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Research Article

Modeling of Ozone Interactions with Various Air Pollutants and Meteorological Factors Using Jaya and Teaching-Learning Based Optimization (TLBO) Algorithms

Nurcan ÖZTÜRK [a,*]

[a] *Department of Civil Engineering, Faculty of Technology, Karadeniz Technical University, Trabzon, TURKEY*
**Corresponding author's e-mail address: nurcan@ktu.edu.tr*
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ABSTRACT

Ozone (O_3), nitrogen oxides (NOx) and carbon monoxide (CO) concentrations and some meteorological parameters measured hourly have been analyzed to examine the interaction patters between O_3 and NOx, CO, air temperature, wind speed, relative humidity, and air pressure by taking into account the diurnal variations of them at urban site (Akçaabat) in Trabzon. Variations of O_3 levels have been modeled via Jaya and Teaching-Learning Based Optimization (TLBO) algorithms considering the effects of certain parameters (NOx and CO concentration, air temperature, wind speed, relative humidity, and air pressure) called as the independent variables. The accuracy of Jaya and TLBO methods has been determined and these methods have been carried out with four different functions: quadratic, exponential, linear and power. Some statistical indices have been applied to evaluate the performance of these models. In conclusion, it is shown that Jaya and TLBO algorithms can be used in the optimization of the regression function coefficients in modelling some air pollutants interactions and the best-fit equation for each parameter is obtained from the quadratic function.

Keywords: *Air pollution, Ozone concentration, Modeling*

Jaya ve Öğretme-Öğrenme Tabanlı Optimizasyon Algoritmalarını Kullanarak Meteorolojik Faktörler ve Çeşitli Hava Kirleticileri ile Ozon Etkileşimlerinin Modellenmesi

ÖZET

Ozon (O_3), azot oksitler (NO_x) ve karbon monoksit (CO) konsantrasyonları ve saatlik olarak ölçülen bazı meteorolojik parametreler, O_3 ile NO_x, CO, hava sıcaklığı, rüzgar hızı, bağıl nem ve hava basıncı arasındaki etkileşim eğilimini incelemek için, onların Trabzon'daki kentsel alanda (Akçaabat) günlük değişimlerini dikkate alarak analiz edildi. Bağımsız değişkenler olarak adlandırılan belirli parametrelerin (NO_x ve CO konsantrasyonu, hava sıcaklığı, rüzgâr hızı, bağıl nem ve hava basıncı) etkilerini dikkate alarak O_3 seviyelerinin değişimleri Jaya ve Öğretme-Öğrenme Tabanlı Optimizasyon (TLBO) algoritmaları ile modellenmiştir. Jaya ve TLBO yöntemlerinin doğruluğu belirlenmiş ve bu yöntemler ikinci dereceden, üstel, doğrusal ve güç olmak üzere dört farklı fonksiyona uygulanmıştır. Bu modellerin başarımını test etmek için bazı istatistiksel belirteçler (ortalama karesel hata, ortalama karesel hatanın karekökü, ortalama mutlak hata, ortalama mutlak yüzde hata ve belirleme katsayısı) kullanılmıştır. Sonuç olarak, Jaya ve TLBO algoritmalarının, bazı hava kirletici etkileşimlerinin modellenmesinde regresyon fonksiyonu katsayılarının optimizasyonunda kullanılabileceği ve her parametre için en uygun denklemin ikinci derece fonksiyonundan elde edildiği görülmüştür.

Keywords: *Hava Kirliliği, Ozon konsantrasyonu, Modelleme*

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I. INTRODUCTION

Photochemical air pollution is formed through the interactions between ozone (O_3) and its main precursors of nitrogen oxides (NO_x) and volatile organic compounds (VOC_s) under intense sunlight. It is known that O_3 has an important function in upper layers of atmosphere as it conserves living organisms from sun radiation, but it is accepted as harmful gas in layers nearer to earth's surface. According to Turkey and European Union countries Air Quality Assessment and Management Regulation, the average O_3 amount of 8 hours must be 120 $\mu g/m^3$ [1]. Potential impacts of O_3 to health are irritation to eyes, nose and throat, as well as its effects on vegetation and materials. Surface O_3 is a major component of photochemical smog characterized by high O_3 owing to complex and non-linear chemistry and meteorology. The concentration of ozone in the atmosphere changes with the formation and transport of ozone, photochemical reactions and meteorological factors. O_3 is produced by the reaction of an oxygen molecule (O_2) with an oxygen atom occurring from the photolysis of nitrogen dioxide (NO_2) by solar radiation. However, O_3 is destroyed by reacting with NO to form NO_2 and O_2. In addition, hydrocarbons and VOC_s in the atmosphere are oxidized to CO, CO_2 and water vapour. The oxidation processes include a number of cyclic stages driven by the hydroxyl radical (OH) leading to reactions with the present NO and therefore, leading to the accumulation of O_3. As these complex reactions happen in the atmosphere, measuring O_3 levels alone cannot help in evaluating photochemical conditions [2-7].

