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The characteristics of ozone concentration over the maritime equatorial stratospheric region derived from the quasi-biennial oscillation

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Abstract. The characteristics of ozone concentration [O₃] over the Maritime Equatorial Stratospheric region until now are not yet fully understood well due to the limitation of data observations. However, there are many techniques to derive ozone concentration data; from satellite, in-situ observation, modeling, etc. We have investigated, then found a good agreement between the characteristics of ozone concentration and Quasi-Biennial Oscillation (QBO). This study mainly concerned with the analysis of the stratospheric zonal wind from Singapore's QBO monthly data at 100-10 hPa layers. Total ozone, ozone mass mixing ratio, and stratospheric temperature were considered in the analysis. Predominant peak oscillation in each layer was investigated by using the spectral technique. The result shows that a strong signal of zonal wind oscillation pattern was evident at 30 hPa layer. As the altitude decreases, zonal wind oscillation decays. Box-Jenkins final model contained 28 months of a seasonal component (5,0,4)(0,1,0)²⁸ and a percentage error of 46.6%, whereas multiple linear regression obtained a quite good correlation score, which was about 0.55.

Keywords : ozone, stratospheric temperature, zonal wind oscillation, Box-Jenkins.

1. Introduction

The study of the equatorial stratospheric region which came to be known as quasi-biennial oscillation or QBO firstly discovered by Ebdon [1] and Reed et al. [2]. This phenomenon is characterized by easterly and westerly winds, which originates from above 30 km and propagates downward through the stratosphere at the speed of 1 km per month. The alternating wind regimes repeat at varying intervals of 22 to 34 months, with an average period of ~28 months [3]. The maximum amplitude of QBO mostly associated with the westerly wind rather than the easterly, and its symmetry toward the equator follows the Gaussian distribution. Even though this phenomenon occurs in the tropics area, but it also influences the stratospheric flow from pole to pole. Therefore, QBO particularly impacts the atmospheric dynamics and changes the circulation of chemical constituents such as O₂, H₂O, and CH₄. Furthermore, it also affects the distribution and transport of trace gases, which may be a factor that causes stratospheric ozone depletion [3].



As proposed by Holton and Lindzen [4], the mechanism of QBO is the result of interaction between the mean flow and the equatorial wave equation mode. They are the first that modeled the QBO based on the planetary equatorial wave propagation, known as Kelvin waves and Rossby-gravity waves. Hence, the QBO only occurs in the equatorial region that caused by these waves, and formed in the region of about 12°N - 12°S [5]. This area provides considerable energy from the release of latent heat in large-scale convective clouds to form planetary scale-waves and push them down to the lower stratosphere.

The QBO in the total ozone (TOZ) amount firstly reported by Funk and Garnham [6]. A large number of studies describe possible connections between this phenomenon and the interannual variation of ozone [7,8]. These studies mainly reported that the QBO influences TOZ amount at about 1–2%, with a high correlation ($r > 0.7$) based on the equatorial zonal wind, especially at 30 and 50 hPa.

Additionally, there is evidence suggesting that the variation of TOZ at $\pm 10^\circ$ latitude is nearly in phase with the zonal winds at 30 hPa. Interannual variability of equatorial TOZ is dominated by the QBO that appears after removing the annual cycle of original data [3]. Moreover, the clear signals in temperature and QBO are revealed in the tropics. The equatorial temperature anomalies associated with the QBO in the lower stratosphere are in the order of $\pm 4\text{K}$, which maximize at near 30–50 hPa. Holton and Tan [5] have proven that QBO will satisfy thermal wind equations if the vertical shifts of zonal wind (wind shear) associated with the temperature in the stratosphere. Based on this result, we then investigate how the zonal wind QBO and stratospheric temperature anomalies are related to the TOZ in the equatorial region. Meanwhile, we thought that the ozone concentration which is TOZ, could be derived from predicted wind QBO over the maritime equator region.

2. Data and Method

2.1 Data

To study the ozone variations, we used the monthly total ozone columns (TOZ) dataset of a MERRA-2 satellite from 1988 to 2018, obtained from <https://disc.gsfc.nasa.gov/datasets/>. While the zonal wind data of this study were taken from Singapore's QBO dataset that available since January 1979 until present. This dataset is observed by regular radiosonde measurements of daily vertical wind profiles at the levels of 100 to 10 hPa. Moreover, stratospheric temperature data from NOAA NCEP-NCAR CDAS-1 reanalysis were also used. This dataset was accessed through the IRI operational website, online data repository and analysis tools. Both zonal wind and stratospheric temperature data were on a month-by-month basis. As a review, the ozone mass mixing ratio data were included in the analysis.

