Estimate BTEX Concentrations Variations in a Petrochemical Parks Area using a Geographically and Temporally Weighted Regression Model

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KEY WORDS: BTEX pollutants; air pollution; Geographically Temporally Weighted Regression (GTWR); petrochemical industrial area.

ABSTRACT: Many studies have considered volatile organic carbons (VOCs) such as BTEX (*toluene, ethylbenzene, mp-xylene, and o-xylene*) as hazardous air pollutants. Besides contributing to the formation of ozone, the further effects of BTEX on health can increase the risk of cancer. The petrochemical industry is a major contributor to BTEX emissions, so determining the variations of these pollutants in the petrochemical industrial area is needed to reduce health risks due to BTEX exposures. In this study, a specific industrial monitoring database was used to collect BTEX data from May 2015 to September 2018 in Kaohsiung Petrochemical Parks area (including Linyuan Industrial Park and Linhai Industrial Park), Taiwan. Land use inventory, MODIS NDVI, digital road network map, temple, Chinese restaurant, thermal power plant, and weather variables were used as potential predictor variables in developing the prediction model. A Geographically Temporally Weighted Regression (GTWR) approach which considers both the spatial and temporal heterogeneity of air pollutants was then conducted to develop the prediction model for estimating the spatial-temporal variability of BTEX concentrations. The results showed that, BTEX concentrations decreased during the study period. The resultant models showed a mid-estimate performance level with the value of Adjusted R^2 for *toluene, ethylbenzene, mp-xylene,* and *o-xylene* was 0.68 (RMSE = 0.93), 0.46 (RMSE = 0.26), 0.53 (RMSE = 0.49); and 0.47 (RMSE = 0.29), respectively. Moreover, the results of model simulation showed that the highest concentrations of *ethylbenzene, mp-xylene,* and *o-xylen*e formed in the industrial zones close to the manufacturing areas while *toluene* was mostly found in the agricultural fields.

1. INTRODUCTION

Some common VOCs, such as Benzene series pollutants (*benzene, toluene, ethylbenzene, mp-xylene, and o-xylene*), are widely used in industry and exert serious adverse effects on environmental air quality. BTEX species have been the subject of many toxicological and health effects studies (Chauhan et al., 2014; Partovi et al., 2018; Zabiegała et al., 2010). Exposure to BTEX concentrations in the ambient air pose harmful health effects such as cancer, teratogenic impacts, and neurological disorders (Chauhan et al., 2014; Esteve Turrillas et al., 2007; Moolla et al., 2015; Xiong et al., 2016; Zabiegała et al., 2010). The petrochemical industry and traffic are major contributors to BTEX emissions (Hsieh et al., 2006; Liu et al., 2018), so determining the variations of these pollutants in the petrochemical industrial area is needed to reduce health risks due to BTEX exposures.

The objective of this study was to depict the spatially varying effect so as to better predict BTEX. First, a Land use regression (LUR) model was adopted to screen the land-use factors for BTEX predictions. However, previous studies overlooked the possibility that the effect of land-use configuration on the air pollutions may not always be constant across the study domain. So, in this study we built the geographically temporally weighted regression (GTWR) model based on land-use factors identified in the LUR model to improve both the spatial and temporal heterogeneity of the pollutants (Huang et al., 2010; Fotheringham et al., 2015). The aim of this study was to investigate the spatially varying relationship between land use configuration and Toluene, Ethylbenzene, mp-xylene, and o-xylene (BTEX in short) in petrochemical park areas in the southern Taiwan.

2. MATERIALS AND METHODS

2.1 Study area and materials

There are two important petrochemical parks located on the lee side of the central mountain range of the southern Taiwan (Fig 1). One is Linhai Industrial Park, located in Siaogang District and Cianjhen District of Kaohsiung, Taiwan. Linhai Industrial Park is a major cluster of heavy industry in Taiwan. There are several of the largest producers in their industries situated in this industrial park, such as steelmaker, ship builder and oil refiner. Furthermore, Linhai Industrial Park also has some manufacturers of machinery, steel, transportation and chemical industry. The total area of the park is about 1,560 ha and the park contains a total of 493 factories (Industrial development bureau, ministry of economic affairs). Another, Lin-Yuan industrial park, located in Linyuan District of Kaohsiung, Taiwan. This park is also an important exclusive petroleum zone in southern Taiwan. The park has a high traffic density and is in an area of newly built low-rise residential buildings and low-rise factory buildings. The total area of the park is about 395 ha and the park contains a total of 32 factories. Both two industrial parks are near the international airport, port, the terminal of national highway and a fossil fuel power plant.

