing slowly towards evening starting at 16:00 hours and night time around 21:00 hours in line with the disappearing of sun and redox process (19). It was supported by (20) which stated that during the nighttime, the  $\text{O}_3$  concentration was far lower than the day-time concentration due to the absence of photochemical reactions. The ozone concentrations continues to its lower value in the morning until the solar radiation present (7). The  $\text{O}_3$  concentration decreases progressively until evening starting at 16:00 hours and then keep on decreasing more gradually during the night-time (21:00 hours) until morning (07:00 hours) because of lack of solar radiation (13). The  $\text{O}_3$  concentration was generally low and in a stable condition because of the absence of photochemical reactions (13). High intensity of solar radiation helps in the ozone concentration formation during the day time (9).

The higher the temperature, the greater the concentration of  $\text{O}_3$ . When the temperature rises above a certain threshold in Malaysia (a tropical country), ozone is diluted because of the increased production of ozone-forming organic compounds ( $\text{O}_3$ ) in the atmosphere (9). It's important to consider the residual (error) when determining the size of the factual model. Errors that show a pattern are interpreted as a sign that the model does not handle all of the methodological data (Fig. 2(a)-(c) and Fig. 3(a)-(c)).  $\text{O}_3$  model residual histograms are shown in Fig. 2(a)-(c). Analyses of the residuals show them to be symmetrical in shape, with zero mean and zero variance. According to the  $\text{O}_3$  model, there is no correlation between the fitted values and residuals because the residuals are in a horizontal band, which indicates that the variance is constant. As can be seen in Fig. 4(a)-(c), the predicted  $\text{O}_3$  concentration at Nilai is plotted against the actual  $\text{O}_3$  concentration (ppm). As a result of using the MLR method, the models' equations are listed in Table III. For example, each precursor has a coefficient, but it doesn't correspond to how much of a factor it has in determining how much ozone is present in the atmosphere (21). Coefficients are analogous to one another when they are transformed into standardised regression, so the largest coefficient may indicate the independent variables that have the greatest influence on  $\text{O}_3$  (22).

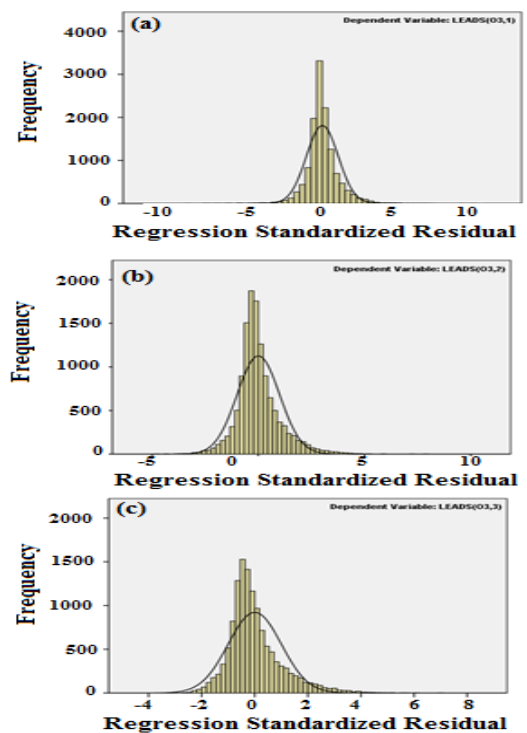


Fig 2: Residual of Multiple Linear Regression (MLR). The residual analysis shows that the residuals were normally distributed with zero mean and constant variance for next-hour (a). The residual analysis shows that the residuals were normally distributed with zero mean and constant variance for next two-hour (b). The residual analysis shows that the residuals were normally distributed with zero mean and constant variance for next three-hour (c).

