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Stratospheric Ozone Forecasting By Multiple Linear Regression Models

التنبؤ بطبقة الأوزون الإستراتوسفيرية بإستخدام نماذج الإرتداد الخطية المتعددة

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الملخص العربى :

يوضح هذا البحث إستخدام تمثيل لبعض النماذج متعددة الإنحدار الخطى من أجل التنبؤ بتركيزات الأوزون على مدينة القاهرة بدلالة بعض المتغيرات الجوية (مثل: الأشعة فوق البنفسجية ، زاوية سقوط الأشعة الشمسية ، و إنعكاسية الأشعة الشمسية) وأيضا مؤشرات لبعض الملوثات (مثل: مؤشر الهباء الجوى ، ومؤشر أكاسيد الكبريت). والبيانات المستخدمة فى هذه الدراسة تمثل فترة حوالى خمسة وعشرون عاما ، ويتضح بدراسة تلك البيانات وتطبيق النماذج المستخدمة فى هذا البحث أن النموذج الرابع هو أفضل النماذج من حيث القياسات الإحصائية المستخدمة .

Abstract: This paper represents a multiple linear regression modeling (LRM) approach in order to predict ozone concentration over Cairo as a function of meteorological parameters (i.e., reflectivity, solar ultraviolet intensity, zenith angle) and pollutants indexes (i.e., aerosol index, and sulfur oxides index). Data for this paper were collected over a period of 25 years. When different combinations of data sets were examined from the test point of view, it was found that the LRM-AI model provides the most reasonable results compared to other lagged models (i.e., LRM, LRM-SOI).

Keywords: Multiple linear regression models, ozone, air pollutants, ultraviolet solar intensity, aerosol index.

1. Introduction

Interest in ozone stems from the fact that such absorption of solar radiation is important in determining not only the thermal structure of the stratosphere, but also the ecological framework for life on the earth's surface [1]. The health of humans, animals, and plants can be affected by increasing ultraviolet radiations, where the ozone decrease is one of the most significant of its impacts [2].

Observations of the total integrated column ozone based on ultraviolet absorption began in the first few decades of the twentieth century [3-5]. Systematic measurements of this type have revealed that the total ozone abundances over many regions of the globe have decreased markedly since about 1980. Indeed, the depletion of the global ozone layer has emerged as one of the major global scientific and environmental issues of the twentieth century. Downward trends are evident in the time series of spatially or time-averaged spring column ozone observations [6-11].

Ozone (O_3) is produced due to the complex photochemical reaction between nitrogen oxide radicals (NO_x) and non methane hydrocarbons and other volatile organic compounds (VOC_x) in the vicinity of UV solar irradiance; also other meteorological parameters can effectively affect ozone concentration [12].

Stratospheric ozone is considered good for humans and other life forms because it absorbs ultraviolet UV-B radiation from the Sun (see Figure 1). If not absorbed, UV-B would reach Earth's surface in amounts that are harmful to a variety of life forms. In humans, increased exposure to UV-B increases the risk of skin cancer, delayed tanning, cataracts, lens capsule deformation, ocular melanoma, sunburn, and a suppressed immune system [13-15]. Because of its capability to absorb the incoming radiation, the stratospheric ozone is a major source of stratospheric heating, which further heats the troposphere [16].

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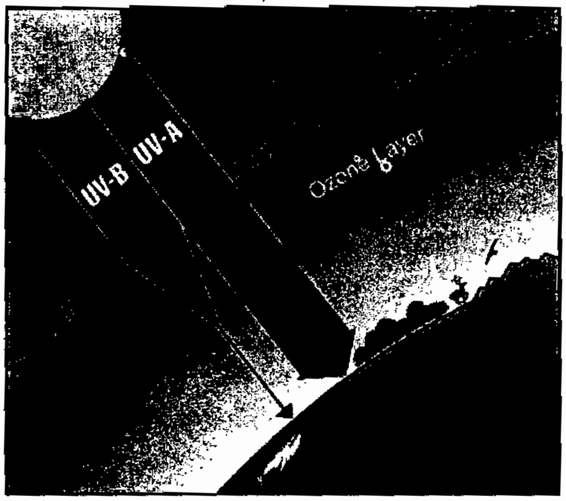

Fig.1 The ozone layer resides in the stratosphere and surrounds the entire Earth. UV-B radiation (280 to 315 nanometer (nm) wavelength) from the Sun is partially absorbed in this layer. As a result, the amount of UV-B reaching Earth's surface is greatly reduced. UV-A (315- to 400-nm wavelength) and other solar radiation are not strongly absorbed by the ozone layer.