Meta-heuristic optimization algorithms solve optimization problems by imitating animal behavior, biological or physical events. Today, a range of meta-heuristic optimization algorithms such as Jaya[8], Teaching-Learning-Based Optimization (TLBO) [9], Artificial Bee Colony (ABC) [10], Coyote Optimization (COA) [11], Cuckoo Search (CS) [12], Crow Search (CSA) [13], Differential Search (DS) [14], Grey Wolf Optimizer (GWO) [15], Harris Hawks Optimization (HHO) [16], Neural Network (NNA) [17], Symbiosis Organisms Search (SOS) [18], Teaching–Learning–Based Artificial Bee Colony (TLABC) [19], Weighted Differential Evolution (WDE) [20] are widely used in solving problems.

In this study, O_3 concentration and its correlation with NO_x, CO and some meteorological parameters in Trabzon (Akçaabat) for 2016 and 2017 datasets obtained from Ministry of Environment and Urban Planning-air quality monitoring stations [21] are modelled using Jaya and TLBO algorithms. There are several studies on estimation algorithms in the literature [22-26].

Jaya algorithm, meaning “victory” in Indian language, was developed by Rao in 2016. This algorithm can maximize the size of a target function by trying to get closer to the best and to get away from the worst among the candidate solutions that are created and refreshed in each iteration [8].

TLBO algorithm simulates the relationship between students and the teacher in the class. The algorithm is consisting of teacher and student stages. The teacher phase represents the education of the students by the teacher. Also, the student phase represents the learning which is the result of the interaction among the students themselves. Further information about the algorithm can be obtained from related reference[9].

The objective of this study is to generate equations being quadratic, exponential, linear and power functions for modeling of O_3 levels via Jaya and TLBO algorithms.

II. METHODOLOGY

Trabzon is a city located at the geographic coordinates of 40°N and 390°E with a population over 779000 with an area of about 4664 km^2. Although there are six different stations measured various pollutants in Trabzon, in this study, Akçaabat station has been chosen because of regional characteristic, providing

different emissions, particularly O_3. Relationships between O_3 emission levels and some meteorological parameters - the other emission (NO_x, CO) levels have been modelled via Jaya and TLBO methods.
In the present work, the objective function of the models is minimization of mean square error (MSE) calculated as follows:

$$\min f(x) = \frac{1}{N}\sum_{i=1}^{N}(P_i - E_i)^2 \tag{1}$$

where N is the number of data sets, E_i is the i^{th} measured O_3 amount, and P_i is the i^{th} estimated O_3 amount for the regression functions. Root mean square error (RMSE), mean absolute error (MAE), mean absolute percentage error (MAPE), and coefficient or determination (R^2) for data sets have been selected to measure the performance of models of Jaya and TLBO.

$$\mathrm{RMSE} = \left[\frac{1}{N}\sum_{i=1}^{N}(P_i - E_i)^2\right] \tag{2}$$

$$\mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}|P_i - E_i| \tag{3}$$

$$\mathrm{MAPE} = \frac{1}{N}\sum_{i=1}^{N}\frac{|P_i - E_i|}{E_i} \tag{4}$$

$$R^2 = 1 - \left(\frac{\sum_{i=1}^{N}(P_i - E_i)^2}{\sum_{i=1}^{N}(P_i - \overline{P}_i)^2}\right) \tag{5}$$

