# GIS BASED URBAN AIR QUALITY MODEL: THE CASE OF $NO_2$

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## INTRODUCTION

Despite improvements in vehicle emission control technology, the rapid growth of vehicle ownership and average trip length during past decades has created an unhealthy air quality in urbanized areas. Traffic emissions are known to be responsible for a substantial share of urban air pollution, such as nitrogen dioxide ($NO_2$), carbon monoxide, volatile organic compounds (VOCs), and particulate matters. Pollutants emitted by motor vehicles influence the spatial and temporal patterns of ambient pollution concentrations. Generally, air pollution concentrations are determined by such factors as the formation and destruction of pollutants through chemical and physical reactions, the intensity and duration of emissions, the uptake and assimilation of pollutants by urban vegetation, and meteorological factors inducing chemical reactions and physical dispersion (Derwent & Hertel, 1998; Harrison, 2001; Seinfeld & Pandis, 2006; Takahashi et al., 2005; US EPA, 2000; WHO, 2006). Among these factors, vehicle emissions are considered a key factor to determine the air quality of urban regions. It is reasonable to expect that, as vehicle-kilometres-travelled (VKT) increase, ambient air pollution concentrations will also increase. Since transportation is responsible for a substantial share of urban air pollution emissions, VKT is considered as a better regressor to explain pollution concentrations than other transportation-related variables, such as traffic counts, area of road, distance to major roads, etc. (Jerrett et al., 2007; Kahyaoğlu-Koračin, Bassett, Mouat, & Gertler, 2009; Kim, 2007; Kim & Guldmann, 2008).

Integrated air quality modelling systems have been developed in several countries for dense urban regions, where pollutants generated by road traffic tend to be present at high concentrations. These systems include both emission inventories and dispersion models. To enhance the credibility of emission inventories, it is necessary to develop up-to-date emission factors and data on actual traffic flows, vehicle speeds, fleet composition, and weather conditions. Dispersion models require significant computational resources to calculate high-resolution air pollution concentrations from both geographical and temporal perspectives. Other approaches to explain the relationships between air pollution concentrations and urban land uses have taken advantage of improvements in geographic information systems (GIS). To explain observed spatial variations in pollution concentrations, land uses identified and measured with GIS procedures are inputs into land-use regression (LUR) models. Pioneering LUR research was initiated in the EU-funded SAVIAH (Small Area

Variations in Air Quality and Health) project (Briggs et al., 1997). The pollution maps predicted with LUR models have been used for epidemiological studies, assessment of long-term exposure to traffic-related pollution, and scenario-based land-use impacts on air quality. Since observed concentrations at air quality monitoring stations (AQMs) and measured land uses around AQMs are used as dependent and independent variables, LUR models are regarded as primarily empirical models. Despite developments in conventional air quality modelling systems and in recent LUR models, the complex interactions between pollution concentrations, traffic flows, land uses, meteorological factors, and chemical reactions have not been satisfactorily investigated. As the spatial and temporal variations in vehicle emissions are expected to significantly impact pollution concentrations, LUR models must be expanded to incorporate traffic flows over both space and time.

The purpose of this research is to (1) understand the system of $NO_2$ concentrations, specifically meteorological impacts on pollution concentrations and pollutants chemistry will be reviewed, (2) analyze the temporal variations of concentrations and compare the differences of concentrations between roadside and urban background AQM, (3) develop a LUR framework to build air quality panel models, accounting for VKT, land uses, and meteorological factors.

# LITERATURE REIVEW

## Chemistry of $NO_2$

When fossil fuels (coal, gasoline, diesel, and natural gas) are burned, nitrogen monoxide (NO) and $NO_2$ gases are released into the atmosphere. Oxides of nitrogen ($NO_x$) are defined as the sum of both NO and $NO_2$. Due to the increase in fossil fuel use, such as road transport, power plants, combustion in industrial and commercial uses, and residential heating, $NO_x$ is a common pollutant (Air Quality Expert Group, 2004). The US EPA (2000) estimates that, in 1998, U.S. on-road and off-road sources contributed 53% of nitrogen oxides, and the EU reports that road transport and other mobile sources account for 57% of $NO_x$, based on CORINAIR (The Core Inventory of Air Emissions in Europe) 1990 inventory (CORINAIR, 2003). In 2000, road transport in the United Kingdom was found to be the largest contributor of $NO_x$ emissions (Air Quality Expert Group, 2004). Because of $NO_x$ emissions, it is expected that urbanized regions are more vulnerable to vehicle emissions than rural ones. According to the Korea Ministry of Environment (2005), the contributions of on-road vehicles to both the national and Seoul Metropolitan region $NO_2$ concentrations are 42.2% and 61.1%, respectively.

NO is derived from nitrogen ($N_2$) in high-temperature combustion processes, such as internal combustion engines, and $NO_x$ emissions released from these engines contain over 90% of NO, which is relatively unstable when compared to oxygen ($O_2$) and $N_2$. The main fate of NO is to react with ozone ($O_3$) in the ambient atmosphere and to be converted into $NO_2$ (Derwent & Hertel, 1998). Typically, directly emitted $NO_2$ represents 5% of emissions by both gasoline and diesel vehicles. However, Carslaw and Beevers (2004) assert that diesel vehicles are responsible for higher primary $NO_2$ emissions (12.7%) than gasoline vehicles (0.6%), based on monitoring results in London. Nonetheless, it is certain that the share of primary $NO_2$ is far smaller than that of directly emitted NO. In urban regions, relatively abundant $O_3$ reacts rapidly with NO to generate $NO_2$.

$$\mathrm{NO} + \mathrm{O_3} \rightarrow \mathrm{NO_2} + \mathrm{O_2} \tag{1}$$

Another chemical reaction creating $NO_2$ is the interaction of NO with organic peroxy radicals ($RO_2\cdot$) and hydroperoxyl radicals ($HO_2\cdot$), where R is an alkyl radical[1]. In these reactions (Eqs. 2 and 3), an abundance of radicals in the atmosphere stimulates the accumulation of $O_3$, because radicals are more active for reactions than $O_3$ (Seinfeld, 1989):

$$\mathrm{NO} + \mathrm{RO_2}\cdot \rightarrow \mathrm{NO_2} + \mathrm{RO}\cdot \tag{2}$$
$$\mathrm{NO} + \mathrm{HO_2}\cdot \rightarrow \mathrm{NO_2} + \mathrm{OH}\cdot \tag{3}$$