2.2 Method

In this present study, we applied spectral analysis techniques, hereafter referred to power spectral density and wavelet. Time series data was decomposed into time-frequency space, then variability dominant modes and variations modes in time would be determined as well [10]. Power spectral density function shows the strength of each variation (energy) as the function of frequency, mostly uses to maintain the magnitude of frequency variations. This method is useful to determine a level in which stratospheric zonal wind has similar characteristics with ozone. As similar to power spectral density, wavelet analysis is known as an effective tool for analyzing local variations of power within a time series by decomposing it into time-frequency space [10]. This method has been used in the previous study e.g. the tropical convection [11], and the El Niño–Southern Oscillation (ENSO) [12,13].

The ozone model was developed to predict the future monthly of TOZ by using zonal wind QBO and temperature data, especially at 30 hPa. As a univariate method, ARIMA (Autoregressive Integrated Moving Average) model was used to derive ozone concentration data from the QBO. This method divided the dataset into a training set for model learning and a testing set for validating an appropriate ARIMA model. For the detail of this method, please refer to Box and Jenkins [14]. In this case, the total ozone column is a single layer property, where an extracted data typically represents the equatorial region in 0° latitude and 100°E longitude. TOZ anomaly was obtained by subtracting monthly dataset

with the average of TOZ from January 1988 to January 2018. Finally, the selected ARIMA model was then compared to the multiple regression model that formed from zonal wind QBO and temperature data.

3. Results and Discussion

Figure 1 shows the PSD of monthly zonal wind data for period of January 1988 – January 2018 which starts from 100 to 10 hPa’s layers. From this figure, it is clearly shown that pre-dominant peak oscillation is about 28 month that related to the Quasi-Biennial Oscillation (QBO) phenomenon.

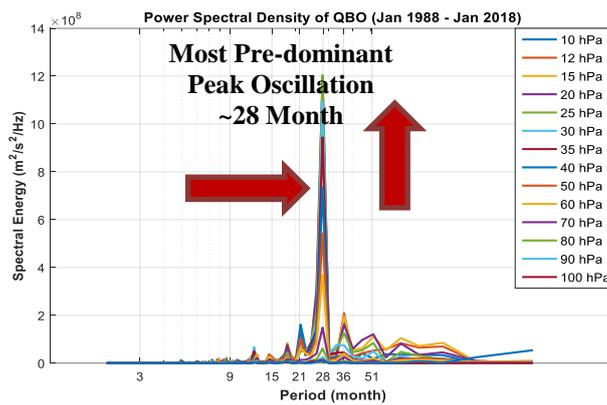


Figure 1. The Power Spectral Density of QBO for period of January 1988 to January 2018.

