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Validation of a Spatiotemporal Land Use Regression Model Incorporating Fixed Site Monitors

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Land use regression (LUR) has been widely adopted as a method of describing spatial variation in air pollutants; however, traditional LUR methods are not suitable for characterizing short-term or time-variable exposures. Our aim was to develop and validate a spatiotemporal LUR model for use in epidemiological studies examining health effects attributable to time-variable air pollution exposures. A network of 42 NO_2 passive samplers was deployed for 12 two week periods over three years. A mixed effects model was tested using a combination of spatial predictors, and readings from fixed site continuous monitors, in order to predict NO_2 values for any two week period over three years in the defined study area. The final model, including terms based on traffic density at 50 and 150 m, population density within 500 m, commercial land use area within 750 m, and NO_2 concentrations at a central fixed site monitor, explained over 80% of the overall variation in NO_2 concentrations. We suggest that such a model can be used to study the association between variable air pollutant exposures and health effects in epidemiological studies.

Introduction

Cohort studies investigating the short-term symptomatic and physiological effects of traffic-related air pollution are most powerful when they use exposure data that encompasses both temporal and spatial variation. Although a number of exposure methods have commonly been used, such as dispersion modeling, land use regression (LUR), use of data from fixed site monitors alone, and proximity based measures, none are ideally suited to this purpose.

Land use regression is sometimes used for estimating the air pollution exposure of households, and hence individuals, in epidemiological studies (*1, 2*). This method uses geographically based attributes to predict the spatial distribution of air pollutants over a defined area. However, most applications of LUR have been limited to describing spatial variation in long-term (often annual) average concentrations of air pollutants, particularly nitrogen dioxide (NO_2). In contrast, fixed site, continuous air pollution monitors collect data with high temporal resolution. However, these monitors are expensive and are usually sparsely distributed in urban environments. Since NO_x and NO_2 have marked concentration gradients over relatively short distances, this sparse distribution makes the network of fixed site monitors unsuitable for epidemiological studies that require information on a small spatial scale (*3*−*7*). Finally, emissions dispersion modeling can be used to estimate air pollutant exposure over time and space (*2, 8*−*11*). However, this method requires a diverse range of data including detailed information on vehicular fleet emissions, other emissions sources, as well as data on meteorology, solar radiation and atmospheric chemistry. Furthermore, the application of this method requires complex computer modeling. These practical difficulties have limited its accessibility in many settings.

A recent review has highlighted the potential for an extension of the LUR approach to address these deficiencies of existing exposure data sources and modeling techniques by including both a spatial and a temporal component in the models (*1*). A technique with these attributes could be used to assign air pollutant exposures to households or individuals over a defined time period. This study addresses this issue by combining data from a fixed site monitor with data from NO_2 passive samplers and geographical attributes to develop and validate a model to predict spatial and temporal variation in NO_2 concentrations within a defined study area.

Materials and Methods

We used data collected in the context of a cohort study (the Air Quality & Respiratory Health Study, AQRHS) investigating the respiratory health impact of a new road tunnel. The AQRHS required the estimation of household exposure to NO_2 for any three month interval between 2006 and 2008.

Study Area and Period. The study area was an approximately 5×10 km^2 region of inner northwestern Sydney incorporating a network of motorways and other major and local roads and traversed by the newly constructed road tunnel (Figure S1 in the Supporting Information). The area is predominantly residential, with pockets of parkland and commercial activities. The study period extended from 1st of January 2006 to 31st of December 2008.

Spatial Predictors. We used layers within geographical information systems (ArcGIS v 9.1) software to examine data on traffic counts, population density, land elevation, and land use as potential predictors of NO_2 exposure. For each point within the study area, the average of the spatial characteristic within a defined radius was evaluated as a predictor of NO_2 concentrations (Table S1 in the Supporting Information).

We used data from vehicle classification surveys, in which vehicles traversing defined points on the road network were classified and enumerated, for the 38 roads in the study area for which these data were available. The surveys were conducted over a one week period during November and December 2004 and again at the same time during 2008. The data from these two surveys were assigned to those roads for the years 2006 and 2008, respectively. Where these survey data were not available, we assigned traffic counts based on information from the Sydney Coordinated Adaptive Traffic

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System (SCATS), a system the NSW Roads & Traffic Authority (RTA) uses to control phasing and timing of traffic signals, where this was available. The SCATS data was also useful for assigning traffic counts for 2007, given that vehicle classification surveys were not carried out for this year. However, neither of these sources could be used for small local roads that were not serviced by traffic lights. We used local government estimates for these local roads, where available, and applied a value of 500 vehicles per day (vpd) as the default for other local roads where counts were not available. Hence, we were able to define traffic volumes for all roads in the study area.