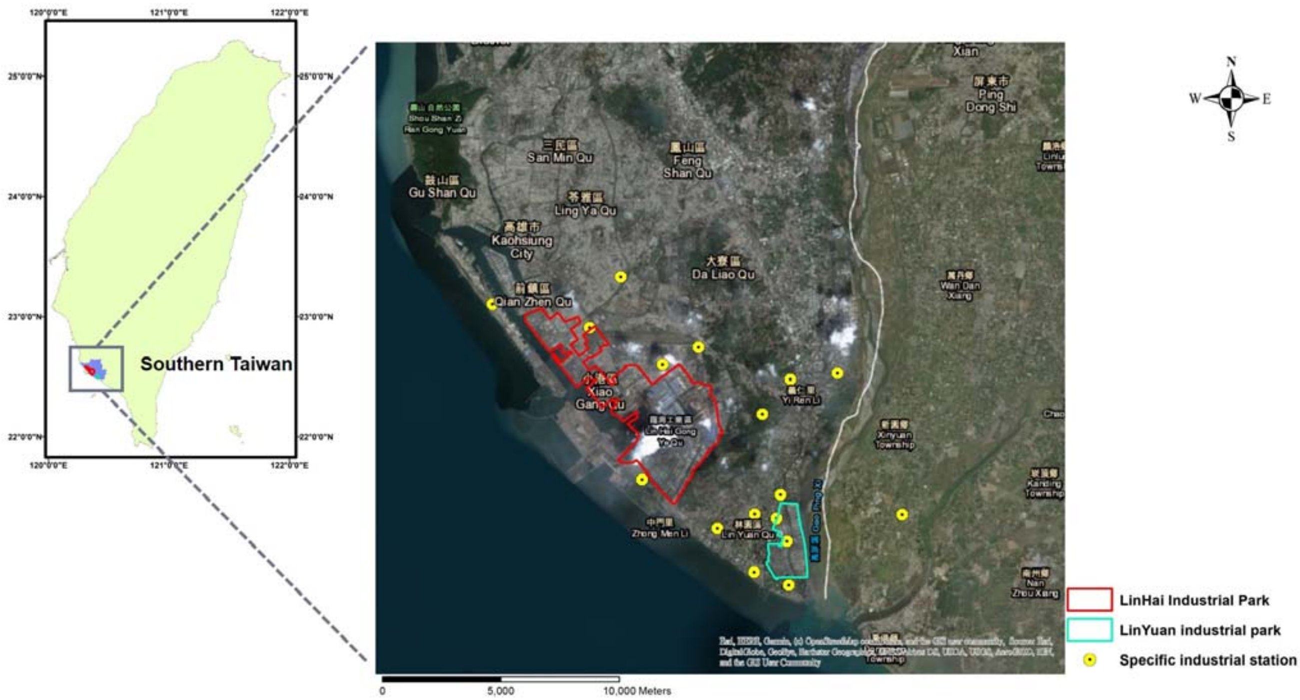

Figure 1. Study sites and the specific industrial monitoring stations.

2.2 Specific industrial monitoring database

The development of special industrial monitoring stations is to consider the impact of industrial areas that contain special industries on the surrounding environment and the health of the people (EPA, 2019). There are five specific industrial parks in Taiwan, including Kaohsiung Linyuan and Linhai industrial park, Yunlin Liuqing industrial park, Taichung Zhongke park, and Tainan Nanke park. Taiwan's EPA has established 35 air quality stations nearby the industrial parks, and there are 19 stations in Kaohsiung (Taiwan EPA, 2019; Fig 1). Linyuan and Linhai industrial park started monitor BTEX from May 2015 and May 2016, respectively. In this study, daily BTEX observations from 2015 to 2018 were used as the study materials. These daily measurements were aggregated into monthly averages for model development, resulting in a total of 489 valid measures.