The main fate of $NO_2$ during daylight is photodissociation with ultraviolet (UV) radiations and reforming NO and a ground-state oxygen atom, $O(^3P)$. The oxygen atom produced in the photolysis of $NO_2$ reacts with $O_2$, generating $O_3$ (National Research Council, 1991). The range of UV wavelength in the $NO_2$ photolysis process is known as around 200 to 400 nm (nanometers, $10^{-9}$ meters) (Derwent & Hertel, 1998; Seinfeld, 1989).

$$\mathrm{NO_2} + h\nu \rightarrow \mathrm{NO} + \mathrm{O}(^3\mathrm{P}) \tag{4}$$

The other chemical removal of $NO_2$ is the reaction with $OH\cdot$, forming nitric acid ($HNO_3$). Since the hydroxyl radical is created with electronically excited oxygen atoms, $O(^1D)$, and water vapour, the presence of short wavelength UV (less than 320 nm) is required. Under usual daytime conditions, the reaction of $NO_2$ and $OH\cdot$ converts around 5% of $NO_2$ per hour (Derwent & Hertel, 1998). The produced $HNO_3$ reacts with ammonia ($NH_3$) to form particulate nitrate ($NO_3^-$).

$$\mathrm{NO_2} + \mathrm{OH}\cdot + \mathrm{M} \rightarrow \mathrm{HNO_3} + \mathrm{M} \tag{5}$$

Understanding the creation and removal processes of $NO_2$ helps explain the temporal and locational variations of $NO_2$ concentrations.

## Air Quality Modelling Approach: Land Use Regression (LUR)

There is much empirical evidence regarding the positive association between traffic flows and air pollutant concentrations. It is reasonable to expect that the contribution of on-road vehicles to the air pollution of urbanized regions is greater than to that of rural areas. In a spatial perspective, the areas adjacent to heavily travelled roads are more susceptible to vehicular emissions than remote areas. The spatial and temporal exceedances of air pollution standards must be examined and estimated, because these hotspots of

[1] Alkyl radicals are generally designated R·, where R represents the chemical formula for alkyl group (Seinfeld & Pandis, 1998).

spatiotemporal exceedances can lead to harmful impacts on human health and natural and man-made environments. There are many studies reviewing the consequences of air pollution, including hedonic models of housing values (Kim, Phipps, & Anselin, 2003), benefit-cost assessment of urban air pollution (Krupnick & Portney, 1991), spatial property assessment (Setton, Hystad, & Keller, 2005), valuing health benefits of clean air (Hall et al., 1992), particulate matter and health outcomes (Dockery et al., 1993; Dominici & Burnett, 2003), PM2.5 and mortality (Franklin, Zeka, & Schwartz, 2007), $NO_2$ and human health (Kraft et al., 2005), air pollution and mortality (Schwartz & Zanobetti, 2000), and epidemiology of traffic-related pollution and asthma (Zmirou et al., 2002).

Since air pollution in urban regions has induced considerable attention from scholars and public administrators, air quality models have been developed while considering the above-mentioned factors in modelling processes. Most of these studies have adopted dispersion methods as key modelling modules, with extensive emission inventories. Integrated modelling systems for air quality management have been developed in several countries, including AirGIS in Denmark (Jensen et al., 2001), Air Quality Information System in Norway (Bøhler et al., 2002), Integrated Model of Urban Land-use and Transportation for Environmental analysis in Canada (Potoglou & Kanaroglou, 2005), Danish Operational Street Pollution Model in Denmark (Berkowicz, Winther, & Ketzel, 2006), Traffic Emission Information System in Hong Kong (Xia & Shao, 2005), GIS based decision support system for estimation of air pollution in Turkey (Elbir & Muezzinoglu, 2004; Elbir, 2004), Urban Dispersion Modelling with road network dispersion in Finland (Karppinen et al., 2000; Karppinen, Kukkonen, Elolähde, Konttinen, & Koskentalo, 2000; Kukkonen, Härkönen, Walden, Karppinen, & Lusa, 2001), and Traffic Emission Modelling and Mapping Suite in England (Namdeo et al., 2002). Air quality models based on dispersion methods require many input data and much computing power to generate acceptable results over both space and time.

As an alternative to these models, LUR models have been recently developed and applied to high-resolution pollution mapping. Generally, traffic related variables are considered as major and significant predictors in LUR equations. In addition, many land uses have been tested as explanatory variables for pollution concentrations. Generally, LUR studies present reliable coefficients of determination ($R^2$), with a range of 0.5 to 0.8, using monitored data (Hoek et al., 2008). With the development of GIS technology, variables potentially related to air pollution concentrations can be obtained in much less time and at lower costs, as compared to dispersion-based approaches, including measures of traffic, land uses, density, and meteorological factors. These variables are assessed for various buffers and used as explanatory variables. Since the explanatory variables used in the regression model are obtained through GIS, it is possible to calculate the values of the explanatory variables for the entire study region. Therefore, the prediction of air qualities in unsampled areas and the mapping of air pollution have been implemented in several LUR studies. $NO_2$ maps have been estimated in Huddersfield, UK, and Amsterdam, Netherlands (Briggs et al., 1997), Toronto, Canada (Kanaroglou et al., 2005), Hamilton, Canada (Sahsuvaroglu et al., 2006), San Diego, CA (Ross et al., 2006), and Oslo, Norway (Madsen et al., 2007). Air pollution maps for particulate matter are also been generated in several studies, including New York City and adjacent counties (Ross, Jerrett, Ito, Tempalski, & Thurston, 2007) and on the European continent (Beelen et al., 2009). Based on the predicted pollution map, an epidemiological study has been implemented in Sadabell, Spain (Aguilera et al., 2008), and long-term exposure to traffic-related pollution has been assessed in the Netherlands (Beelen, Hoek, Fischer, Brandt, & Brunekreef, 2007). Since land uses in urban areas determine movements of freight and passengers, poorly designed urban development plans can increase the levels of vehicle emissions, resulting in temporal and spatial pollution hotspots. Scenario-based future land-use plans were introduced to evaluate impacts on air quality in Southwest California (Kahyaoğlu-Koračin et al., 2009). As expected, traffic-related variables, such as traffic density, traffic volume, VKT, distance from highway, and length of highway, high density residential areas (population density), commercial areas, and industrial land uses, are all positively correlated with $NO_2$ concentrations (Aguilera et al., 2008; Beelen et al., 2007; Briggs et al., 1997; Gilbert, Goldberg, Beckerman, Brook, & Jerrett, 2005; Kahyaoğlu-Koračin et al., 2009; Ross et al., 2006; Sahsuvaroglu et al., 2006; Smith et al., 2006). On the other hand, open space, including urban forests, parks, and water bodies, is negatively correlated with $NO_2$ concentrations (Henderson, Beckerman, Jerrett, & Brauer, 2007; Kanaroglou et al., 2005).