In a more mathematical language, the statistical time series analysis approach in forecasting the atmospheric and environment pollution has been proved viable by a number of researchers. Multiple linear regression models have been widely used for ozone forecasting, and well specified regressions can provide reasonable results [12,17]. Not only are there numerous direct links between weather conditions and the ozone production factors mentioned above, but there are also equally important feedbacks among the many variables. The net result is a highly complex system of ozone formation mechanisms that displays the compounded effects of multiple chemical and meteorologically related nonlinearities [18-20].

In most of past works, MLR models have been developed with other meteorological variables as predictors. In none of the MLR models of ozone concentration, pollution indexes have been used as predictor instead of pollutants concentrations. Since all other meteorological variables have their own chaotic characteristics and complexities, their inclusion to the input set would incorporate more complexity in the forecasting [21-24]. The present approach viewed the prediction problem from a different point of view while performance of MLR models has been compared with each other.

2. Data

We present here the development of a multiple linear regression model that can be used to estimate stratospheric ozone concentration on the basis of erythemal UV irradiance, aerosol index, solar zenith angle, sulfur oxides index, and reflectivity [25,26]. These data was obtained from TOMS' website [27]. The TOMS' data have a daily global coverage over $1^0 * 1.25^0$ (latitude by longitude) grids. The total relative uncertainty in the radiance calibration is estimated to be <3% (though somewhat higher at high latitudes). For more detailed descriptions of the different sources of uncertainty the reader is referred to [28]. But, one of the main shortcomings in using satellite data is that, the TOMS instruments provide one measurement per day near local noon.

The seasonal variation in the columnar ozone time series from 1979 to 2005 is shown in fig.2, and in a qualitative sense, it shows downward trends of about 4.9% in winter/spring and about 4.8% in summer/autumn. The illustrated data summarize the average values of the corresponding records for Cairo (30°4'N, 31°16'E).

UV radiation is the most important factor affecting ozone concentration. Fig.3, shows the downward seasonal variation in Erthymal-UV irradiance time series in (mW/m^2) from 1999 to 2005. The results reveal a decrease in UV data series over time despite significant decrease in the columnar ozone. It is not surprising that the UV irradiance does not follow the ozone trend, because the sensitivity of the TUVR radiometer peaks at long wavelength where ozone does not absorb. Other factors (e.g. aerosol, air pollution) may cause this decrease in UV [26]. A quantity known as aerosol index is a logical choice to use as a parameter for indicating UV attenuation due to scattering and absorbing processes. The results of Hsuet al. [29], and Herman et al. [30] have demonstrated the feasibility of using this index to characterize the temporal and spatial distributions of the tropospheric aerosols. Under most conditions, the aerosol index is positive for absorbing aerosols and negative for non-absorbing aerosols. UV absorbing aerosols include smoke produced by biomass burning, black carbon from urban activities, mineral dust, sea salt particles and ash. Non-absorbing aerosols are primarily sulphate aerosols. Aerosol index (AI) is defined by the following equation:

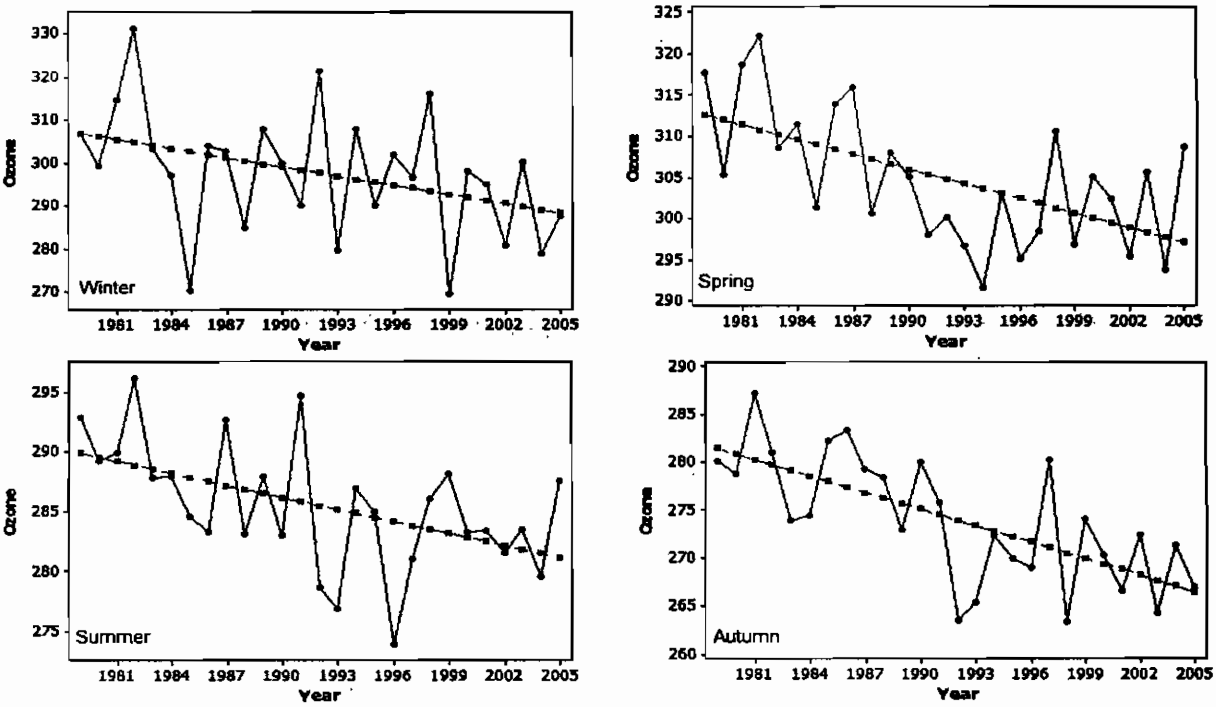

Fig.2 The seasonal variation in the columnar ozone time series in DU from 1979 to 2005

$$AI = -100\left\{log_{10}\left(\frac{I_{340}}{I_{380}}\right)_{meas} - log_{10}\left(\frac{I_{340}}{I_{380}}\right)_{calc}\right\} \quad (1)$$

Where the subscript "meas" is the backscatter radiance measured by total ozone mapping spectrometer at a given wavelength, and the subscript "calc" indicates the radiance calculated using a radiative transfer model for a pure Rayleigh atmosphere. Actually, the scattering and the absorbing processes affect the UV budget in away depending on aerosol type and surface albedo [31]. For this case the effect of surface albedo can be considered insignificant, since the areas where the measurements are performed have almost the same albedo through the year. Fig.4 shows the