Jaya and TLBO algorithms have been applied to reach optimum coefficient of the regression functions (quadratic, exponential, linear and power) formed with eight delayed data sets. For example, these regression functions have been created depending on time for two independent variables and two delayed data sets as follows:

$$\begin{aligned} Y(t) = {} & w_1 + w_2 \cdot X_1(t-2) + w_3 \cdot X_1(t-1) + w_4 \cdot X_1(t) + w_5 \cdot X_2(t-2) + w_6 \cdot X_2(t-1) \\ & + w_7 \cdot X_2(t) + w_8 \cdot Y(t-2) + w_9 \cdot Y(t-1) \end{aligned} \tag{6}$$

$$\begin{aligned} Y(t) = {} & w_1 + exp\big(w_2 + w_3 \cdot X_1(t-2) + w_4 \cdot X_1(t-1) + w_5 \cdot X_1(t) + w_6 \cdot X_2(t-2) + w_7 \\ & \cdot X_2(t-1) + w_8 \cdot X_2(t) + w_9 \cdot Y(t-2) + w_{10} \cdot Y(t-1)\big) \end{aligned} \tag{7}$$

$$\begin{aligned} Y(t) = {} & w_1 \cdot X_1(t-2)^{w_2}.X_1(t-1)^{w_3}.X_1(t)^{w_4}.X_2(t-2)^{w_5}.X_2(t-1)^{w_6}.X_2(t)^{w_7}.Y(t \\ & -2)^{w_8}.Y(t-1)^{w_9} \end{aligned} \tag{8}$$

$$\begin{aligned} Y(t) = {} & w_1 + w_2 \cdot X_1(t-2) + w_3 \cdot X_1(t-1) + w_4 \cdot X_1(t) + w_5 \cdot X_1(t-2).X_1(t-1) + w_6 \\ & \cdot X_1(t-2).X_1(t) + w_7 \cdot X_1(t-1).X_1(t) + w_8 \cdot X_1(t-2)^2 + w_9 \\ & \cdot X_1(t-1)^2 + w_{10} \cdot X_1(t)^2 + w_{11} + w_{12} \cdot X_2(t-2) + w_{13} \cdot X_2(t-1) \\ & + w_{14} \cdot X_2(t) + w_{15} \cdot X_2(t-2).X_2(t-1) + w_{16} \cdot X_2(t-2).X_2(t) + w_{17} \\ & \cdot X_2(t-1).X_2(t) + w_{18} \cdot X_2(t-2)^2 + w_{19} \cdot X_2(t-1)^2 + w_{20} \cdot X_2(t)^2 \\ & + w_{21} + w_{22} \cdot Y(t-2) + w_{23} \cdot Y(t-1) + w_{24} \cdot Y(t-2).Y(t-1) + w_{25} \\ & \cdot Y(t-2)^2 + w_{26} \cdot Y(t-1)^2 \end{aligned} \tag{9}$$

Population size and maximum number of cycles of the algorithms have been taken 20 and 8000, respectively. The algorithms have been programmed in MATLAB (2014).

III. RESULT AND DISCUSSION

The main statistics of the data sets are given in Table 1. There is a negative correlation between O_3 concentration and NO_x, CO and relative humidity, while air tempereture, wind speed and air pressure have a positive correlation.

Table 1. *The main statistics of the data sets*

Data sets	Unit	Min	Mean	Max	Standart Deviation	Coefficient of variation	Correlation
NO_x	µg/m³	11	35.056	197	21.733	61.995	-0.245
CO	µg/m³	111	1618.634	4151	924.303	57.104	-0.223
Air temperature	°C	0	15.973	29	7.216	45.175	0.051
Wind speed	m/s	1	1.603	3	0.509	31.755	0.196
Relative humidity	%	31	73.896	96	11.12	15.049	-0.194
Air pressure	mbar	998	1013.131	1035	6.262	0.618	0.11

When the findings obtained from models developed with TLBO and Jaya algorithms are examined, it is seen that the best relationship between dependent variable and independent variables is between NO_x-relative humidity and O_3 and the worst relationship is between air pressure and O_3. Considering the functions used in modeling these relationships, it is understood that the function giving the smallest error is quadratic, and the function giving the largest error is the exponential function(Table 2 and 3).

