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Multivariate methods to predict ground level ozone during daytime, nighttime, and critical conversion time in urban areas

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ABSTRACT

Ground–level ozone (O_3) is known to exhibit strong daily variations that lead to complexity of the pollutants' analysis and predictions. This study aimed to introduce and explore the variations in O_3 concentrations during daytime (DT), nighttime (NT), and critical conversion time (CCT) using multiple linear regression (MLR) and principal component regression (PCR) analyses. The original variables and principal component analysis (PCA) results were used as the input for MLR analysis. Hourly averages of six air pollutants and four meteorological parameters at Shah Alam during 1999–2009 were selected for this study. The monitoring records in 2010 were used to assess the developed models using several performance indicators. Results showed that the MLR model during DT exhibited optimal performance in terms of normalized absolute error, index of agreement, prediction accuracy, and coefficient of determination (R^2) with values of 0.2762, 0.9211, 0.8581, and 0.7354, respectively. PCR during CCT also showed significantly higher performance than that during DT and NT. This result was evidenced by higher percentage of total variances, which could be explained by the selected variables in PCA during CCT.

Keywords: *MLR, PCR, performance indicators, NO_2 photolysis, NO titration*

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1. Introduction

Ground–level ozone (O_3), a secondary air pollutant from anthropogenic activities, is one of the critical air pollutants that is always associated with degrading air quality worldwide. It is also a greenhouse gas in both the stratosphere and troposphere (Chattopadhyay and Chattopadhyay, 2012). Exposure to O_3 may harm human health via respiratory diseases, and lead to a decrease in lung function (Banan et al., 2013). In the presence of sunlight, nitrogen dioxide (NO_2) undergoes photochemical reactions to produce free oxygen atom (O), which later reacts with oxygen molecules (O_2) to form O_3 (Duenas et al., 2004; Azmi et al., 2010). Once O_3 is created, it is destroyed through several pathways, such as nitric titration and surface deposition (Abdul–Wahab et al., 2005).

The dependency of O_3 formation toward UV light is associated with its clear daily variations. As a result, significant differences exist between daytime (DT) and nighttime (NT) O_3 based on the diurnal plots (Han et al., 2011; Reddy et al., 2011; Ghosh et al., 2013). Various studies reported that the daily maximum O_3 concentration is reached at late afternoon, similarly this value is reached at approximately 2 pm in Malaysia (Duenas et al., 2004; Azmi et al., 2010; Ghazali et al., 2010). O_3 concentration variations show an interesting pattern in the morning because of the increment in O_3 precursors emitted by various anthropogenic activities. Jimenez–Hornero et al. (2010) mentioned that O_3 reaches the lowest concentration in the morning because of the higher rate of NO titration. Once the minimal point is reached, O_3 starts to increase with rising NO_2 concentration, thereby promoting NO_2 photolysis. The point when the NO_2 photolysis rate is higher than the NO titration rate is very crucial in ground–level O_3 chemistry because the difference in the chemical reaction's rate is expected to result in O_3 accumulation. Toh et al. (2013) reported that air pollutants, such as O_3, are very responsive to changes in meteorological parameters. Thus, elevated O_3 levels are often associated with intense solar radiation, high temperature, minimal rainfall, low wind speed, and low relative humidity.

The study of ozone variations is complex because of various possible precursors, photochemical processes, and meteorological factors (Chattopadhyay and Chattopadhyay, 2012; Toh et al., 2013). In addition, the interactions among O_3, its precursors, and meteorological parameters occur within a wide range of temporal and spatial scales (Abdul–Wahab et al., 2005). In explaining the variations in O_3 concentration, various approaches have been applied. There are five multivariate techniques, such as multiple linear regression (MLR), principal component analysis (PCA), cluster analysis, Fourier analysis, and artificial neural networks which have been exploited to explain the variability in large air pollution data (Sousa et al., 2007; Ozbay et al., 2011; Dominick et al., 2012). In Malaysia, Ghazali et al. (2010) reported that the use of MLR in predicting O_3 at an urban station is efficient and it is a highly useful tool in providing early information to the public. PCA, as a multivariate technique, has been used in ground–level ozone studies worldwide (Abdul–Wahab et al., 2005; Ozbay et al., 2011).

According to the literature, data on O_3 prediction using PCA in tropical areas, such as Malaysia, are unavailable. The present study aimed to present the results of MLR analyses using the original variables and principal components (PCs) as the inputs for three different time periods, namely, DT, NT, and critical conversion time

(CCT) in Malaysia. This study is the first to attempt to introduce and explore the possibilities of explaining the variation in O_3 concentration using CCT of ground–level O_3 formation in the study area.