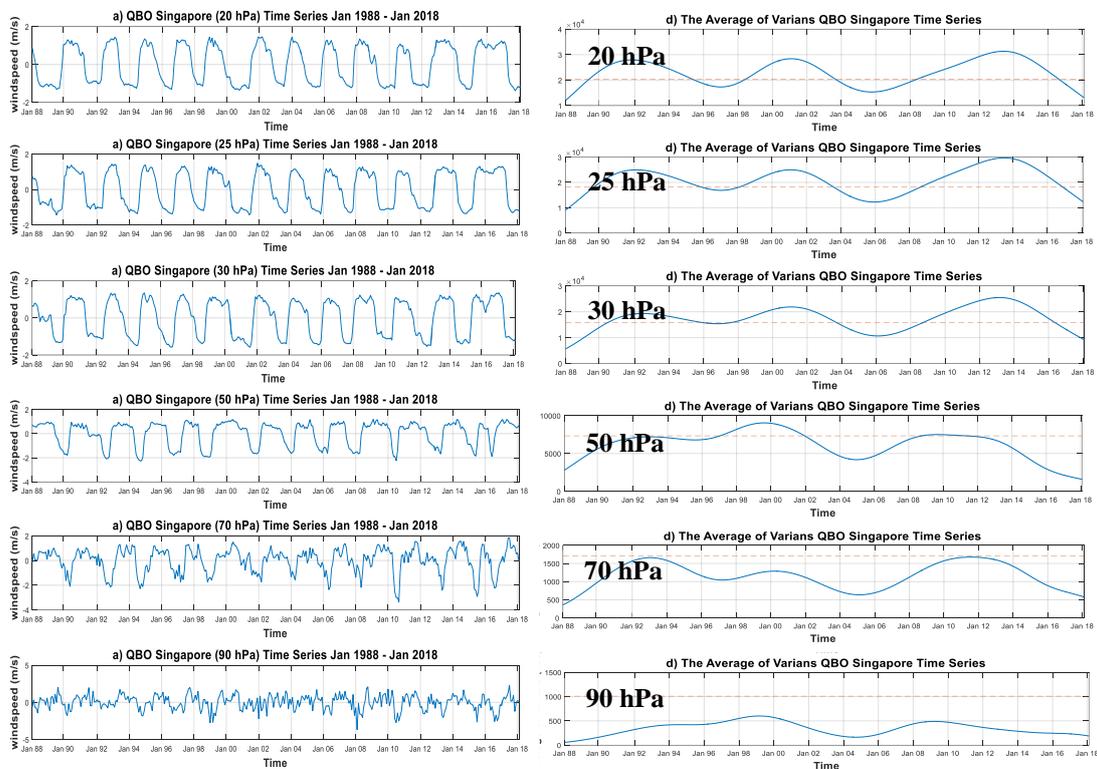


Figure 2. Time series of zonal wind (left-hand panel) and the average of varians (right-hand panel) at 20, 25, 30, 50, 70, and 90 hPa layers for period of January 1988 to January 2018.

From figure 2, in the left panel, we can see a similar oscillation pattern at the upper layer of the stratosphere (20 – 30 hPa), whereas inconsistency appears at 50 hPa until the bottom layer. The same result is also displayed by the average of variance for each layer as shown in the right panel. A periodic easterly and westerly phase of wind is clearly shown in the layer of 20-50 hPa. Along with a decrease in the altitude, zonal wind oscillation decays by the stratospheric disturbance. It can be seen from the random oscillation of QBO signal that turns up in the bottom layer.

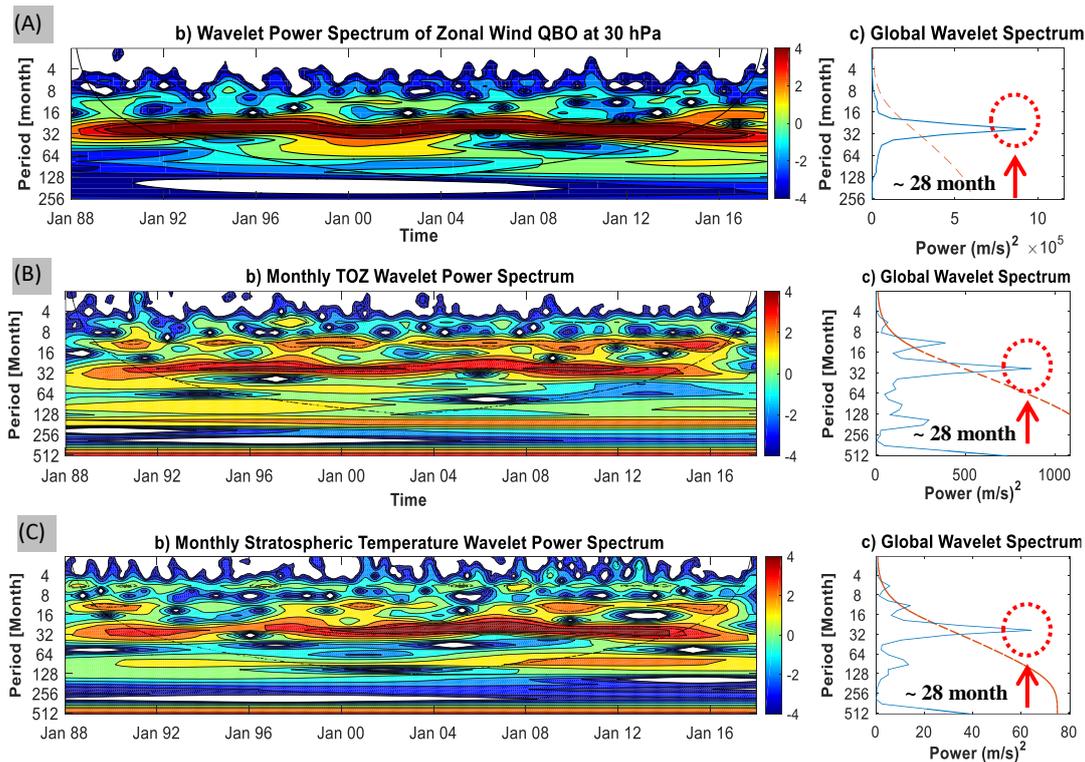


Figure 3. Wavelet analysis of (A) zonal wind QBO at 30 hPa (B) total ozone column and (C) stratospheric temperature at 30 hPa for period of January 1988 to January 2018.