# METHOD

## Data

Air pollution concentrations in 2003 have been measured at 34 AQMs and are reported in both the Seoul Metropolitan government website (Seoul Metropolitan Government, 2008) and in the Annual Report of Air Quality in Korea (National Institute of Environmental Research, 2004). As illustrated in Figure 1, AQMs are distributed over the Seoul Metropolitan area, with at least one AQM in each district. Out of the 34 AQMs, 27 are classified as urban background AQMs, monitoring the average air quality and assessing whether air quality standards are attained. The other 7 AQMs are located near crowded traffic links to measure the air quality of roadsides.

The Seoul Development Institute (SDI) releases transportation network and OD matrix data for the Capital region of Korea every year. The network and OD data cover the Seoul, Incheon, and Gyeonggi regions. These OD and network data are used in traffic assignment models. The OD table and network involve 1,142 traffic zones, divided into 1,129 internal and 13 external zones. The OD system includes auto, taxi, and bus OD tables. According to the report, “The Standard Guideline of Pre-feasibility Study for Road and Railroad Sectors” (Korea Development Institute, 2004), the surveyed average numbers of people per vehicle are 1.46 and 14.99 for automobile and bus, respectively. These values are used to convert person trip to vehicle trip. As freight OD data are not available in 2003, freight flows are not included in the traffic assignment process. Therefore, the assigned volumes on each link can be expected to be less than the actual traffic flows. The distances between traffic emissions and receptors are important in determining the concentrations at receptors. To identify the impacts of traffic emissions on the concentrations at AQMs, several circular buffers with a radius varying from 500 meters to 5,500 meters are delineated around each AQM. The VKTs on the transportation links within the circular buffers are estimated as follows: (1) the traffic flow of each transportation link is estimated with a traffic assignment model; (2) the buffers are intersected onto the traffic network; (3) the attributes of the intersected links are calculated using ArcGIS® and Python® scripts. To account for the wind-direction (WD) effects on traffic emissions, the circular buffer is subdivided into eight sectors, each sector is overlaid onto the assigned network, and then the VKTs for each sector are computed using the above process, and then weighted by the WD frequency. WD-weighted VKT (WVKT) is calculated as the sum of the eight sectors' VKT. Using available hourly traffic counts data, the estimated daily VKTs are divided into hourly VKTs.

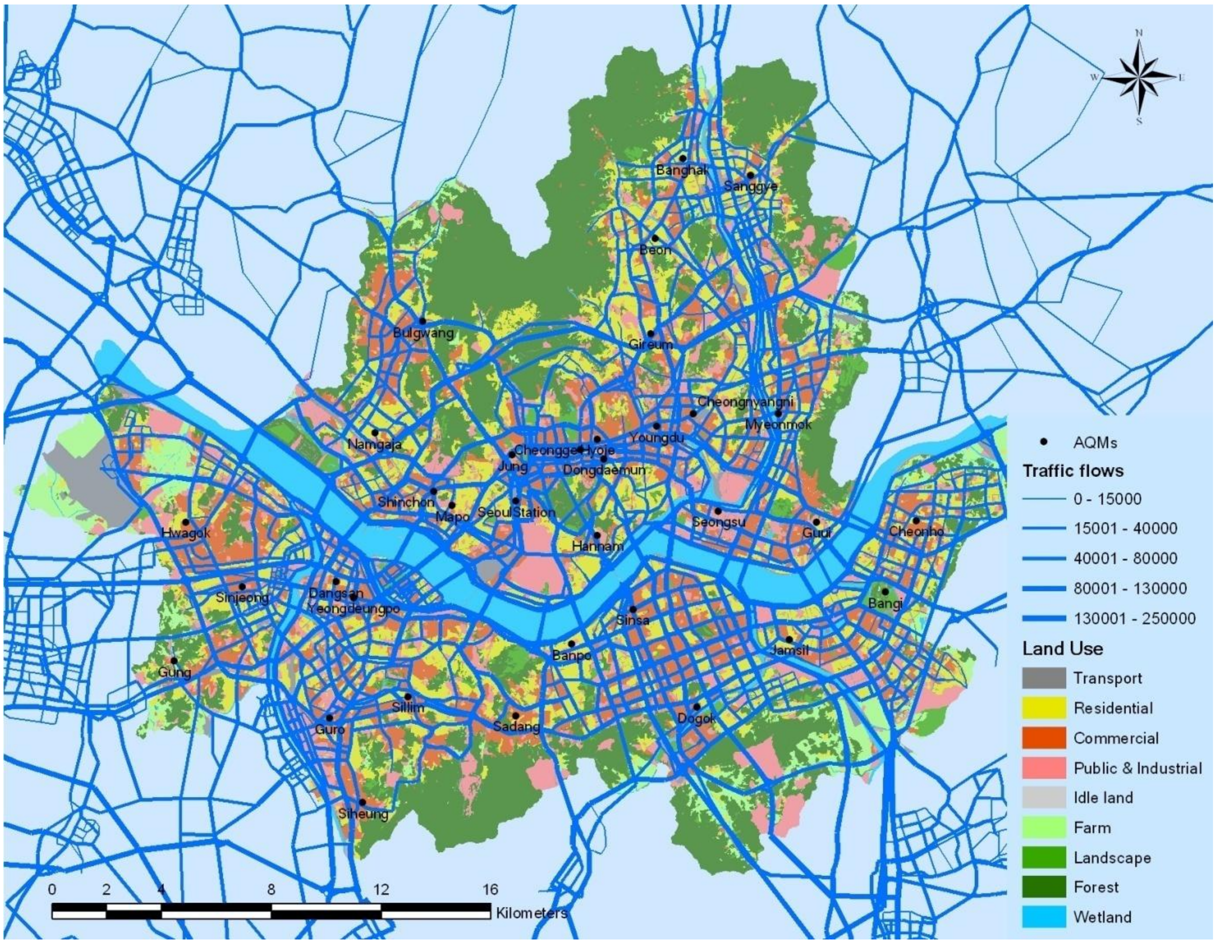

Figure 1 AQM location, traffic assigned network, and land-use classification

Traffic counts data are more accurate for simulating vehicle emission than the results of traffic assignment method. Traffic counts data in the Seoul city have been collected at 4 different road classifications, including the CBD (26 locations), Han River bridges (19 locations), arterial roads (36 locations), and cordon line (38 locations). The number of traffic counts stations, however, is limited to calculate VKTs which can be used as the proxies of vehicle emissions in the LUR models. As seen in Figure 1, the locations of AQMs are distributed across the entire city and the links required calculating VKTs for each AQM are numerous, it is not possible to use traffic counts data in the LUR approaches. Since traffic assignment methods have been developed with diverse theoretical backgrounds, it is necessary to evaluate the results of assigned traffic volumes with the monitored traffic counts.