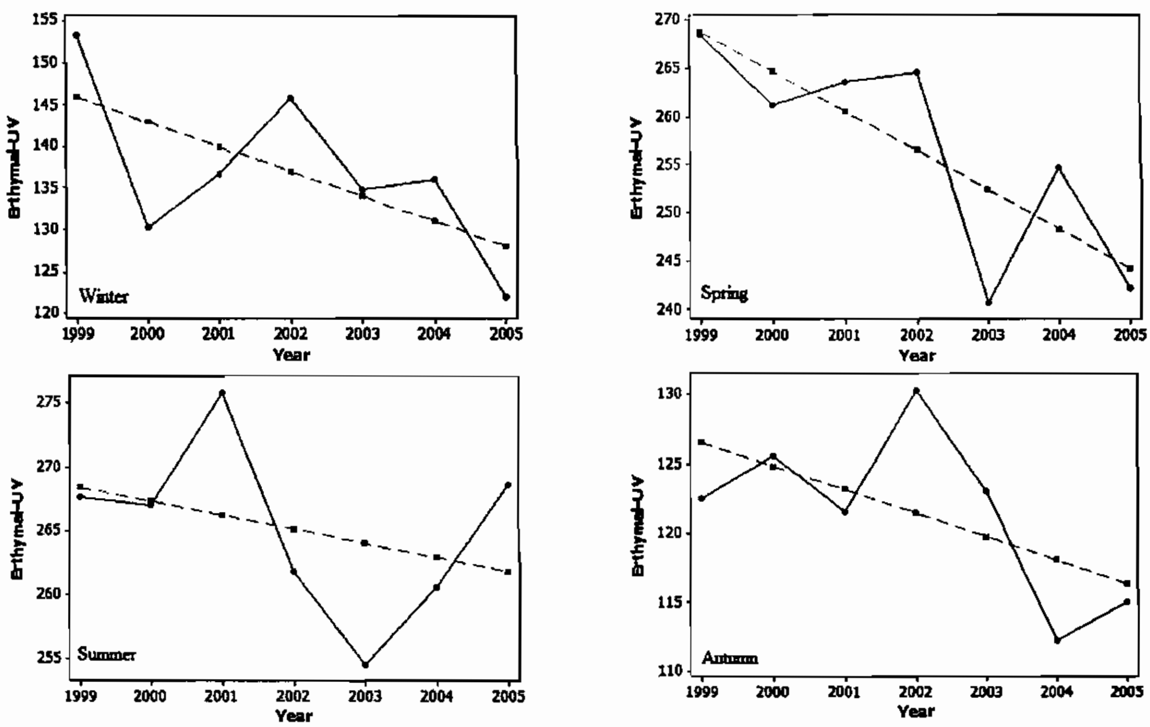

Fig.3 The seasonal variation in Erthymal-UV irradiance time series in (mW/m^2) from 1999 to 2005

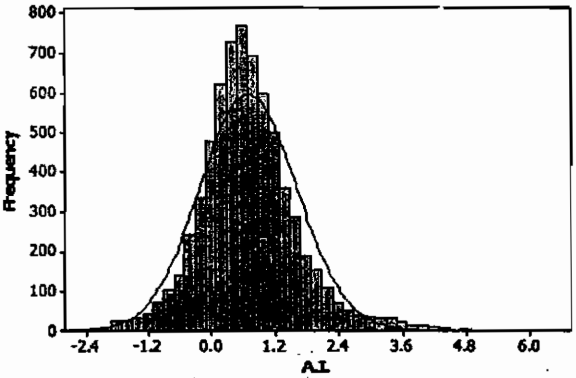

Fig.4 The frequency of aerosol index for the period 1979–2005

frequency diagram of the TOMS aerosol index for the period 1979–2005.

The next relevant factor influencing ozone concentration is the solar zenith angle (SZA). The SZA is one of the most important factor, because it determines the path length of UV radiations through the atmospheric ozone and other absorbers [32,33]. The larger SZA means that the UV radiation has to travel a longer optical path length through the atmosphere; hence, less amount of UV radiation will reach the ozone layer, which leads to less formation of ozone particles. Fig.5 shows the relation between SZA and ozone concentration.

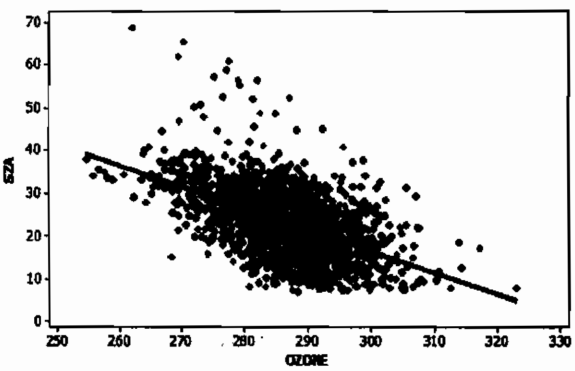

Fig.5 The relation between SZA and ozone concentration, less ozone concentrations DU for larger SZA

The solar irradiance reflected up to a spacecraft from the surface of the earth can be used to calculate reflectivity. Reflectivity calculated for specific bandwidths is needed for the calculation of total column ozone from the TOMS and OMI instruments. Reflected radiation can come from two surfaces, the ground, and the tops of clouds. Reflectivity is determined from the measurements at 380 nm, or 360 nm in the case of Earth Probe satellite. Clouds are clearly defined and recognizable in images produced using TOMS and OMI reflectivity data.