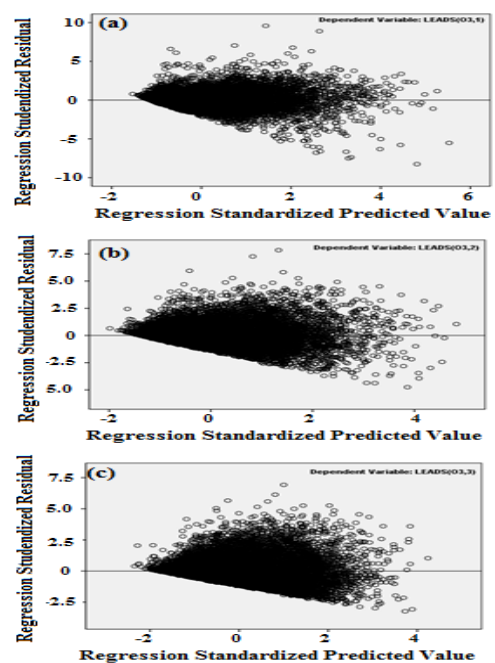


Fig 3: Testing assumption of variance and uncorrelated with mean equal to zero for Multiple Linear Regression (MLR). The residuals are uncorrelated because the residuals are contained in a horizontal band and hence obviously that variance is constant for next-hour (a). The residuals are uncorrelated because the residuals are contained in a horizontal band and hence obviously that variance is constant for next two-hour (b). The residuals are uncorrelated because the residuals are contained in a horizontal band and hence obviously that variance is constant for next three-hour (c).

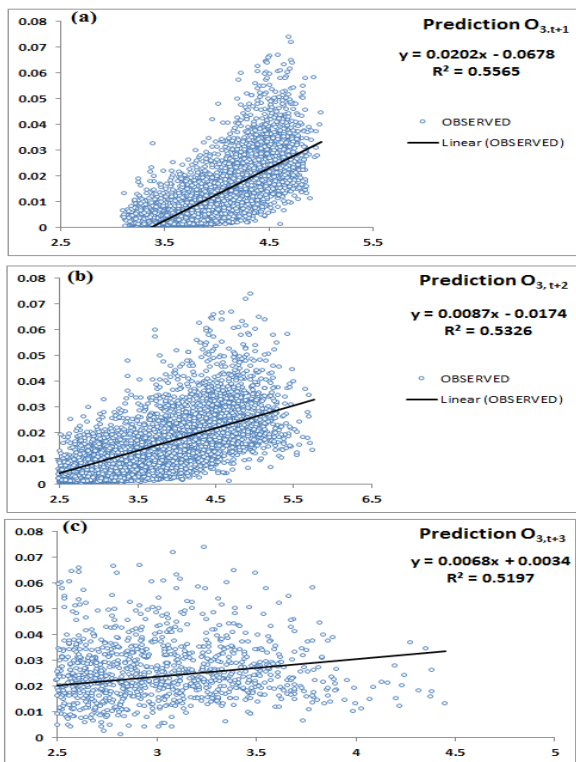


Fig 4: Scatter plot of forecasted O<sub>3</sub> concentration (ppm) against observed O<sub>3</sub> concentration (ppm) at Nilai. The models showing the prediction of O<sub>3</sub> concentration for the next-hour (a). The models showing the prediction of O<sub>3</sub> concentration for the next two-hour (b). The models showing the prediction of O<sub>3</sub> concentration for the next three-hour (c).

**CONCLUSION**

In conclusion, the ozone concentrations are fluctuating during the day and night time as a result of solar radiation and temperature inversion, respectively. The ozone concentrations are significantly correlated with the meteorological factors and air pollutants which these parameters influence the ozone formation at the study area. It indicates because of nitrogen start to decrease in value when the presence of sunlight with high temperature produces. The predicted coefficients for the three next one, two, and three hours are R<sup>2</sup>=0.5565, R<sup>2</sup>= 0.5326, and R<sup>2</sup>= 0.5197, respectively. The developed MLR models are the most suitable model for forecasting the prediction of O<sub>3</sub> concentration to the next hours.

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