Diverse land-use patterns around AQMs have been measured with GIS techniques and used as input variables in the $NO_2$ models to explain pollution concentrations varied over space and time. SDI has released the first biotope map of Seoul, Korea, in 2000 and an updated map was published five years later, including 24,847 land parcels.[2] Each land parcel has been classified into urban or non-urban land uses, with 9 middle classes and 64 detailed classes. The middle-class land-uses classification is illustrated in Figure 1. The non-urban land uses include forest, open space, river, stream, and wetland. The urban land uses are sub-classified as residential, commercial, transportation, industrial, urban infrastructure, public facilities, industrial, denuded, and inaccessible areas.

## Model Specification

Physical environments, such as VKTs and land use shares, around AQMs are calculated and used as explanatory variables in the $NO_2$ LUR models. Pollution concentrations monitored at each AQM are used as the dependent variables with these predictors. VKTs of all links in the Seoul transportation network are estimated based on the results of traffic assignment. Areas of five land uses, such as residential, commercial, industrial, transportation, and vegetative area, are calculated using a biotope map and satellite image. Land-use variables are applied WD frequency and then re-calculated as WD-weighted land uses (WLU). Meteorological factors induce chemical and physical reactions, consequently, leading to the creation, destruction, and dispersion of pollutants. Hourly measured solar radiation, temperature, humidity, and wind speed are included in panel regression models to investigate the meteorological impacts on concentrations. In order to compare the different impacts of explanatory variables on pollution concentrations across the four seasons, concentrations measured weekdays are averaged over for each season and then four seasonal hourly panel data sets are constructed. Interaction terms between the dummy variables and the other regressors are included in the models. VKTs vary over space (AQMs) and time (24 hours). In contrast, land uses are time-invariant and meteorological variables, such as solar radiation, temperature, wind speed, and humidity, are space-invariant. Hourly meteorological variables are averaged over each season. Four seasonal regression models are formulated and their estimates are compared. WVKT and WLU variables are recomputed for each season. The proposed panel regression model is expressed as:

$$C_{it}^{p} = \alpha + \sum_{j=1}^{J} \beta_j X_{itj} + \sum_{j=1}^{J} \gamma_{jl} \left( X_{itj} \times D_R \right) + \sum_{j=1}^{J} \delta_{jl} \left( X_{itj} \times D_D \right) + u_{it} \tag{6}$$

Since roadside AQMs tend to be more impacted by vehicle emission than background AQMs, the concentration at roadside AQMs are generally higher for directly emitted pollutants. The introduction of interaction terms between the basic explanatory variables and the locational dummy variable ($D_R$) will allow for testing the effects of the original regressors under different locational conditions. In addition, the chemical reaction

[2] http://www.seoul.go.kr/info/organ/subhomepage/urban_new/library/mode_8_04.html

rates are different in daytime and night-time. Including a daytime dummy variable ($D_D$) and related interaction terms may help assess these temporal differences.

If serial correlation is present in panel data, estimation without correcting for auto-correlation is inefficient. If the error structure is assumed to be first-order autoregressive, the Parks method (Parks, 1967) can be considered for estimating the regression model. The specification of the first-order autoregressive error term is as follows:

$$u_{it} = \rho_i u_{i,t-1} + \varepsilon_{it} \quad (7)$$

where $\rho_i$ is the first order autoregressive parameter, which is estimated for each cross-section. Since there are fixed effects with regard to (w.r.t.) space (AQMs) and time (hours), the above error specification has limitations in differentiating these effects. According to Kmenta (1986), the use of dummy variables is a cover-up of the incomplete knowledge regarding the true model. However, the traffic emissions and solar radiation variables are expected to create different impacts between roadside and background areas. In addition, the impacts of the original regressors vary, depending on the intensity of solar radiation. Therefore, it is reasonable to assume that the two proposed dummy variables and their interactions with the regressors will help capture these locational and temporal differences. Panel data including hourly measured pollution concentrations can be expected to have strong positive autocorrelation, and therefore the estimation method should correct for autocorrelation. The error specification in Eq. (7) and the introduction of both cross-sectional and time-series dummy variables should produce a realistic model. Parks method is used to estimate the parameters of the $NO_2$ seasonl panel regression models.[3]

# TEMPORAL VARIATIONS OF POLLUTION CONCENTRATIONS

It is widely accepted that traffic emissions are the major source of $NO_2$ concentrations in urban regions (Jo & Park, 2005; Carslaw & Beevers, 2004a; Fujita et al. 2003). Observed traffic counts and diurnal variations of $NO_2$ concentrations are reviewed for the four seasons. As shown in Figure 2, the hourly patterns of $NO_2$ concentrations for both roadside and background AQMs are similar in all four seasons. Roadside AQMs display a steep increase in the morning, commencing around 6 AM when morning traffic increases, then make a plateau at midday in Spring and Fall, continually increase in Summer, and slightly decline in Winter. In the case of background AQMs, the concentration patterns are similar across the four seasons; double peaks during the day, the highest after the evening traffic peak, and a deep trough during daytime are observed.

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[3] http://support.sas.com/documentation/cdl/en/etsug/60372/HTML/default/etsug_panel_sect033.htm

If the number of time-series units is less than the number of cross-section units, then the Parks method produces an error message that the phi matrix is singular. To fix this problem, the number of cross-sectional observations is reduced to the number of time-series observations. In order to compare the different impacts of background AQMs and roadside AQMs, 17 out of the 27 background AQMs are randomly selected. In the case of roadside AQMs, all 7 AQMs are selected. Therefore, the number of observations for the estimation of the panel models in this research is 576 (24 AQMs × 24 hours).