Sulfur occurs in Earth's atmosphere as a variety of compounds, in both gaseous and aerosol forms, and has a range of natural and anthropogenic sources. Emissions of SO_2 and other sulfur species have been the subject of particular attention, given the impact that sulfur may have on the Earth's radiative budget, through the direct scattering of sunlight, and also indirectly via modification of cloud albedoes and lifetimes, which impacts on the stratospheric ozone formation [34]. Most sulfur enters the atmosphere as gaseous sulfur dioxide (SO_2), a dangerous air pollutant. Sulfur dioxide has a lifetime in the atmosphere of about a day, before being deposited to the surface or oxidized to sulfate (SO_4^-) aerosol [35]. SO_2 emissions can be assessed based on the sulfur oxides index "SOI" which is an open-end scale, that relates directly to the amount of SO_2 produced [36].

3. Methods

The intricacies of ozone formation make day-to-day operational prediction of ozone quite difficult. One of the best ways to capture these complex interactions is through the use of photochemical models used mainly for research and planning (e.g., the Urban Airshed Model) [12]. But such models are unsuitable in many operational settings because they require significant computer and staffing commitments, as well as many complex chemical and meteorological inputs (precursor concentrations, mesoscale meteorological measurements, etc.). Thus, while such models are theoretically sophisticated and desirable for forecasting, they are not practical choices in many locations. The most common alternative is to employ a multivariate statistical approach, which is widely used in operational ozone forecasting and research oriented statistical modeling [37-40]. Multiple (multivariate) linear regression is the most popular of these techniques, and it has the general form:

$$Y_i = b_0 + b_1 X_1 + b_2 X_2 + \ldots + b_k X_k + i \qquad (2)$$

Where, for a set of i successive observations, the predictand variable Y is a linear combination of an offset b_0, a set of k predictor variables X with matching b coefficients, and a residual error. When the regression equation is used in predictive mode, (the difference between actual and predicted values not accounted for by the model) is omitted because its expected value is zero. Note that regression models are inherently linear, although curvilinear relationships can be incorporated via polynomial terms in the regression, and known relationships can be pre-specified by transforming a nonlinear predictor variable into a more linear form (e.g., by taking a logarithm) before using it in the model.

Regression models of ozone pollution typically incorporate from one or two input variables [24] to as many as 313 variables (reflecting a range of weather data from several atmospheric levels that are potentially correlated with ozone concentrations) [37] A stepwise multiple regression procedure is commonly used to produce a parsimonious model that maximizes accuracy with an optimally reduced number of predictor variables. In most locations, temperature is the meteorological variable most highly correlated with ozone, although wind speed, variables related to UV, and atmospheric moisture are sometimes included in regression models. In this paper, five variables are used to reflect the most important effect which are (reflectivity, ultraviolet solar intensity, solar zenith angle, aerosol index, and sulfur oxides index).

Because daily maximum ozone concentrations are partially dependent on the previous day's concentrations, ozone data display strong serial correlation. In contrast, regression models assume that observations are statistically independent events. To avoid this weakness while still incorporating the importance of persistence, some investigators have used a lagged ozone concentration (typically a value from the previous day) as an additional predictor variable in the model [12,24,37]. If the regression is performed in an explanatory mode (for interpretation of coefficients or significance testing), then this strategy is statistically somewhat awkward, because the inclusion of serially correlated ozone data does not necessarily aid understanding of weather-ozone relationships. In contrast, the inclusion of lagged data in regression modeling is desirable when used in a predictive mode, frequently improving the accuracy of predictions.