A traffic density variable was created in GIS by creating a circle with a defined radius around each point in a map layer. The length of the portion of each line (meters) that fell within the circle was calculated. Each line was weighted by its assigned traffic volume (vehicles per day). The weighted lengths of these lines were summed, and the total divided by the area of the circle (square kilometers) to yield a weighted traffic density for each point within the study (*12*). Population density was obtained by applying a kernel density function to census population data for 2006 (*13*). Population data from the census is aggregated to Mesh Blocks, which typically contain 30–60 households. Land use variables were constructed by calculating the area of a particular land type (square meters), within buffers of different radii (Table S1 in the Supporting Information).

Measured Concentrations of NO_2. NO_2 concentrations were measured at 42 sites in the study area using passive diffusion samplers prepared and analyzed by the Commonwealth Scientific & Industrial Research Organization (CSIRO) (*14*). Their lower limit of detection was 0.5 ppb. The locations of the sampler sites were chosen to represent a wide range of traffic exposure conditions: from very quiet background levels in residential streets (estimated traffic counts up to 500 vehicles per day) and near bush land settings, to curbside locations on the most heavily trafficked roads in the area. The devices were deployed for three two week periods between September and December in each of 2006, 2007, and 2008 and also, at a subset of 11–13 sites, on three two weeks periods between March and June 2008. One in five randomly chosen locations was sampled in duplicate. Where duplicate sampler readings differed by more than 30% (2% of duplicate pairs), these results were excluded from the analysis.

There were four ground level fixed site air quality monitors in the study area that recorded NO_2, measured using the chemiluminescent method, wind direction, wind speed, and ambient temperature (at 2 m and 10 m height above ground level), as well as other pollutants, every five minutes throughout the study period (abbreviated as CBW, CBE, GBW, GBE). The sites were chosen by government and the community to reflect urban background concentrations. They were operated by Ecotech Pty Ltd., a National Association of Testing Authorities (NATA) accredited agency. Validated data were audited by an independent company.

We did not deploy passive samplers during the first half of 2006 and 2007. For those years, we used two week average NO_2 concentrations from the four fixed site monitors as if they had been passive samplers located at those sites. This provided some data on year round variation in NO_2 in the study area, although it was limited to those four locations.

Model Fitting. The dependent variable in the model was the NO_2 concentration, measured by the passive samplers as described above. The distribution of NO_2 concentrations was highly skewed to the right; and hence, values were log-transformed resulting in an approximate normal distribution. We used values for NO_2 for each sampler to represent NO_2 concentration at the designated location during the two week period when that sampler was exposed.

The traffic density, population density, elevation, and land use variables were tested as predictors of spatial variation. To model temporal variation, average NO_2 concentrations for the relevant two week periods from the background fixed site monitor readings were used. These fixed site monitor readings were incorporated in three ways. In model 1, the average of the four fixed site monitors was used. Model 2 used the nearest fixed site monitor reading. Model 3 used just the most central monitor in the study area, CBW. Categorical variables representing year, season, and their interaction with fixed site monitor were also tested.

While a least-squares regression model could have been used, we implemented a hierarchical mixed effects model with random effects to account for the spatial correlation of the passive samplers. This model can be represented by the following random intercepts mixed model:

$$\log(\mathrm{NO_2})_{ij} = \beta_{0ij} + \beta_1 X_{ij} + \beta_2 Y_{ij} + \beta_3 Z_{ij} \ldots$$

$$\beta_{0ij} = \beta_0 + u_{0j} + e_{0ij}$$

$$u_{0j} \sim N(0, \sigma^2_{uo})$$

$$e_{0ij} \sim N(0, \sigma^2_{e0})$$

where the subscripts i and j represent the NO_2, site levels of the model, β_1, β_2, β_3, and so forth represent the coefficient estimates for the fixed model predictors, and u_{0j} and e_{0ij} represent the site random effect and model error term, respectively. We tested several correlation structures and selected the one that yielded the smallest value for the Akaike Information Criteria (AIC). Data for the entire three year period were included in a single model. Initially, LSR with R^2 selection was used to identify the best predictors for inclusion in the final model (using a significance level of 0.05). The R^2 selection method determines the subset of independent variables that optimizes the R^2 of the model for a given number of variables. Model variables were checked for collinearity, and those with a Variance Inflation Factor (VIF) greater than 3 were excluded.