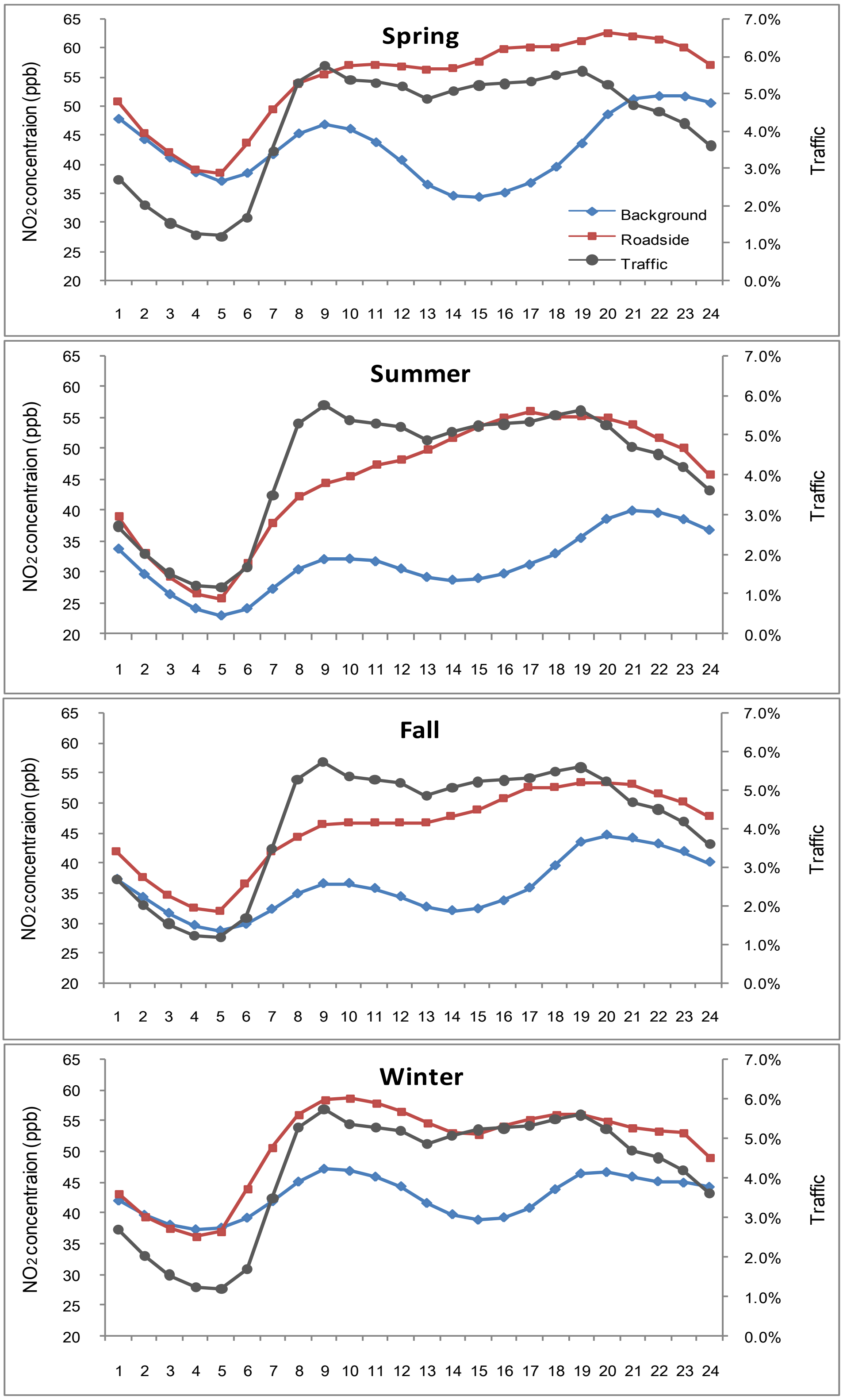


Figure 2 Variations of hourly traffic volumes and hourly $NO_2$ average concentrations at roadside and background AQMs in the four seasons

There are two notable phenomena in this seasonal comparison. One is that the depth of the trough is shallow in the roadside pattern, as compared to the background one. The reason may be that, during daytime, UV rays stimulate the photolysis of $NO_2$, but near the roadside freshly emitted NO from the tail pipe is abundant, so that the effects of photolysis are alleviated. The other interesting phenomenon is that the hour of daily peak concentration at background AQMs is changing along with the season. With plenty of daylight, as in Summer and Fall, the peak occurs at 22:00; however, in Winter and Spring, the peak hour starts earlier, at 19:00 and 20:00 PM, respectively. The occurrence of the time lag for the $NO_2$ peak concentration at background AQMs can also be explained by the photolysis of $NO_2$. The evening highest $NO_2$ concentration can be explained by the reaction between the accumulated ozone in daytime and the NO emission in evening traffic peak.

# RESULTS FOR $NO_2$ PANEL MODELS

The estimation results for the $NO_2$ panel regression models are presented in Table 1. The results point to positive and very significant coefficient estimates for WVKT (buffer radius 5000meter) across the four seasonal models. Emissions from traffic flows are the direct sources of $NO_x$, and most of the $NO_x$ are emitted in the form of NO, which is quickly transformed into $NO_2$ by reaction with $O_3$ (Eq. 1), organic peroxy radicals (Eq. 2), and hydroperoxy radicals (Eq. 3). In the urban atmosphere, these two radicals are generated in the process of anthropogenic and biogenic VOCs oxidation. Solar radiation has a negative impact on $NO_2$ concentrations, because $NO_2$ is decomposed by UV radiation (Eq. 4) during daytime. The coefficient estimates for solar radiation are negative and significant in all models. Since the intensity of UV radiation is lower during the cold season, the coefficient estimate for Winter solar radiation is, as expected, the smallest in absolute term among the four models.

Since NO gases emitted from vehicles are more likely to be converted into $NO_2$ at roadside locations, higher $NO_2$ concentrations are generally observed there. The $NO_2$ models include two significant interaction variables related to the roadside dummy variable. The coefficient estimates for the WVKT interaction term are positive, supporting the theory that roadside areas represent favourable conditions for high $NO_2$ concentrations. In addition, a significant interaction variable related to the daytime dummy variable is also included in the $NO_2$ models. During daytime, negative and positive impacts on $NO_2$ concentrations occur simultaneously. The negative effects include $NO_2$ photodissociation and decreased space heating during the warm season. In contrast, anthropogenic activities generally take place during daytime, leading to more $NO_x$ emissions. The coefficient estimates for the daytime interaction variable with WVKT are negative in Spring and Winter, and positive in Summer and Autumn, indicating that the negative effects are dominant in Spring and Winter, and the positive effects in Summer and Autumn. However, the effects in Spring and Winter are less significant. The coefficient estimates for the solar radiation interaction variables are also positive, indicating that the negative impact of solar radiation on $NO_2$ concentrations is reduced at roadside areas. As background areas are more favourable for generating $O_3$, the rate of $NO_2$ photodissociation is greater in background areas than in roadside areas.