Four multiple linear regression models are performed to compare with each other for each season. The first model is the unlagged model (URM), which doesn't depend on the previous day's concentration of ozone, it depends only on reflectivity, ultraviolet solar intensity, solar zenith angle, aerosol index, and sulfur oxides index. The other models depend on the previous day's ozone concentration. The second model, implemented by variables reflectivity, ultraviolet solar intensity, solar zenith angle, aerosol index, and sulfur oxides index, concluding the previous day's ozone concentration (LRM). The third model, implemented by variables reflectivity, ultraviolet solar intensity, solar zenith angle, and aerosol index, as the third model after eliminating the sulfur oxide index from the model (LRM-SOI). The fourth model, implemented by variables reflectivity, ultraviolet solar intensity, solar zenith angle, aerosol index, and sulfur oxides index concluding the previous day's ozone concentration, but after eliminating negative values from the aerosol index (LRM-AI).

4. Results

In our work, multiple regression modeling was performed, without transforming any input variables or employing a stepwise variable-selection procedure. The latter was done to maximize explained variance, coefficient of determination (R^2), and to keep the results in comparable form, thereby offsetting the minor loss in parsimony caused by having all variables in the regression. Regressions were run on the MINITAB® software package.

The reliability of the model has been assessed using statistical measures, such as coefficient of determination (R^2), mean bias error (MBE), root mean square error (RMSE), mean absolute error (MAE), and mean absolute percentage error (MAPE). High values of R^2, and Low values of MBE, RMSE, MAE and MAPE indicate better correlation [41-43].

The coefficient of determination (R^2), used to illustrate the relationship between observed and estimated values, (which account for variability explained by the given model) was provided for the whole period (see table 1). Fig. 6 shows the scatter plots of the measured and estimated datasets. According to Fig. 6 the results obtained by the proposed model are generally satisfactory and shows a good correlation between observed and estimated values. In (table 1), an analysis of the results at the individual season's shows that the season's has little impact on the value of R^2, for lagged models it varies between 0.567 to 0.699, (about 0.13 variation), and for unlagged model it varies between 0.155 to 0.541, (about 0.39 variation), thus indicating the goodness of the fitting for lagged models over unlagged model.

Table 1: R^2 compared between models and seasons

	R^2			
	URM	LRM	LRM-SOI	LRM-AI
Winter	0.315	0.643	0.652	0.655
Spring	0.541	0.699	0.691	0.695
Summer	0.367	0.659	0.644	0.657
Autumn	0.155	0.567	0.572	0.580

The MBE (mean bias error) is technically a difference, but it is included here because it succinctly summarizes the average over- or under-prediction of ozone in each model. The MBE values are small, and the sizes of the standard errors indicate no discernible differences between models. Comparing models, all models tend to slightly over-predict. These subtle variations in MBE may be attributable to slight differences in information between the training data set and the independent test data set for each city, rather than any overall structural tendency in the models.

MBE varies between 0.7% (in the first quarter of the year "winter") and 0.03% (in the Third quarter of the year "summer"), as shown in (table 2). It is clear that the best MBE (lowest values) appears in fourth model (LRM-AI) of all quarters, and the worse MBE (highest values) appears in the first model (URM) of all quarters.

Table 2 MBE implies the over-prediction of ozone in all models

	MBE %			
	URM	LRM	LRM-SOI	LRM-AI
Winter	0.733	0.373	0.367	0.365
Spring	0.189	0.123	0.120	0.118
Summer	0.060	0.032	0.032	0.031
Autumn	0.291	0.147	0.131	0.128

The mean absolute error (MAE) is simply the average absolute value of all such deviations, without exponentiation; the root mean square error (RMSE) is the square root of the mean of all squared residuals (the root is taken to return the result to the original metric which, in this case, is DU of ozone). MAE has the benefit of being fairly intuitive to interpret, and it is not sensitive to outliers, but RMSE is widely used and is more amenable to additional statistical analyses.

In (table.3), it indicates that MAE ranges between 4 DU (for fourth model (LRM-AI) in summer) and 19.7 DU (for first model (URM) in winter). Values for MAE are also illustrated, to highlight the pattern of model errors. Generally, the fourth model (LRM-AI) performs better, as do both kinds of models incorporating lagged ozone data. Thus, that model has the overall lowest MAE values and the first model (URM) the highest.