2.3 Geo-spatial database

Several GIS databases were used to derive land use variables for GTWR model development, including residential areas, farm, forest, park, water, airport, and port from the National Land Use Inventory of 2012; road patterns from the digital road network map, it consists of the national highways, provincial highways, county road, village street, and express ways; industrial park from the 2010 digital map of industrial parks.

To estimate the emissions as a result of unique local culture activities such as joss money burning and use of frying oil, we also considered the number of temples, cemeteries, crematoria and restaurants, and their locations from the landmark databases of 2008. Distance to the nearest power plant and garbage incinerator was also calculated and incorporated in the analysis. Moreover, surrounding greenness (e.g. trees and vegetation) from 2015 to 2018 was characterized by NASA's MODIS Normalized Difference Vegetation Index (NDVI) database with 50×50 m^2 spatial resolution. All of these geo-spatial variables are abstracted circular buffer ranges surrounding each air quality monitoring site, the buffer radius was 50m, 150m, 250m, 500m, 750m, 1000m, 1250m, 1500m, 1750m, 2000m, 2500m, 3000m, 4000m, and 5000m, to represent the neighborhood land-use/land cover allocations. Fig 2 shows the framework of spatial modelling of BTEX pollutants distribution using GTWR.

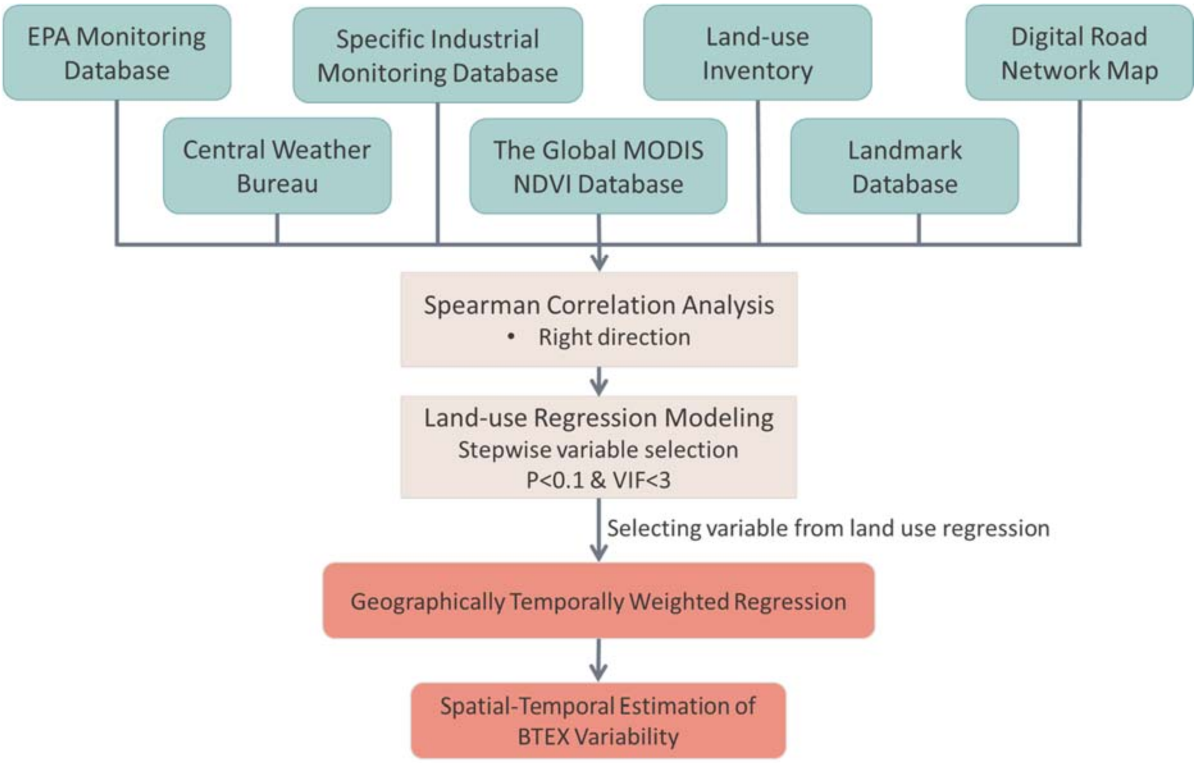

Figure 2. Framework of spatial modelling of BTEX pollutants distribution using GTWR.