Since our analysis only focussed on 30 hPa layer, we applied the wavelet technique to investigate when the strong signal has occurred. Then, we obtained the pre-dominant peak oscillation of 30 hPa was still 28 month. The same method was also used for monthly TOZ and stratospheric temperature. From the global wavelet spectrum, we saw that pre-dominant oscillation of ozone was around 28 months, with two other oscillation in 6 and 12 months. It means that the variation of ozone concentration and temperature at the stratospheric layer were affected by the wind QBO, Annual Oscillation (AO) and Semi-Annual Oscillation (SAO) as shown in figure 3.

Then, we concentrate to analyze the comparison between TOZ against QBO and temperature anomalies over the maritime equatorial stratospheric region, started from January 2001 to December 2017 as shown in figure 4. From here, we can see a good pattern of both parameters. Ozone concentration in the stratosphere is a combination of the transport mechanism and photochemical process at the layer of ~30 – 20 hPa [15]. Figure 4(a) shows that there is a difference of ozone concentration when the westerly and easterly phase of QBO occurred. Generally, it increases in the westerly phase and conversely, decreases in the easterly phase. Thereby, the oscillation of zonal wind at 30 hPa layer influenced the ozone fluctuation. The transport mechanism in the stratosphere was not only associated with the wind regimes, but also the temperature. A negative anomaly of temperature described the low

of temperature at the easterly phase of QBO and related to the descending rate of ozone which resulted in ozone depletion as shown in figure 4(b). In other words, a negative anomaly of TOZ was associated with negative anomaly of temperature, hence the ozone absorbed solar and infrared radiation. The stratospheric layer with slight ozone concentration will cause a limited amount of absorbed radiation, so the temperature is low.

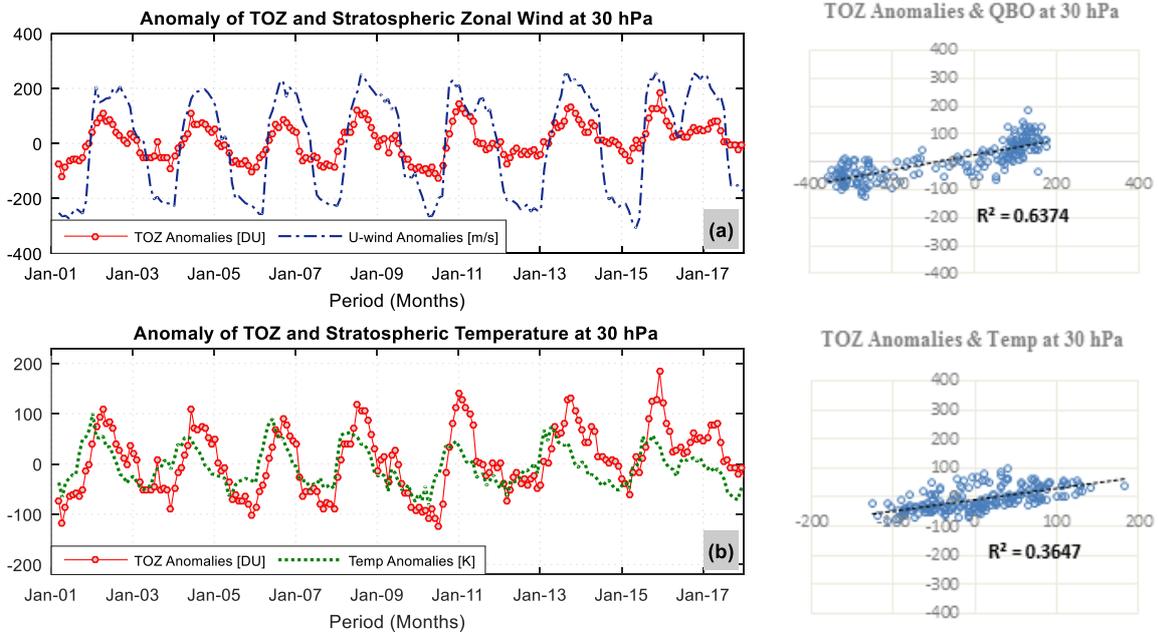


Figure 4. Time series comparison of TOZ anomalies against (a) stratospheric zonal wind and (b) temperature at 30 hPa during the 2001-2017 period (left panel) and scatter plot for (a) and (b) (right panel).