2. Methodology

2.1. Location of sampling station

The air quality and meteorological parameters used in this study were collected from Shah Alam monitoring stations (N0 3°4.636, E 101°30.373), a major city located about 25 km west of Kuala Lumpur, the capital of Malaysia (Figure 1). The city is served by six major highways, which experience heavy traffic in the morning and late afternoon rush hours (Azmi et al., 2010). Mohamed et al. (2011) reported that Shah Alam is a heavily industrialized area with high pollution, with a population of more than half a million, and high traffic density. Various studies have selected the city as an important urban area in Malaysia (Azmi et al., 2010; Ghazali et al., 2010; Latif et al., 2012). Climatically, Shah Alam has a tropical rainforest climate, with March being the warmest month. Seasonal heavy rains are common in November during the Northeast Monsoon (Azmi et al., 2010). The monitoring station is located in a large residential area near several industrial areas, such as Subang Industrial Park and Glenmarie Industrial Park (Azmi et al., 2010; Ghazali et al., 2010). Weak prevailing winds in the area may cause air pollutants to be trapped in stagnant air (Mohamed et al., 2011). Thus, high ozone concentrations are observed at Shah Alam with several exceedances when the hourly average surpasses the Malaysia Ambient Air Quality Guidelines limit of 100 ppb per 1 h (Ghazali et al., 2010).

2.2. Data collection

Continuous hourly air quality data from January 1999 to December 2010 were obtained from the Air Quality Division of the Department of Environment, Ministry of Natural Resources and Environment of Malaysia. This study utilized 10 variables that were divided into two groups. One group comprised six air pollutants, such as ground–level ozone (O_3), nitrogen dioxide (NO_2), nitric oxide (NO), sulfur dioxide (SO_2), carbon monoxide (CO), and particulate matter with aerodynamic diameter less than 10 µm (PM_{10}). The other group was composed of four meteorological parameters, such as temperature, relative humidity, wind speed, and incoming solar radiation.

These variables were selected based on their relationship with ozone. NO_2, NO and CO are principle precursors to ozone production (Clapp and Jenkin, 2001; Seinfeld and Pandis, 2006; Ahamad et al., 2014). Whereas, (Ultraviolet B) UVB is the main ingredients in ozone photochemical reactions and without UVB, the reactions could not be completed (Tiwary and Colls, 2009). The relationship between O_3 and temperature is obtained through UVB and high relative humidity which indicates wet or rainy conditions that can promote ozone scouring. Furthermore, wind is considered as a dispersion agent to any air pollutant in the atmosphere. Additionally, PM_{10} and SO_2 are primary air pollutants that are being emitted from similar sources to ozone precursors. Therefore, increases in these pollutants may provide indication in increasing ozone concentrations.

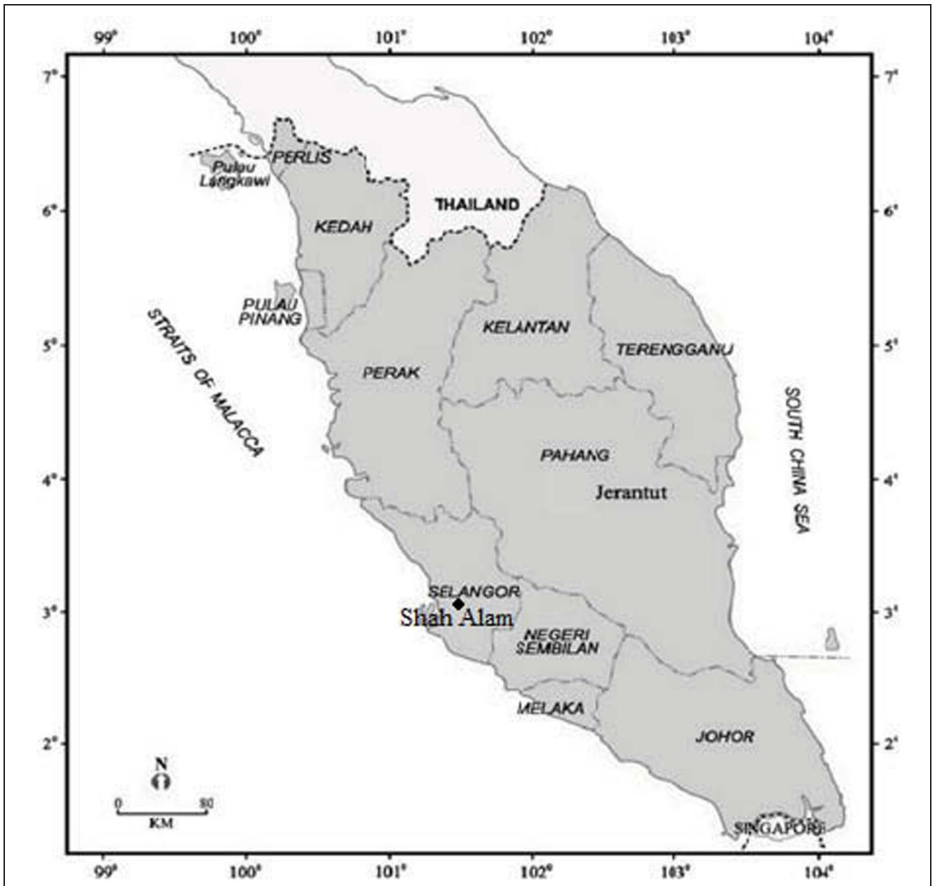

Figure 1. *Location of Shah Alam in Peninsular Malaysia.*