In order to make a comparison with the ratio method, the average passive sampler reading at each site for each year was using to construct an LUR model (model 5). However, given the absence of passive sampler readings for the first half of 2006 and 2007, and the small number of sites used during the first half of 2008, only Spring values (September to December) were used, giving a four month average for each year. The ratio of the average CBW reading for the two weeks that each passive sampler was deployed was divided by the average CBW reading for the four month Spring period and used to adjust the four month passive sampler readings as predicted by the LUR.

Validation. We used leave one out cross validation (LOOCV) to assess the predictive validity of models 1, 2, and 3 (*15*). This involved refitting the model excluding all data (that is, all periods sampled) for one site at a time rather than excluding one measurement at a time for each site. This allowed us to assess both spatial and temporal predictive validity. The agreement between the predicted and observed values for each site was ascertained as an indicator of the validity of the model (*16, 17*) and included the calculation of bias, upper and lower limits of agreement, the intraclass correlation coefficient (ICC) and mean square error (MSE). We also calculated the R^2 and the type 1 squared semipartial correlation coefficient (PCORR1) for the equivalent LSR implementation of the optimal model to provide an alternative indication of model fit and the contribution of each variable to the model.

We also tested the agreement between the LUR model estimates for the site of a fifth fixed site monitor (AMS) in

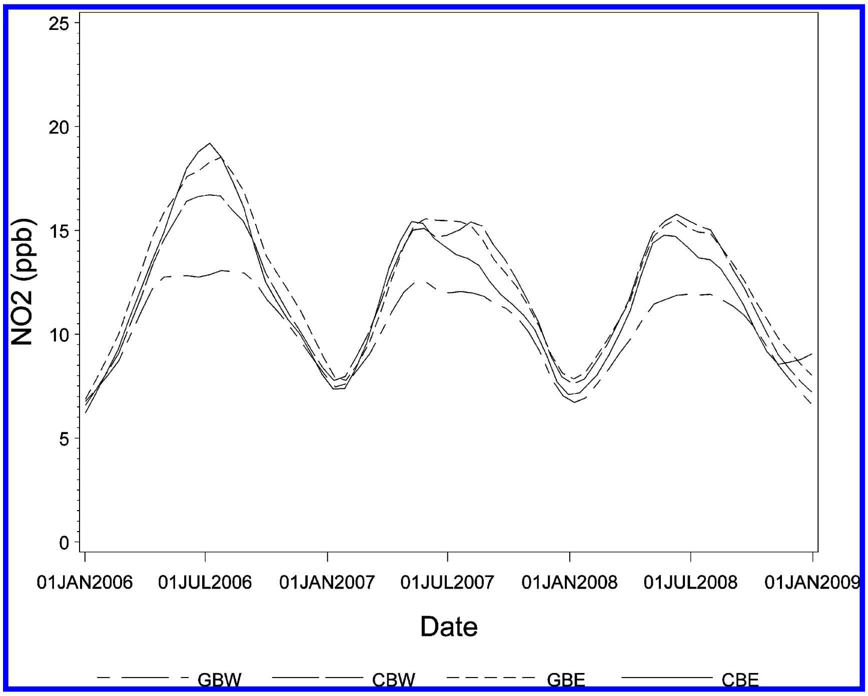

FIGURE 1. NO_2 concentrations (smoothed Lowess) at the four fixed site monitors, January 2006 to December 2008.

TABLE 1. Agreement between Observed Passive Sampler NO_2 (ppb) and That Predicted by the LUR Models (Using LOOCV)

model	covariates	bias	limits of agreement		ICC[a]	mean square error
			upper	lower		
1	TD50, TD50_150, PD500, COM750, $FIXED_{mean}$	0.017	2.64	−2.60	0.89	1.72
2	TD50, TD50_150, PD500, monitor, $FIXED_{nearest}$	−0.006	2.74	−2.76	0.88	1.89
3	TD50, TD50_150, PD500, COM750, $FIXED_{CBW}$	0.004	2.61	−2.60	0.90	1.69
4	$FIXED_{nearest}$	0.110	5.34	−5.11	0.51	6.80
5	TD50, TD50_150, PD500, COM750, year	0.20	4.38	−3.98	0.73	4.34

[a] Intraclass correlation coefficient.

the study area and observed values at that site during the period of September to December 2008. Data from this fixed site monitor were not used in developing the regression models.

