Ambient Formaldehyde Concentration Prediction from the Relationship of Formaldehyde, Ozone and 1,3-butadiene

Paitoon Mueanpetch, Winai Somboon, and Woranut Keotsinchai

***Abstract*—**The mathematical ambient formaldehyde modeling was established using the relationship between formaldehyde (FD), ozone and 1,3-butadiene (BD) concentration data collected at Map Ta Phut Industrial Estate (MTPIE) area, Rayong province, Thailand. The concentrations of formaldehyde and ozone were related with linear method, exponential method, logarithm method and power function method and it was found that all methods gave the R^2 values more than 0.5. The models were built on all four relationship methods and used to predict the ambient formaldehyde concentration during January 2012 to April 2013. The simulation data were compared to collect data at the same period of time. It was found that the logarithmic relationship of [FD] = 4.336 ln[Ozone] - 11.59 was fitted the collected data best with less than 28.3% MAPE.

***Keywords*—**1,3-butadiene,Formaldehyde prediction modeling, Map Ta Phut Industrial Estate, Ozone

I. Introduction

FORMALDEHYDE is a toxic air pollutant generated from many aspects such as combustion process, forest burning and the atmospheric photochemical oxidation of organic compounds. The World Health Organization (WHO) has reported in 2002 that 70 – 90% of total atmospheric formaldehyde was occurred by the photochemical formation [1]. The reaction of many hydrocarbon compounds such as methane, isoprene, biogenic and anthropogenic terminal alkenes compound, could interact with the oxidizing agents and produced formaldehyde (FD) [2]. Methane is a common substance which used to describe the formaldehyde formation. When methane interacts with hydroxyl radical, resulted in FD and nitrogen dioxide (NO_2) [3]. In addition, FD can produce form the reaction between ozone and unsaturated hydrocarbon compounds such as alkenes then convert to FD and other carbonyl compounds, for example 1,3-butadiene, 3-methyl-1-butene, α-pinene (in perfume) etc. [4]-[8]. However, the reaction which investigated in a laboratory was not conforming to the reaction obtained under ambient air.

Paitoon Mueanpetch, Department of Chemistry, Faculty of Science, King Mongkut's University of Technology Thonburi, Bangkok, 10140 Thailand (Corresponding e-mail: Iddariss@gmail.com)

Assoc.Prof.WinaiSomboon (Ph.D), Department of Chemistry, Faculty of Science, King Mongkut's University of Technology Thonburi, Bangkok, 10140 Thailand (e-mail: Winai.som@kmutt.ac.th)

Asst.Prof.WoranutKeotsinchai (Ph.D.), Department of Mathematic, Faculty of Science, King Mongkut's University of Technology Thonburi, Bangkok, 10140 Thailand (e-mail: Woranut.keo@kmutt.ac.th)

The statistical method which gained interest was used to study the relationship of ambient FD and other pollutants. Friedfeld et al. studied the contribution of primary and secondary source to FD concentration by using the regression model coupled with time series. The results showed that the using of the linear regression which distinguished primary (carbon monoxide; CO) and secondary (Ozone) contributions to predict FD concentration [9].

In this study, the correlated of ambient formaldehyde (FD), ozone and 1,3-butadiene (BD) concentration in Map Ta Phut Industrial Estate (MTPIE) area were studied by using mathematical modeling including regression, exponential and logarithmic equation. These models were compared with the collected data and the most suitable one to predict the ambient FD concentration.

II. Procedure

A. The collected data

Two fence line monitoring stations were operated by the Map Ta Phut Industrial Estate (MTPIE), Rayong province, Thailand. These sites were collected continuous by measurement of FD, ozone and BD concentrations. The data was collected during January 2011 to April 2013. The Ozone and the FD concentrations were detected by using the differential optical absorption spectroscopy system (DOAS). The BD concentration was used online gas chromatograph instrument. The collected data was converted from hourly concentration to monthly concentration.

B. Relation study and Modeling application

The linear regression, exponential and logarithmic function were applied to study the relationship between the monthly FD, ozone and BD concentration. The correlation of ozone-FD and BD-FD were compared. The equation of the high correlations was converted to the FD prediction models.

C. Comparison of predicted and collected formaldehyde

The predicted FD concentrations were compared with the collected FD data and mean absolute percentage error (MAPE) was determined.

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III. Result and Discussion

A. The pollutants concentration

In 2011, the concentration of FD, Ozone and BD showed the changing concentration level in Fig. 1. The variation of the FD concentrations was corresponded to ozone concentration. The concentration of FD and ozone which occurred in winter was high, while the BD concentration was low by the atmospheric reaction.

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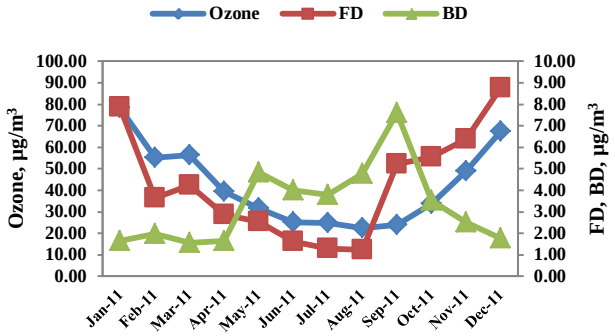

Fig. 1 The monthly concentration of the ambient formaldehyde (FD), ozone, and 1,3-butadiene (BD) in 2011.