2.4 Land use regression

LUR is a commonly-used predictive method for capturing ambient air pollution gradients (Jerrett et al., 2005; We et al. 2017; Wu et al. 2018), and it has been shown to have advantages for characterizing spatial relationships between local emissions and intra-urban pollution variations (Clougherty et al., 2013; Hoek et al., 2008; Michanowicz et al., 2016a, 2016b). LUR normally combines distributed pollution measures at multiple sites with a set of potentially predictive geographic source covariates, to develop a multiple linear regression model that can be rendered in a geographic information system (GIS) to estimate air pollution levels in unmeasured areas (Wu et al., 2017). In the first step, we used the stepwise variable selection procedure to build the LUR model, which could identify the significant land-use factors affecting BTEX, and then we can build the GTWR model based on the important spatial predictors selected by the LUR model.

2.5 GTWR

GTWR is a local linear regression model that can account for both spatial and temporal non-stationarity simultaneously (Huang et al. 2010; Fotheringham et al. 2015). The GTWR design embodies a local weighting scheme wherein Geographically Weighted Regression (GWR) and Temporally Weighted Regression (TWR) become special cases of GTWR. In short, the GTWR model based on the LUR model. The land-use predictors remain fixed, but their coefficients vary over the study domain. In other words, the constant coefficient was replaced by local varying coefficients (Weize et al., 2019). The local coefficient estimates were obtained by weighting neighboring observations using a distance-adjusted kernel function (Fotheringham et al., 1996). Here, we run the GTWR tool in ArcGIS 10.5, and configured the kernel type and bandwidth method parameters as 'Fixed' and 'cross validation'. The resultant models were then applied to estimate the spatial-temporal variability of BTEX pollutants in the petrochemical park areas in the southern Taiwan.

3. RESUITS AND DISCUSSION

3.1 Descriptive statistics of measured BTEX concentrations

Fig. 3 shows the annual averages of the measured BTEX levels over the study years, the annual value (mean ± standard deviation) of Toluene, Ethylbenzene, o-Xylene, mp-Xylene measurements were 3.23±0.09, 0.49±0.02, 0.51±0.02, and 0.81±0.04, ppb, respectively. From the figure, the Toluene level obviously decreased during the study years; the Ethylbenzene level slightly decreased; the o-Xylene and the mp-Xylene level almost had the same trend.