Table 2. *Results of TLBO algorithm model*

Independent Variable	Dependent Variable	Function	MSE	RMSE	MAE	MAPE	R^2
Relative Humudity	O_3	Linear	24.9541	4.9954	3.8567	0.0826	0.7225
	O_3	Power	24.9017	4.9902	3.8801	0.0833	0.7231
	O_3	Exponential	25.8241	5.0817	3.9591	0.0852	0.7128
	O_3	Quadratic	22.8448	4.7796	3.7002	0.0792	0.7459
Air Pressure	O_3	Linear	26.1388	5.1126	3.9375	0.0846	0.7093
	O_3	Power	26.2456	5.1231	3.9597	0.0853	0.7081
	O_3	Exponential	27.6076	5.2543	4.0609	0.0876	0.6930
	O_3	Quadratic	24.1535	4.9146	3.8693	0.0829	0.7314
CO	O_3	Linear	26.4889	5.1467	3.9919	0.0852	0.7054
	O_3	Power	26.6624	5.1636	4.036	0.0863	0.7035
	O_3	Exponential	27.8172	5.2742	4.0894	0.0878	0.6906
	O_3	Quadratic	24.11	4.9102	3.7942	0.0803	0.7319

Table 2 (continuation). *Results of TLBO algorithm model*

Independent Variable	Dependent Variable	Function	MSE	RMSE	MAE	MAPE	R^2
NO_X	O_3	Linear	25.088	5.0088	3.9106	0.0832	0.7210
	O_3	Power	25.0103	5.001	3.9343	0.084	0.7218
	O_3	Exponential	25.9412	5.0933	3.9984	0.0853	0.7115
	O_3	Quadratic	23.3103	4.8281	3.7382	0.0792	0.7408
NO_X-Relative Humudity	O_3	Linear	20.5103	4.5288	3.485	0.0742	0.7719
	O_3	Power	20.6423	4.5434	3.5139	0.0754	0.7704
	O_3	Exponential	21.5837	4.6458	3.6256	0.0777	0.7600
	O_3	**Quadratic**	**19.5954**	**4.4267**	**3.4084**	**0.0723**	**0.7821**
NO_X-CO	O_3	Linear	24.1502	4.9143	3.7867	0.0804	0.7314
	O_3	Power	24.2741	4.9269	3.85	0.0821	0.7300
	O_3	Exponential	25.4763	5.0474	3.9186	0.0834	0.7167
	O_3	Quadratic	22.8192	4.7769	3.7425	0.0789	0.7462
NO_X-Air Temperature	O_3	Linear	24.0054	4.8995	3.7834	0.0806	0.7330
	O_3	Power	24.1707	4.9164	3.8135	0.0815	0.7312
	O_3	Exponential	25.1732	5.0173	3.9114	0.0838	0.7200
	O_3	Quadratic	22.2127	4.713	3.6721	0.0776	0.7530
NO_X-Relative Humudity-Wind Speed	O_3	Linear	20.8774	4.5692	3.5222	0.0752	0.7678
	O_3	Power	21.1807	4.6023	3.5513	0.0762	0.7644
	O_3	Exponential	21.6881	4.657	3.6596	0.0785	0.7588
	O_3	Quadratic	19.8181	4.4518	3.4388	0.0734	0.7796
NO_X-Air Temperature-Wind Speed	O_3	Linear	22.6849	4.7629	3.6651	0.078	0.7477
	O_3	Power	23.0582	4.8019	3.7316	0.0795	0.7436
	O_3	Exponential	23.9079	4.8896	3.7838	0.0812	0.7341
	O_3	Quadratic	21.8516	4.6746	3.6214	0.0769	0.7570

Table 3. *Results of Jaya algorithm model*

Independent Variable	Dependent Variable	Function	MSE	RMSE	MAE	MAPE	R^2
Relative Humudity	O_3	Linear	25.0469	5.0047	3.8678	0.0829	0.7214
	O_3	Power	24.9278	4.9928	3.8823	0.0833	0.7228
	O_3	Exponential	28.4483	5.3337	4.1710	0.0886	0.6836
	O_3	Quadratic	23.0213	4.4041	3.3021	0.0796	0.7320
Air Pressure	O_3	Linear	26.3712	5.1353	3.9638	0.0854	0.7067
	O_3	Power	26.3020	5.1286	3.9693	0.0855	0.7075
	O_3	Exponential	28.4661	5.3354	4.1563	0.0900	0.6834
	O_3	Quadratic	25.8934	5.0643	3.8432	0.0842	0.7120