B. Relationship between FD, ozone and BD

The correlation of ozone and FD concentration (Ozone-FD) was highly in positive (R^2 = 0.585) but the correlation of BD and FD (BD-FD) was lower than 0.5. The results in Fig. 2 and Fig. 3 showed the correlation of Ozone-FD which studied and applied by the linear equation to a formaldehyde prediction model followed in (1)

$$[FD] = 0.103[Ozone] - 0.099 \quad (1)$$

Where, [*FD*] is the ambient formaldehyde concentration (µg/m^3) and [*Ozone*] is the ambient ozone concentration (µg/m^3).

Moreover, the relationship between ozone and FD by exponential and logarithmic equation (in Fig. 4 and Fig. 5) provided the correlation (R^2) of each equation more than 0.5, as alike linear model. The exponential and logarithmic equations were applied to predict modeling as following (2) and (3). The relationship between ozone and FD in this study corresponded to the secondary FD production by the precursor contribution study by [9].

$$[FD] = 1.136 \exp 0.026[Ozone] \quad (2)$$

$$[FD] = 4.336 \ln[Ozone] - 11.59 \quad (3)$$

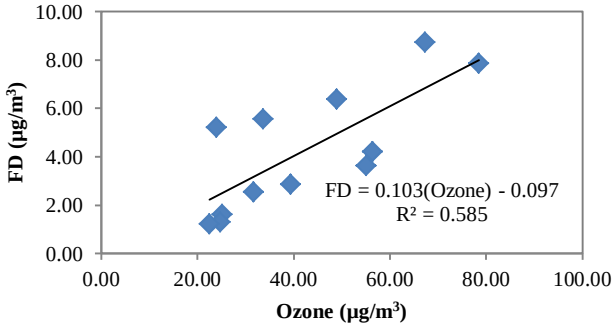

Fig. 2 The linear relationship of the ambient ozone and FD concentration.

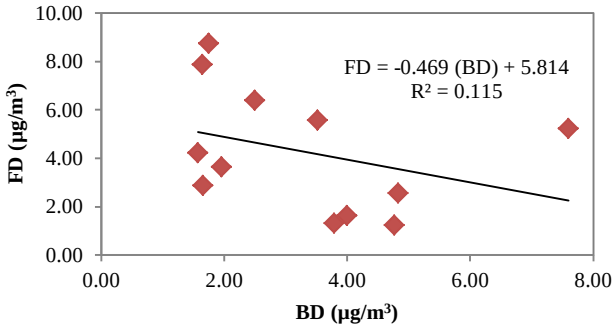

Fig. 3 The linear relationship of the ambient BD and FD concentration.

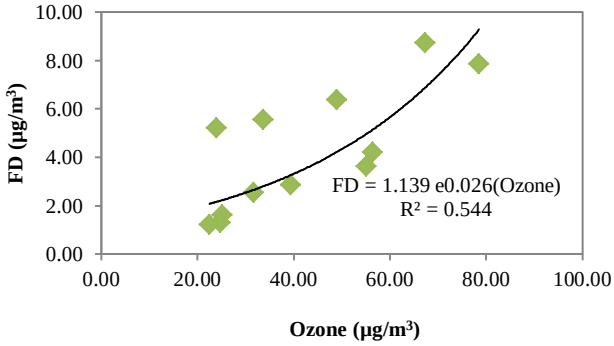

Fig. 4 The exponential relationship of the ambient Ozone and FD concentration

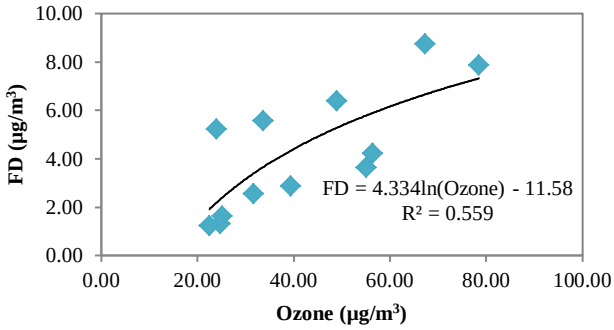

Fig. 5 The exponential relationship of the ambient Ozone and FD concentration.

C. The result of comparison

The FD prediction models (Eq. 1 – 3) were used to calculate FD concentration during January, 2012 to April, 2013. The calculated FD was compared with the collected FD in the same period by using MAPE method. The results showed the difference between the predicted and the collected FD concentration by modeling calculation as listed in Table 1.

TABLE I
THE COMPARISON OF COLLECTED AND PREDICTED AMBIENT FD CONCENTRATION

Model	R^2	MAPE
$[FD] = 0.103[Ozone] - 0.099$	0.585	29.6
$[FD] = 1.136\exp(0.026[Ozone])$	0.544	36.9
$[FD] = 4.336\ln[Ozone] - 11.59$	0.560	28.3

The logarithmic model has appropriate model for the ambient FD prediction that has the lowest difference value (MAPE 28.3%). This reason was supported the logarithmic model that suitable for ambient FD prediction and conclusion, although the R^2 value of linear model was higher than that of logarithmic model.

IV. CONCLUSION

This study indicated that the ambient concentration of ozone and FD were related more than BD. The correlation of ozone and FD concentration could be a prediction model including linear regression, exponential and logarithmic models to predict the FD concentration. The predicted FD concentration was compared with the collected FD concentration. The suitable model was the logarithmic model that provided the R^2 values as higher than 0.5 and the predicted ambient FD concentration was nearly the collected FD data (the lowest MAPE). This study could reduce the instrumental limitation for the FD concentration measurement in the field area, and help preliminary to evaluate the FD concentration evaluation for environmental planning. This research used a year collected data and studied in the specific area.

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