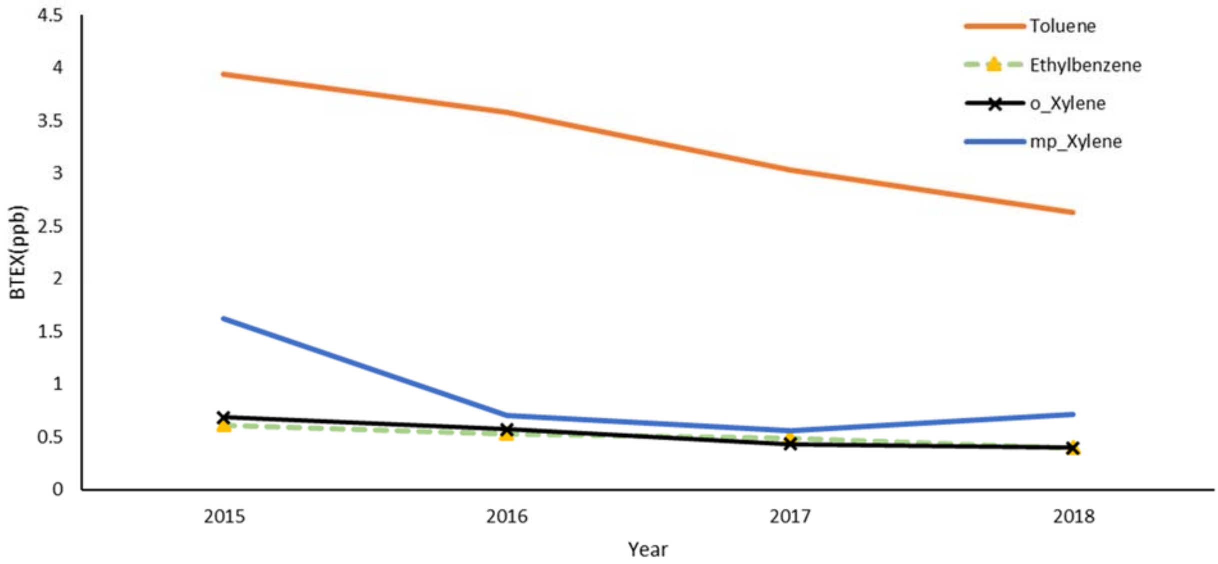

Figure 3. Annual averages of the measured BTEX concentrations over the study years.

3.2 GTWR model development

The results of BTEX GTWR models are presented in Table 1. The resultant models showed a mid-estimate performance level with the value of Adjusted R^2 for toluene, ethylbenzene, mp-xylene, and o-xylene was 0.68 (RMSE = 0.93), 0.46 (RMSE = 0.26), 0.53 (RMSE = 0.49); and 0.47 (RMSE = 0.29), respectively. Based on the selected predictor variables, the number of temples was selected as an important predictor variable to predict the four types of BTEX pollutants concentrations.

Table 1 Coefficient estimates, overall performance of the developed BTEX GTWR model.

	BTEX GTWR model			
Predictor variable	Toluene	Ethylbenzene	mp-xylene	o-xylene
Intercept	-1.12 (-2.69, 0.29)*	0.76 (0.57, 0.95)	0.50 (0.41, 0.56)	0.91 (0.74, 1.06)
NO_X (ppm)	0.12 (0.09, 0.17)	-	-	-
SO_2(ppb)	0.25 (-0.04, 0.64)	-	-	-
UV	-	$-5.57*10^{-2}$ (-0.08, -0.03)	-	-0.06 (-0.07, -0.04)
Non-irrigated $crops_{2500m}$	$7.48*10^{-3}$ (0.005, 0.01)	-	-	-
Fruit $orchard_{50m}$	-	-	-	$3.36*10^{-4}$ (0.00002, 0.0005)
Paddy rice + Non-irrigated $crops_{250m}$	$-1.56*10^{-3}$ (-0.003, -0.0008)	-	-	-
$Temple_{250m}$	0.37 (0.002, 0.67)	0.10 (0.02, 0.14)	0.21 (0.10, 0.30)	0.14 (0.09, 0.17)
Manufacturing $industry_{250m}$	-	$3.12*10^{-4}$ (0.0002, 0.0005)	-	-
Manufacturing $industry_{50m}$			$4.20*10^{-4}$ (0.0002, 0.0007)	$2.96*10^{-4}$ (0.0002, 0.0004)
Winter	-	-	0.25 (0.16, 0.35)	-
Fall	-	-	0.11 (0.01, 0.23)	-
Distance to the nearest airport	-	-	-	$-1.63*10^{-5}$ (0.00002, 0.00001)
Distance to the nearest Industrial park	$-3.35*10^{-4}$ (-0.0006, -0.0001)	-	-	-
Model performance	R^2= 0.68	R^2= 0.46	R^2= 0.53	R^2= 0.48
	ADJ R^2= 0.68	ADJ R^2= 0.46	ADJ R^2= 0.53	ADJ R^2= 0.47
	RMSE= 0.93	RMSE= 0.26	RMSE= 0.49	RMSE= 0.29

*Coefficient estimates: Median (Q1, Q3)

3.3 Spatial distribution of predicted BTEX concentrations

The results of GTWR model simulation are presented in Fig 4. Higher BTEX concentrations appeared in the industrial zones and close to the manufacturing areas. In contrast, Toluene was mostly found around the agricultural fields. Ethylbenzene, mp-xylene and o-xylene pattern were very similar, indicated that manufacturing industry is the most important emission sources for them. Non-irrigated crops field burning may be one of emission sources of Toluene, but paddy rice can improve the air quality by removing the pollutants from the air, the high concentration was found around the agricultural fields. There are some circular blocks with higher concentration appear in Fig 4 is the distribution of temples, indicated that temple also plays a role in this study.