Software. We used ArcGIS 9.1 for GIS analysis. A Geocentric Datum of Australia 1994 to Map Grid of Australia 1994 Zone 56 (Universal Transverse Mercator, using the GRD80 Ellipsoid) transformation was used in all GIS processing. Regression analysis was carried out using SAS 9.1 (SAS Institute, Cary, NC).

Results and Discussion

Table S2 in the Supporting Information shows summary data for the passive samplers for each period they were deployed over the three years of the study. Data from the fixed site monitors demonstrate both spatial and temporal variation in NO_2 concentrations (Figure 1). There was a marked seasonal trend in NO_2 concentrations, which were higher in the winter months. This trend was evident at all four continuous monitoring sites.

The LSR analysis identified a best set of variables for inclusion in the hierarchical mixed effects model. Predictors that were found to be significant across all the models included population density within 500 m (PD500), traffic density within 50 m (TD50), traffic density between 50 and 150 m (TD50_150), area of commercial land use within 750 m (COM750), and a dummy variable representing the nearest fixed site monitor (monitor). A mixed effects model was then fitted using these predictors. An exchangeable correlation matrix for the random effect was found to produce the smallest AIC. Table 1 show the agreement statistics for the different models using LOOCV. Model 4 shows these agreement statistics where only the nearest fixed site monitor to the passive sampler was used. The residuals for the LUR models were normally distributed with a mean of zero, and there were no unusually influential observations. Although the improvement was small, the use of a mixed model produced better agreement statistics than the equivalent LSR model. For instance, the MSE for model 3 was 1.76 using least-squares regression compared to 1.69 using the mixed model. The limits of agreement and bias were also larger using LSR. This is because the mixed model is able to take into account correlation for readings belonging to a particular site and produce more efficient estimates of coefficients. It is not possible to provide an R^2 value for a mixed model; however, the equivalent LSR implementation of model 3 yields an R^2 of 0.83.

Based on the agreement statistics, the model using just the one fixed site monitor (model 3) performed marginally better than the one using the mean fixed site readings (model 1). The ICC for models 1, 2, and 3 were excellent (ICC = 0.88−0.90) and much better than the agreement between the observed values and those derived from the nearest fixed site monitor (model 2, ICC = 0.51, Table 1 and Figure S2 in the Supporting Information). Although not strictly comparable because only Spring data were modeled, the ratio method (model 5) did not perform as well as models 1 to 3.

TABLE 2. Parameters from Model 3 Land Use Regression Mixed Model for Predicting log NO_2

predictor	estimate	lower CI	upper CI	*P*	PCORR1[a]
intercept	2.22	2.15	2.25	<0.0001	–
TD50	0.67	0.57	0.76	<0.0001	0.35
TD50_150	0.40	0.21	0.60	<0.0001	0.066
PD500	33.49	21.70	45.28	<0.0001	0.037
COM750	0.46	0.12	0.80	0.008	0.012
$FIXED_{CBW}$	0.061	0.057	0.065	<0.0001	0.37

[a] Values based on the equivalent LSR implementation using the same predictor variables.

Table 2 lists the variables of model 3, including coefficient estimates, confidence intervals, and significance.

Figure 2 compares predictions of model 3 for NO_2 concentrations at the location of the new fixed site monitor (AMS) with prediction using the ratio method and nearest fixed site monitor. While model 3 follows the levels of the AMS readings over the four months fairly closely, readings predicted with the ratio method tend to overestimate the AMS readings at the start. The nearest fixed site monitor to this site, GBE, was 700 m away from the AMS monitor and underestimates the AMS readings. Figure 3 shows maps using model 3 to predict average levels of NO_2 for January/February 2006 and May/June 2006.