Table 3 MAE indicate the absolute average value of all such deviations

	MAE (DU)			
	URM	LRM	LRM-SOI	LRM-AI
Winter	19.71	13.74	13.52	13.41
Spring	10.02	8.13	7.97	7.94
Summer	5.59	4.06	4.08	4.01
Autumn	11.42	7.85	7.36	7.23

The results for RMSE follow a remarkably similar pattern to MAE, but with slightly higher values because of the outlier sensitivity. The RMSE results show the broad quarter-based dependency on mean of observations, as well as the better performance of fourth model (LRM-AI) and another both forms of lagged model (lowest RMSE of 5 DU (for fourth model in summer), highest of 25.7 DU (for first model in winter), as shown in (table 4). Both the MAE and RMSE results provide interesting contrasts in prediction errors between the various quarters. Summer has smallest MAE and RMSE.

Table 4 RMSE indicate the performance of models related to seasons

	RMSE (DU)			
	URM	LRM	LRM-SOI	LRM-AI
Winter	25.78	18.61	18.48	18.41
Spring	13.74	11.12	10.92	10.84
Summer	6.97	5.11	5.14	5.05
Autumn	14.97	10.72	10.08	9.98

Mean Absolute Percentage Error (MAPE), measures the accuracy of fitted time series values. It expresses accuracy as a percentage. It ranges between 1.4% (for the best model (LRM-AI), in the summer quarter), and 6.6% (for (URM), in the autumn quarter), as shown in (table 5).

Table 5 MAPE measures the accuracy of fitted time series values

	MAPE %			
	URM	LRM	LRM-SOI	LRM-AI
Winter	6.66	4.58	4.51	4.47
Spring	3.23	2.62	2.57	2.57
Summer	1.96	1.42	1.43	1.41
Autumn	4.14	2.84	2.68	2.63