Table 3 (continuation). *Results of Jaya algorithm model*

Independent Variable	Dependent Variable	Function	MSE	RMSE	MAE	MAPE	R^2
CO	O_3	Linear	27.5249	5.2464	4.0798	0.0871	0.6937
	O_3	Power	27.7776	5.2704	4.1210	0.0883	0.6909
	O_3	Exponential	29.9449	5.4722	4.2226	0.0906	0.6668
	O_3	Quadratic	26.7520	5.1732	3.9877	0.0834	0.7182
NO_X	O_3	Linear	26.0840	5.1073	3.9975	0.0853	0.7097
	O_3	Power	25.8172	5.0811	4.0216	0.0859	0.7127
	O_3	Exponential	27.6407	5.2574	4.1382	0.0883	0.6924
	O_3	Quadratic	24.9367	5.0122	3.9562	0.0809	0.7238
NO_X-Relative Humudity	O_3	Linear	22.6981	4.7642	3.6572	0.0778	0.7474
	O_3	Power	22.1524	4.7066	3.6758	0.0794	0.7535
	O_3	Exponential	27.3535	5.2301	4.0873	0.0878	0.6956
	O_3	**Quadratic**	**20.2672**	**4.4910**	**3.0435**	**0.0685**	**0.7925**
NO_X-CO	O_3	Linear	26.7909	5.1760	4.0365	0.0863	0.7019
	O_3	Power	29.5671	5.4376	4.2719	0.0886	0.6710
	O_3	Exponential	30.2055	5.4960	4.2862	0.0946	0.6639
	O_3	Quadratic	26.1360	5.0645	3.9031	0.0823	0.7080
NO_X-Air Temperature	O_3	Linear	25.6974	5.0693	3.9716	0.0845	0.7140
	O_3	Power	26.3697	5.1351	4.0540	0.0870	0.7066
	O_3	Exponential	27.7133	5.2643	4.1176	0.0886	0.6916
	O_3	Quadratic	24.3560	5.0192	3.7396	0.0810	0.7235
NO_X-Relative Humudity-Wind Speed	O_3	Linear	23.8372	4.8823	3.6551	0.0786	0.7347
	O_3	Power	21.9946	4.6898	3.6256	0.0776	0.7552
	O_3	Exponential	24.8762	4.9876	3.8821	0.0844	0.7232
	O_3	Quadratic	21.5493	4.5239	3.5927	0.0740	0.0765
NO_X-Air Temperature-Wind Speed	O_3	Linear	25.4261	5.0424	3.9448	0.0845	0.7171
	O_3	Power	27.6849	5.2616	4.1076	0.0864	0.6919
	O_3	Exponential	31.3367	5.5979	4.3522	0.0941	0.6513
	O_3	Quadratic	24.3786	5.0213	3.3826	0.0823	0.7195

Optimum coefficients (w_i) of the independent variables (x_i) from these regression functions by both algorithms have been obtained. Obtained optimum coefficients from Jaya analysis of linear function explaining relationship between NO_x emission levels - relative humidity and O_3 emission levels are shown as an example in Table 4.

Table 4. *The coefficient obtained from Jaya analysis*

Coefficients									
w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_{10}
0.027	0.094	-0.072	0.049	-0.010	0.165	0.047	-0.036	0.372	-0.614
Coefficients									
w_{11}	w_{12}	w_{13}	w_{14}	w_{15}	w_{16}	w_{17}	w_{18}	w_{19}	w_{20}
0.035	0.007	-0.017	0.119	0.033	0.098	0.030	0.038	-0.332	0.070
Coefficients									
w_{21}	w_{22}	w_{23}	w_{24}	w_{25}	w_{26}	w_{27}			
0.032	-0.002	0.078	0.056	0.034	0.121	0.545			

Figure 1 illustrates a comparison of the measured O_3 with the predicted ones from the determined quadratic function by depending on NO_X and relative humidity. Figure 2 also supplies a different presentation of the performance for the obtained best fitting model via Jaya analysis. If the points gather around the diagonal, smaller error and greater R^2 values are obtained.