Since $NO_x$ gases are emitted from commercial, residential, and industrial land uses, the signs of coefficients for these land uses are expected to be positive. The estimate coefficients for commercial and industrial areas are positive, but those of residential areas are inconsistent across the seasons. During Summer season, fossil fuel consumption is small in residential areas, and therefore much reduced $NO_x$ emissions are expected, leading negative effect may occur in Summer. The negative estimate coefficients for Spring and Winter models are unexpected results, calling for further research.

Generally, higher temperatures reduce the consumption of fossil fuels, leading to decreased $NO_x$ emissions, thus explaining the negative coefficient of temperature in Winter. However, the coefficient estimates for temperature are positive for the Spring, Summer, and Autumn models, possibly because of the coincidences of high traffic flows and high temperatures during daytime, and low traffic flows and low temperatures during night-time. Wind speed presents more complicated interactions compared to other meteorological factors, because strong wind expedite the dispersion of pollutants but light wind is known to facilitate the photochemistry of pollutants because of scattering effects. The threshold for differentiating these two effects, however, has not been clarified yet. As wind speed in Spring and Winter is generally higher than in the other seasons, dispersion effects are expected to be dominant for these two seasons. However, the coefficient estimates for Spring and Winter are positive. To explain the patterns of wind speed effects on pollution concentration, it is necessary to investigate in advance when the conditions for dispersion or scattering effects would occur. Finally, humidity has generally negative impact on pollution concentrations. This is only true in Winter, and the unexpected results of humidity effects also call for further research. The two dummy variables for roadside AQMs and daytime are not included in the final models, because the estimate coefficients are insignificant and the inclusion of these dummy variables causes the change of signs for the other regressors.

Table 1 Results of $NO_2$ panel regression models estimation

| Season | Spring | | | Summer | | | Autumn | | | Winter | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Explanatory Variables | Parameter | t Value | Pr > \| t \| | Parameter | t Value | Pr > \| t \| | Parameter | t Value | Pr > \| t \| | Parameter | t Value | Pr > \| t \| |
| Intercept | -151.80 | -32.05 | <.0001 | -323.25 | -66.01 | <.0001 | -93.85 | -12.77 | <.0001 | 43.48 | 36.36 | <.0001 |
| WVKT_R5000 | 1.48 | 21.82 | <.0001 | 1.31 | 16.73 | <.0001 | 2.09 | 33.50 | <.0001 | 2.02 | 48.21 | <.0001 |
| Commercial_R4500 | 5.91 | 20.86 | <.0001 | 2.36 | 10.92 | <.0001 | 3.65 | 9.68 | <.0001 | 0.82 | 6.66 | <.0001 |
| Residential_R1000 | -0.15 | -0.60 | 0.550 | -1.33 | -10.56 | <.0001 | 2.32 | 9.59 | <.0001 | -2.43 | -17.26 | <.0001 |
| Industrial_R4500 | 2.70 | 11.84 | <.0001 | 0.65 | 3.48 | 0.001 | 1.85 | 8.04 | <.0001 | 1.32 | 27.29 | <.0001 |
| Solar Radiation | -31.24 | -49.16 | <.0001 | -19.24 | -89.18 | <.0001 | -11.89 | -29.32 | <.0001 | -8.83 | -33.18 | <.0001 |
| Wind Speed | 8.49 | 13.38 | <.0001 | 6.18 | 43.08 | <.0001 | -3.36 | -9.18 | <.0001 | 2.34 | 9.91 | <.0001 |
| Temperature | 8.95 | 42.04 | <.0001 | 10.37 | 80.32 | <.0001 | 5.30 | 21.31 | <.0001 | -0.03 | -0.25 | 0.801 |
| Humidity | 1.19 | 27.75 | <.0001 | 1.47 | 52.19 | <.0001 | 0.71 | 13.73 | <.0001 | -0.15 | -8.70 | <.0001 |
| WVKT × Roadside Dummy | 0.20 | 2.40 | 0.017 | 0.56 | 9.32 | <.0001 | 0.14 | 4.59 | <.0001 | 0.72 | 21.11 | <.0001 |
| Solar × Roadside Dummy | 8.89 | 29.20 | <.0001 | 9.79 | 51.61 | <.0001 | 6.24 | 31.47 | <.0001 | 2.59 | 8.13 | <.0001 |
| WVKT × Daytime Dummy | -0.07 | -2.17 | 0.030 | 0.17 | 20.17 | <.0001 | 0.17 | 7.46 | <.0001 | -0.06 | -2.56 | 0.011 |
| $R^2$ | 0.980 | | | 0.995 | | | 0.983 | | | 0.981 | | |

# ELASTICITY ANALYSIS

The original regressors and diverse interaction terms have been selected as significant explanatory variables across the four seasonal panel models. It is difficult, however, to directly interpret the impacts of these variables on $NO_2$ concentrations, and therefore elasticities of the estimated model w.r.t. these variables are considered. Since WVKT and solar radiation are major factors to determine the $NO_2$ concentrations, these two variables selected to be analyzed. The derivative functions of the $NO_2$ models w.r.t. these two variables are calculated and then elasticities are computed across all input data.

Summary statistics for the calculated elasticities w.r.t. the WVKT and solar radiation variables are presented in Table 2. The hourly elasticities for these two variables are compared across roadside AQMs and background AQMs, and across the four seasons. Traffic flows have positive impacts on $NO_2$ concentrations at both locations and in all seasons. Higher elasticities are observed at roadside AQMs. A 1% increase in WVKT at background AQMs induces an average 0.13% to 0.23% increase in $NO_2$ concentrations. In contrast, for roadside AQMs, a 1% increase in WVKT leads to an average 0.17% to 0.29% increase. Two reasons explain these differences in the elasticities w.r.t. WVKT: (1) roadside areas are directly influenced by traffic emissions, and (2) NO emissions from tail pipes immediately react with ambient $O_3$, generating $NO_2$. In addition, if radicals, such as $RO_2\cdot$ and $HO_2\cdot$, are present in the atmosphere, NO reacts with these radicals instead of $O_3$. Generally, these radicals are associated with VOCs oxidation, and anthropogenic and biogenic VOCs are abundant in the urban atmosphere. Therefore, NO emissions can be easily converted into $NO_2$.