Please note, the similar result is also obtained by Hermawan [10] that compared QBO and ozone anomalies from AIRS satellite over Kototabang, West Sumatera. Hereafter, we made the scatter plot between TOZ anomalies with QBO and stratospheric temperature at 30 hPa layer as shown in the right panel of figure 4. We found a good agreement based on the coefficient determination, which is 0.64 to QBO and 0.36 to temperature. It means that 64% of TOZ anomaly can be explained by the QBO phenomenon.

Finally, to derive ozone concentration from Quasi-Biennial Oscillation data, we used Box-Jenkins or so-called ARIMA method. The first step of the method is the identification of stationarity of the data by time series plot, autocorrelation functions (ACF) and partial autocorrelation functions (PACF) of the whole dataset. Then, the next step is the determination the order of AR and MA processes from the PACF and ACF patterns which useful to consider the initial model. Based on the least square criteria, the model parameters were calculated. A diagnostic test consisted of the significance parameter and residual white noise test was applied to the initial model (right panel of figure 5). If the model passed the test, it will be used to forecast ozone concentration for the next period. As in the spectral analysis above, the QBO contains seasonal variation which oscillates around 28 months. Therefore, Box-Jenkins final model was SARIMA (5,0,4)(0,1,0)²⁸ with model equation, $Y_t = 0.3Y_{t-1} + 1.11Y_{t-2} + 0.2Y_{t-3} - 0.87Y_{t-4} + 0.16Y_{t-5} + e_t - 1.09e_{t-1} + 0.36e_{t-2} + 1.29e_{t-3} + 0.44e_{t-4} - e_{t-28} + 1.09e_{t-29} - 0.36e_{t-30} - 1.29e_{t-31} - 0.44e_{t-32}$ and percentage error of 46.6%

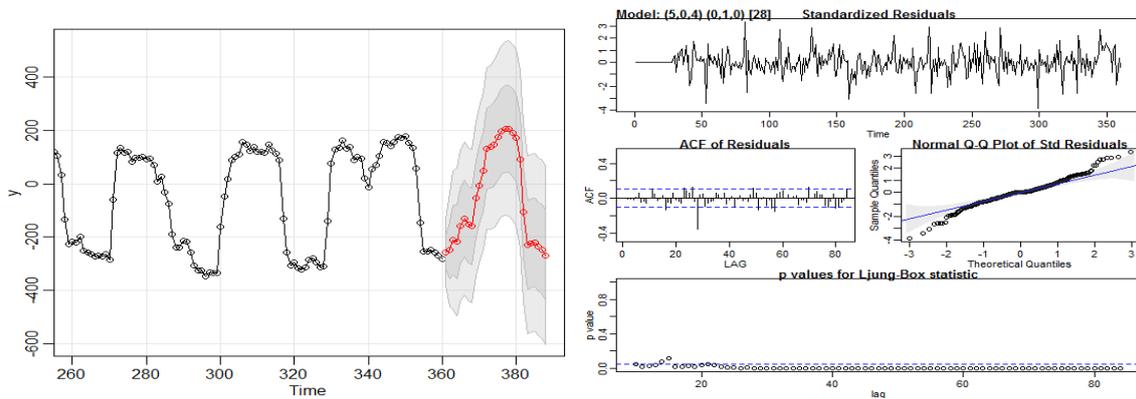


Figure 5. The forecast model of QBO at 30 hPa layer (left panel) and the result of diagnostic testing (right panel) from January 1988 to December 2017.

We have divided the QBO into 2 dataset, which were a training and a testing set. For model validation, comparison between the data observation and model has been done. The dataset of testing started from April 2008 to December 2017, were validated for each 28 months as shown in figure 6 below.