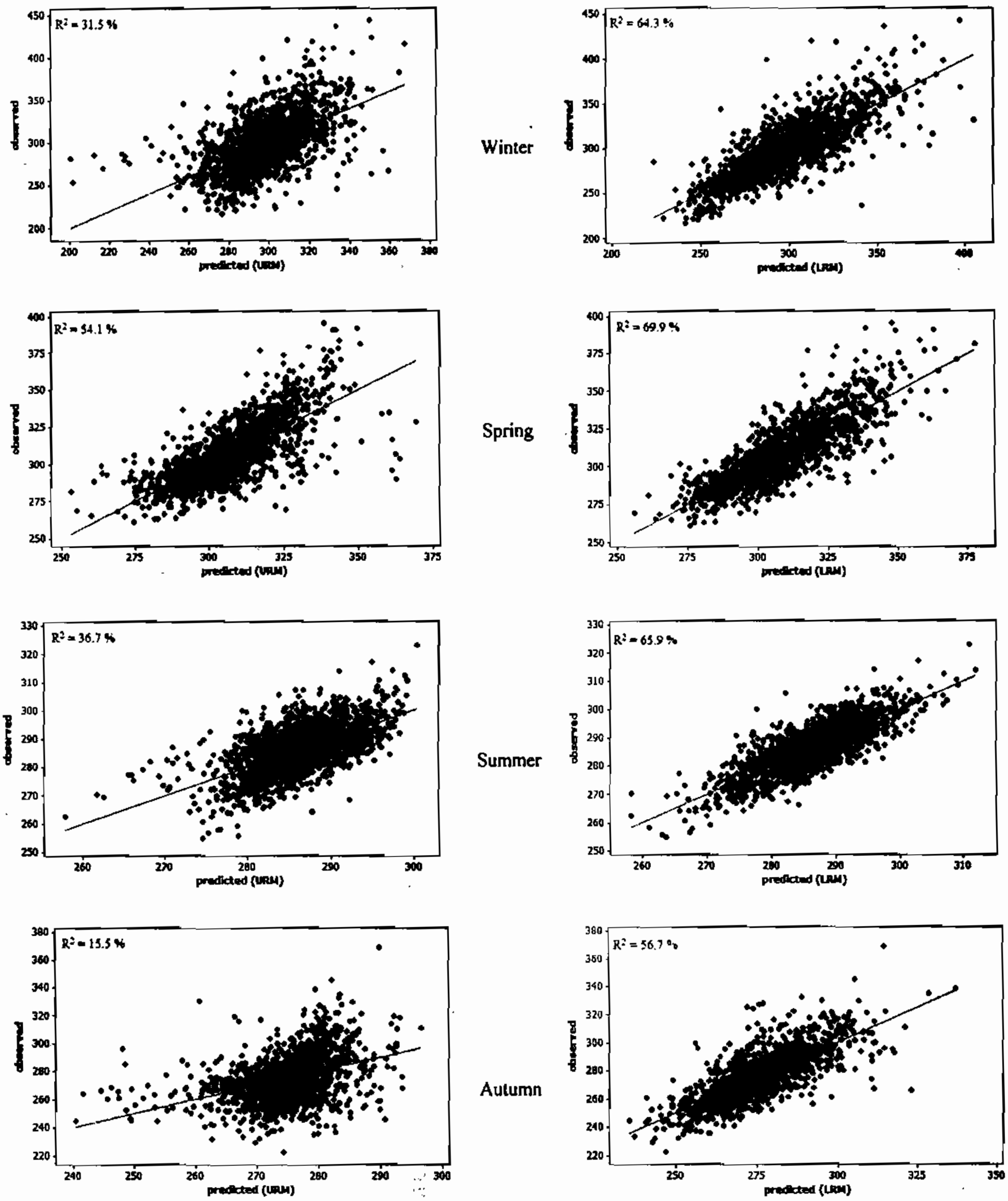

Fig.6 Correlation between observed & predicted ozone in DU (indicating thc efficiency of LRM model over URM model)

5. Conclusions

This paper shows the Multiple linear regression (MLR) modeling approach in order to predict ozone concentration over Egypt as a function of meteorological parameters (reflectivity, ultraviolet solar intensity, and solar zenith angle (SZA)) and pollutants indexes (aerosol index, and sulfur oxides index). The four MLR models were used to prepare a regression model were compared with each other. It was found that the lagged models (LRM, LRM-SOI, and LRM-AI) give an acceptable response more than unlagged model (URM), and the fourth model (LRM-AI) provide the most reasonable results than the other lagged models (LRM, LRM-SOI).

Appendix A

One of the most common indicators used in error analysis is the mean absolute error. This term is used similar to variance. The MAE of an estimator Y_i with respect to the estimated parameter X_i is defined as

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left|\hat{Y}_i - X_i\right| \quad (3)$$

Where n is the number of data points. The MAPE is measure of accuracy in a fitted time series

$$MAPE = \sum_{i=1}^{n}\left|\frac{Y_i - X_i}{Y_i}\right| \quad (4)$$

We used the MBE to describe how much the estimator underestimates or overestimates the situation. The MBE was determined using the following equation:

$$MBE = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{Y_i - X_i}{X_i}\right) \quad (5)$$

The mean squared error (MSE) of an estimator is the square of the amount by which the estimator differs from the quantity to be estimated. The difference occurs because the estimator does not account for information that could produce a more accurate estimate. The RMSE which gives an idea of the magnitude of the non-systematic error is then simply defined as the square root of the MSE. The mathematical formula of the RMSE is given by

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)^2} \quad (6)$$

In general, correlation coefficient, r, indicates the strength and direction of a linear relationship between two random variables. The correlation coefficient is 1 in case of an increasing linear relationship and -1 in case of a decreasing linear relationship, and some value in between in all other cases, indicating the degree of linear dependence between the variables.

$$r = \frac{\sum_i (Y_i - \bar{Y})\cdot(X_i - \bar{X})}{\{[\sum_i (Y_i - \bar{Y})^2]\cdot[\sum_i (X_i - \bar{X})^2]\}^{0.5}} \quad (7)$$

Where, $\bar{Y}$ is the estimated mean value.

The coefficient of determination (R^2), used to illustrate the relationship between observed and estimated values, and it equals the square of the correlation coefficient and it varies between 0 to 1.

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