Table 2 Summary statistics for the elasticities w.r.t. WVKT and solar radiation in the $NO_2$ models

| Variable | AQM | Season | Min | 10th Pctl | Lower Quartile | Median | Mean | Upper Quartile | 90th Pctl | Max |
|---|---|---|---|---|---|---|---|---|---|---|
| WVKT | Background | Spring | 0.01 | 0.04 | 0.06 | 0.12 | 0.13 | 0.18 | 0.23 | 0.31 |
| | | Summer | 0.01 | 0.05 | 0.08 | 0.15 | 0.16 | 0.24 | 0.29 | 0.37 |
| | | Autumn | 0.02 | 0.07 | 0.11 | 0.22 | 0.23 | 0.33 | 0.40 | 0.61 |
| | | Winter | 0.01 | 0.05 | 0.09 | 0.16 | 0.17 | 0.24 | 0.27 | 0.38 |
| | Roadside | Spring | 0.05 | 0.08 | 0.12 | 0.17 | 0.17 | 0.22 | 0.25 | 0.28 |
| | | Summer | 0.08 | 0.12 | 0.17 | 0.22 | 0.23 | 0.29 | 0.33 | 0.47 |
| | | Autumn | 0.07 | 0.14 | 0.20 | 0.27 | 0.29 | 0.39 | 0.47 | 0.61 |
| | | Winter | 0.10 | 0.14 | 0.20 | 0.28 | 0.28 | 0.36 | 0.41 | 0.51 |
| Solar Radiation | Background | Spring | -2.58 | -1.50 | -0.95 | -0.21 | -0.52 | 0.00 | 0.00 | 0.00 |
| | | Summer | -1.24 | -0.92 | -0.62 | -0.19 | -0.33 | -0.02 | 0.00 | 0.00 |
| | | Autumn | -0.65 | -0.42 | -0.26 | -0.04 | -0.14 | 0.00 | 0.00 | 0.00 |
| | | Winter | -0.33 | -0.22 | -0.14 | -0.02 | -0.07 | 0.00 | 0.00 | 0.00 |
| | Roadside | Spring | -0.97 | -0.67 | -0.46 | -0.13 | -0.24 | 0.00 | 0.00 | 0.00 |
| | | Summer | -0.30 | -0.24 | -0.19 | -0.07 | -0.10 | -0.01 | 0.00 | 0.00 |
| | | Autumn | -0.21 | -0.14 | -0.09 | -0.02 | -0.05 | 0.00 | 0.00 | 0.00 |
| | | Winter | -0.19 | -0.12 | -0.07 | -0.01 | -0.04 | 0.00 | 0.00 | 0.00 |

Since ambient $NO_2$ is decomposed by UV radiation, the elasticities of the $NO_2$ functions w.r.t. solar radiation are negative. During night-time, the photodissociation of $NO_2$ does not occur, providing a zero elasticity. Since the Summer season has the shortest night-time, zero impacts are less frequently observed in the Summer than in the other seasons.

Background areas are more favourable conditions for generating $O_3$, suggesting that UV impacts on $NO_2$ solar decomposition are greater in background areas. In addition, the impacts of direct $NO_x$ emissions are smaller in background areas, leading to $NO_2$ concentrations that are more sensitive to solar radiations in background areas. Therefore, stronger negative elasticities are observed at background AQMs than at roadside AQMs. For example, a 1% change in solar radiation in Spring induces an average 0.52% decrease at background AQMs, but the same change at roadside AQMs leads to only an average 0.24% decrease.

The patterns of average hourly elasticities w.r.t. the WVKT and solar radiation on $NO_2$ concentrations are illustrated in Figures 3 and 4. Since roadside areas are directly impacted by traffic emissions, the hourly elasticities w.r.t. WVKT are higher at roadside AQMs across the four seasons. The patterns of hourly elasticities match the hourly traffic flow patterns (see Figure 2). Traffic flow patterns are characterized by two peaks, in the morning and the evening, and sustaining volumes during daytime. The elasticities display similar patterns, except for the evening traffic peak.

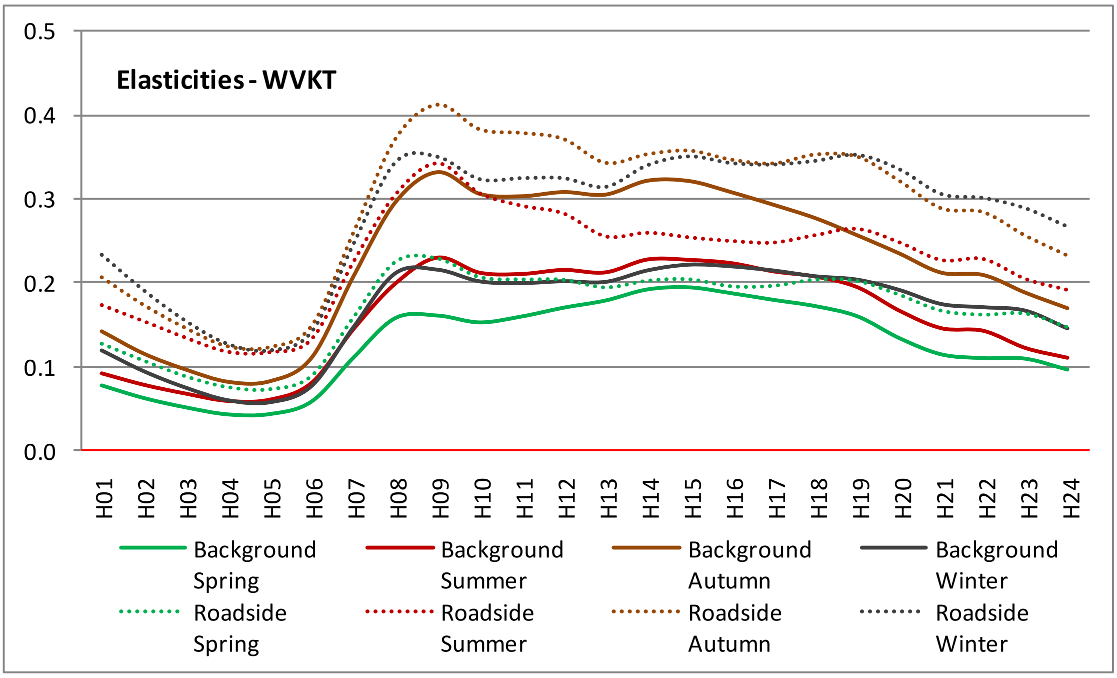


Figure 3 Average hourly-seasonal elasticities w.r.t. WVKT in the $NO_2$ models

The hourly elasticities w.r.t. solar radiation at background AQMs are lower than those at roadside AQMs across the four seasons. Since the intensity of solar radiation in Spring and Summer is higher than in the other seasons, the negative impacts of solar radiation on $NO_2$ concentrations are greater during these seasons than during the other seasons in both the background and roadside cases. $NO_X$ emissions from space heating are added to traffic emissions in Spring, leading to higher $NO_2$ concentrations in Spring than in Summer. Higher $NO_2$ concentrations in Spring provide more opportunities for solar radiation to actively decompose $NO_2$, which may explain the more sensitive elasticities w.r.t. solar radiation in

Spring. Weak solar radiation in Winter lead to lower $NO_2$ decomposition both for roadside and background AQMs.