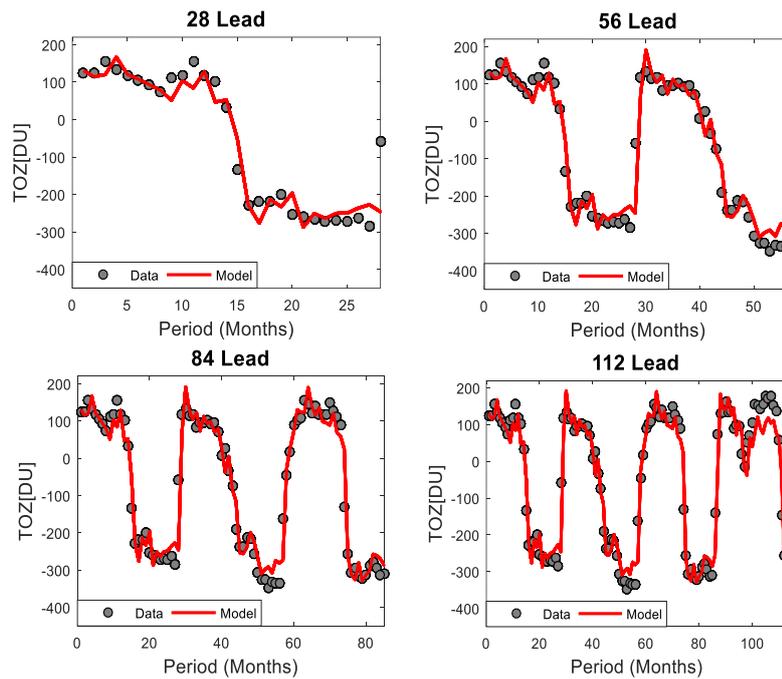


Figure 6. The model validation of SARIMA (5,0,4)(0,1,0)²⁸

If we include the temperature at 30 hPa in the analysis, then developed a multiple linear regression model (figure 7) to derive ozone concentration data, we obtained the correlation score was 0.55. Meanwhile, the model with 2 predictors is still good enough to explain the ozone concentration.

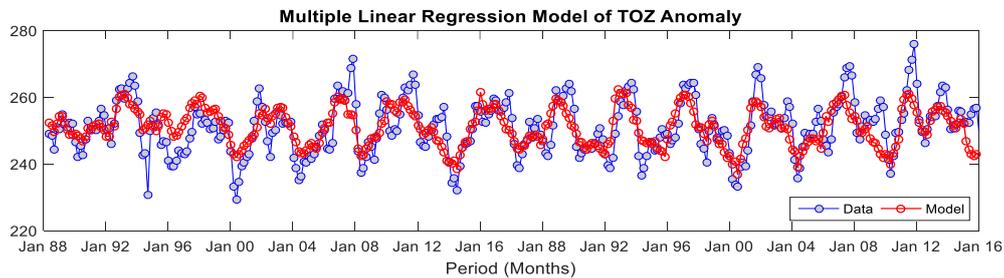


Figure 7. Comparison of TOZ with multiple linear regression model

4. Conclusion

The behavior of ozone concentration at the equatorial region is important to be investigated due to the ozone depletion. Since equatorial TOZ is well correlated with the zonal wind and stratospheric temperature, in this present study we have investigated the QBO and the temperature to derive ozone concentration data. The pre-dominant peak oscillation of QBO from Power Spectral Density (PSD) and wavelet is around 28 months, as the same as temperature oscillation. The result shows that zonal wind oscillation pattern was evident by a strong signal at 30 hPa layer. Zonal wind oscillation decays by the decreasing of the altitude. As the results of the TOZ comparison to zonal wind and temperature anomaly for a period of January 2001 to December 2017, the coefficient determinations (R^2) were obtained about 0.64 and 0.36, respectively. Both parameters look similar to each other. For this reason, we developed a model prediction of ozone concentration using Box-Jenkins and multiple linear regression (MLR). Box-Jenkins final model contains seasonal component of 28 month $(5,0,4)(0,1,0)^{28}$ with the model equation is $Y_t = 0.3Y_{t-1} + 1.11Y_{t-2} + 0.2Y_{t-3} - 0.87Y_{t-4} + 0.16Y_{t-5} + e_t - 1.09e_{t-1} + 0.36e_{t-2} + 1.29e_{t-3} + 0.44e_{t-4} - e_{t-28} + 1.09e_{t-29} - 0.36e_{t-30} - 1.29e_{t-31} - 0.44e_{t-32}$ and percentage error of 46.6%, whereas MLR obtained a fairly good correlation score, that was about 0.55.

Acknowledgments

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