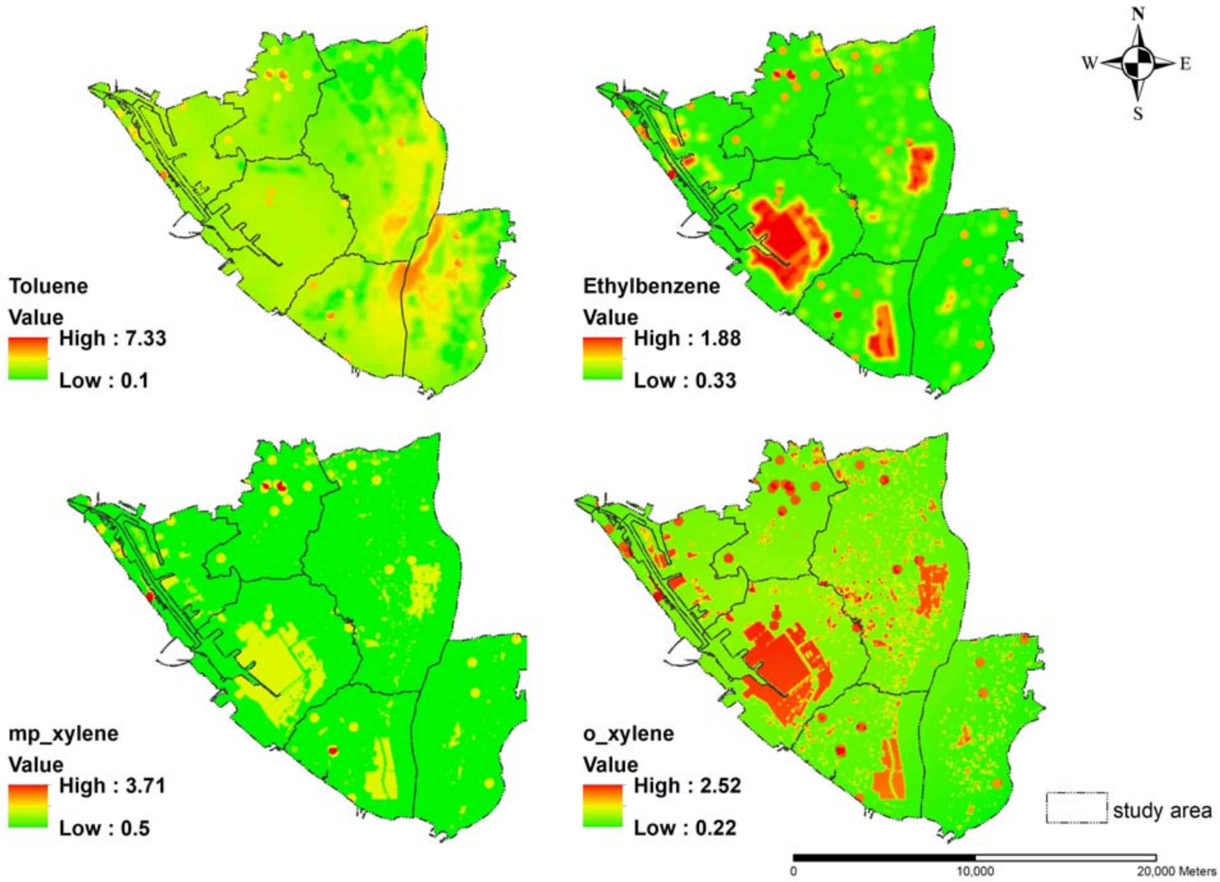

Figure 4. Annual averages of the measured BTEX concentrations over the study years.

4. CONCLUSIONS

The land-use configurations have different effects on Toluene and other BTEX in petrochemical parks area. Higher Toluene concentrations found around the agricultural fields, others appeared in the industrial zones and close to the manufacturing areas. Spatial distribution of predicted BTEX concentrations provided references for city land-use regulation strategies to reduce neighboring BTEX concentration levels. Moreover, this GTWR method could be similarly used in future studies to develop new GTWR models for other pollutants in others area.

Acknowledgements

This study was grant supported by the National Health Research Institutes (NHRI-108-EMGP02).

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