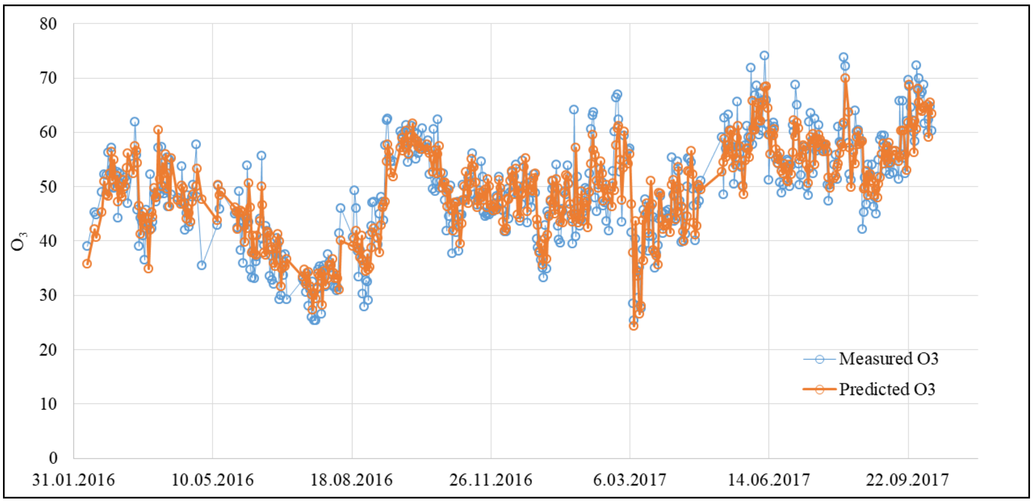

Figure 1. *The comparison of the measured O_3 with the predicted (depending on NO_X - relative humidity) ones varying by time*

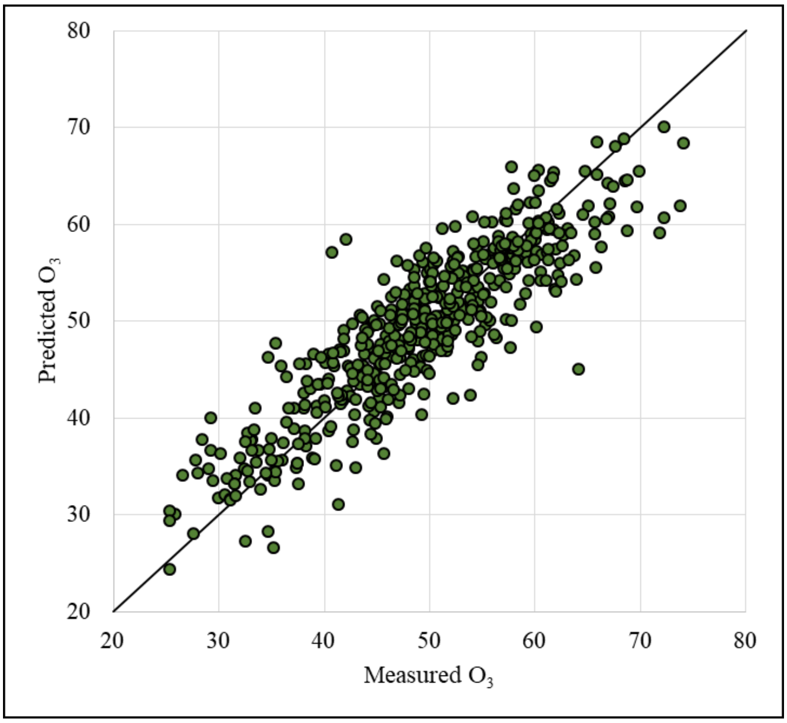

Figure 2.*The comparison of the measured O_3 with the predicted (depending on NO_X – relative humidity) ones by JAYA algorithm model*

IV. CONCLUSION

In order to model which chemicals and meteorological factors are more effective in the formation of O_3, which is a component of photochemical air pollution, the data set was first analyzed, and then the relationship between O_3 concentration and some parameters was modeled with Jaya and TLBO algorithms. When the main statistics of the data sets were analyzed, it was observed that the O_3 concentration was negative correlation between NO_x, CO and relative humidity, while it was positively correlated with other parameters. According to the data obtained from both algorithms, the best fit equation between ozone and NO_X - relative humidity is obtained from the quadratic function. Also, the results of the study show that the quadratic function provide the best fit equation for each parameter. Higher correlations of ozone with NO_X-relative humidity than of ozone with the other independent variables are found pointing that NO_X and relative humidity are highly effective on modelling of ozone. However, the Jaya model shows the relationship between ozone with NO_X and relative humidity by a slightly higher correlation than the TLBO model. On the other hand, lower correlations pointed that the ozone formation in this region depends on many meteorological and chemical factors. Results of both models suggest that formation of surface ozone pollution is much more closely related to the amount of NO_X and relative humidity rather than other parameters.

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