As discussed, solar radiation has a negative impact on the concentrations of directly emitted pollutants during daytime. The OH· radical has a key role in initiating the oxidations of VOCs, leading to the formation of $O_3$ and $HNO_3$. $HNO_3$ removes both OH· and $NO_2$ from the atmosphere, and therefore increasing the generation of $HNO_3$ limits the recycling of OH· and $HO_2$·, resulting in decreasing $NO_2$ concentrations. Since the chemical reactions of these pollutants are interrelated each other, a single regression equation has limitations to explain the correct relationships between pollution concentrations and explanatory variables. Since the creation and destruction reactions occur simultaneously and the concentrations of interrelated pollutants are jointly determined with to the influence of UV radiation and precursors concentrations, simultaneous equations model would be an appropriate approach to investigate these relationships.

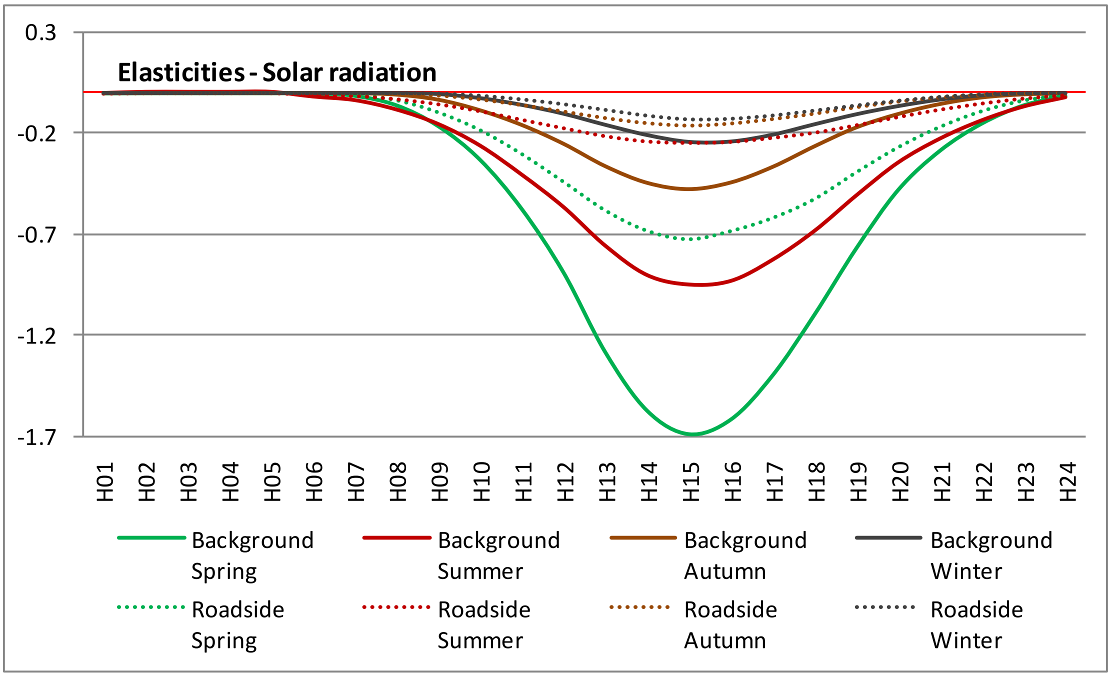


Figure 4 Average hourly-seasonal elasticities w.r.t. solar radiation in the $NO_2$ models

# DISCUSSION

In this research, $NO_2$ air quality panel models have been formulated and estimated, accounting for the impacts of WVKT, land uses, and meteorological factors on hourly-averaged concentrations across the four seasons. Advanced GIS techniques are widely applied to calculate explanatory variables, such as WVKT and land uses. Locational and daytime dummy variables are included in the panel models to assess the impacts of AQM general location and daytime variations on pollution concentrations. Traffic emissions, proxied by WVKT, have positive impacts in the $NO_2$ panel models. The analyses of hourly-seasonal elasticities show that the impacts of WVKT vary along the hours of the day, depending on the locations of the AQMs. Solar radiation has negative impacts on $NO_2$

concentrations. These two effects are consistent to the estimation results across the four seasons. The emissions from tail pipes contain abundant NO gas, leading to $O_3$ titration (Eq. 1), and thus WVKT display positive effects on $NO_2$ concentrations. However, $NO_2$ is decomposed by UV radiation, and therefore solar radiation has strong negative impacts on $NO_2$ concentration.

Since $NO_2$ is directly emitted vehicle flows and generated by chemical reactions (Eqs. 1 to 3), roadside areas are favourable conditions to accumulated $NO_2$ concentration than urban background areas. The OH· radicals produced under UV radiation react chemically with $NO_2$, leading to a decrease in the concentration. Since background regions provide good conditions for the regenerations of OH· radicals, solar radiation have greater negative impacts on the concentrations of $NO_2$ in background regions. The hourly elasticities w.r.t. solar radiation indicates that the negative impacts peak when the solar radiation also peak. The estimates of panel regression models support these theoretical assumptions.

Fossil fuel combustion from commercial, industrial, and residential areas have generally a positive impact on $NO_2$ concentration. However, these effects vary, depending on the seasons. It is reasonable to expect that the emission rates of urban land uses are different, depending on the intensity of anthropogenic activities across the hours of the day and the seasons. Land-use variables in this research, however, are time-invariant, and thus only spatial differences have been accounted for in the $NO_2$ panel models. To investigate the temporal impacts of land uses, it is necessary to include the temporal profiles of human activities across land uses. Diverse proxy variables, such as hourly demand for electricity, LNG, and water, would be used to measure these temporal profiles.

The air quality models based on emission inventories and dispersion processes have limitations for developing pollution maps for urban regions, because of large data and computational requirements. In contrast, since improvements in GIS techniques allow for the easy collection of land-use and transportation data needed for urban-scale air quality analysis, LUR approach presented in this research suggests that the potential to be developed as high-resolution air quality maps, which can then be used for the assessment of epidemiological impacts, the location/allocation of public facilities, and the evaluation of pollution mitigation policies.

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