The use of data from fixed site monitors in our model differs from use of these data in previous studies where they were used to limit bias in the comparison of annual averages across sites (*5*) or to adjust passive samplers where measurements were not carried out concurrently (*18*). In these applications, the ratio of air pollution readings from a fixed site monitor to the average reading over a year was used as an adjustment factor. Similarly, a study investigating the effect of traffic related air pollution on birth weight used average daily NO_2 concentration measured at a fixed site monitor over nine months of gestation to adjust local NO_2 concentrations estimated using an LUR model (*19*).

It is possible to use these correction techniques to provide temporal adjustment to annual estimates from an LUR model. However, there are two key advantages to our approach. First, a traditional LUR model that estimates annual averages forces the researcher to exclude passive sampler sites from the model where there are any missing values for that site, reducing study power, and potentially biasing the results. Since missing sampler values in this context are likely to be missing at random, the implicit imputation inherent in using a mixed model allows all passive sampler measurements to be incorporated into the prediction model. Second, because two week passive sampler readings are modeled directly, we believe our method produces better estimates. This is evident in the results of model 5.

There have also been other attempts in modifying LUR models to estimate air pollutant concentrations within a time and a spatial dimension simultaneously. One of these studies incorporated hourly data on wind speed, wind direction, and cloud insulation to construct a hybrid source area (SA)-LUR model (*20*) to estimate concentrations of NO_2 and NO_x for Vancouver (*21*). As well as including these time-dependent predictors, these investigators also modified the standard LUR approach by using the distance traveled by wind within 1 h as the radius of the concentric circles (kernels) around points within the study area. Another study used data from a fixed site air pollution monitor, together with meteorological conditions, day of the week, cumulative traffic density within 100 m, and other data, to form a nonparametric regression modeling nonlinear effects on the distribution (*22*). The advantage of our approach is that, by using actual measurements from continuous monitors, one is better able to capture temporal influences that cannot be modeled from meteorological information alone. Our approach is also computationally simpler and does not require detailed meteorological information.

In this application of the model, we were fortunate to have data for four fixed site monitors within the relatively small study area. Intuitively, our models work by utilizing the spatial information of the variables such as traffic density to adjust the background levels from the fixed site monitor. The four fixed site monitors were positioned to measure background pollution; however, although of low traffic volumes, GBW and more significantly CBE were placed quite

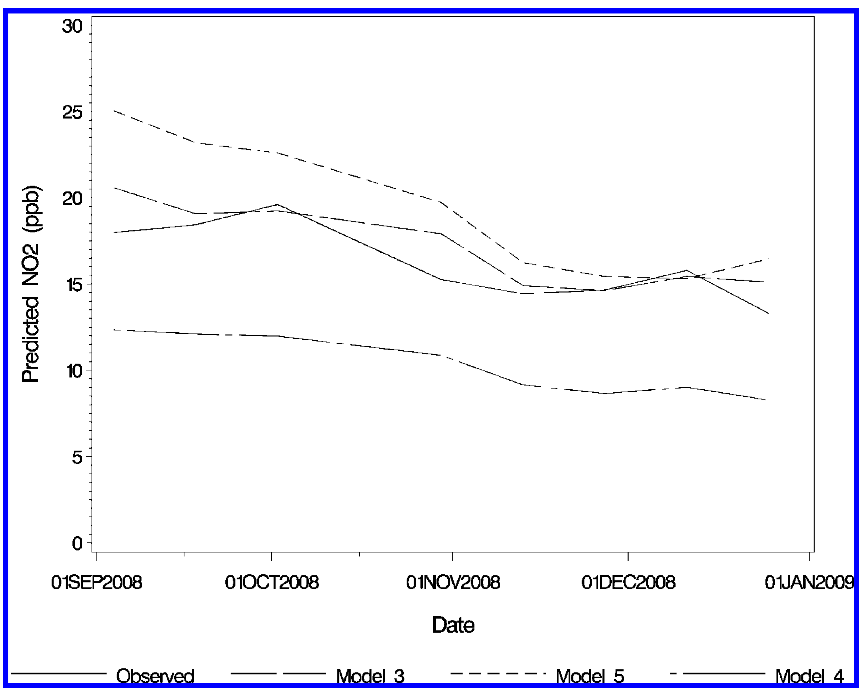

FIGURE 2. NO_2 concentrations at the fixed site monitor AMS, with LUR (model 3), ratio method (model 5), and nearest fixed site monitor (model 4) predictions for that site, September to December, 2008.

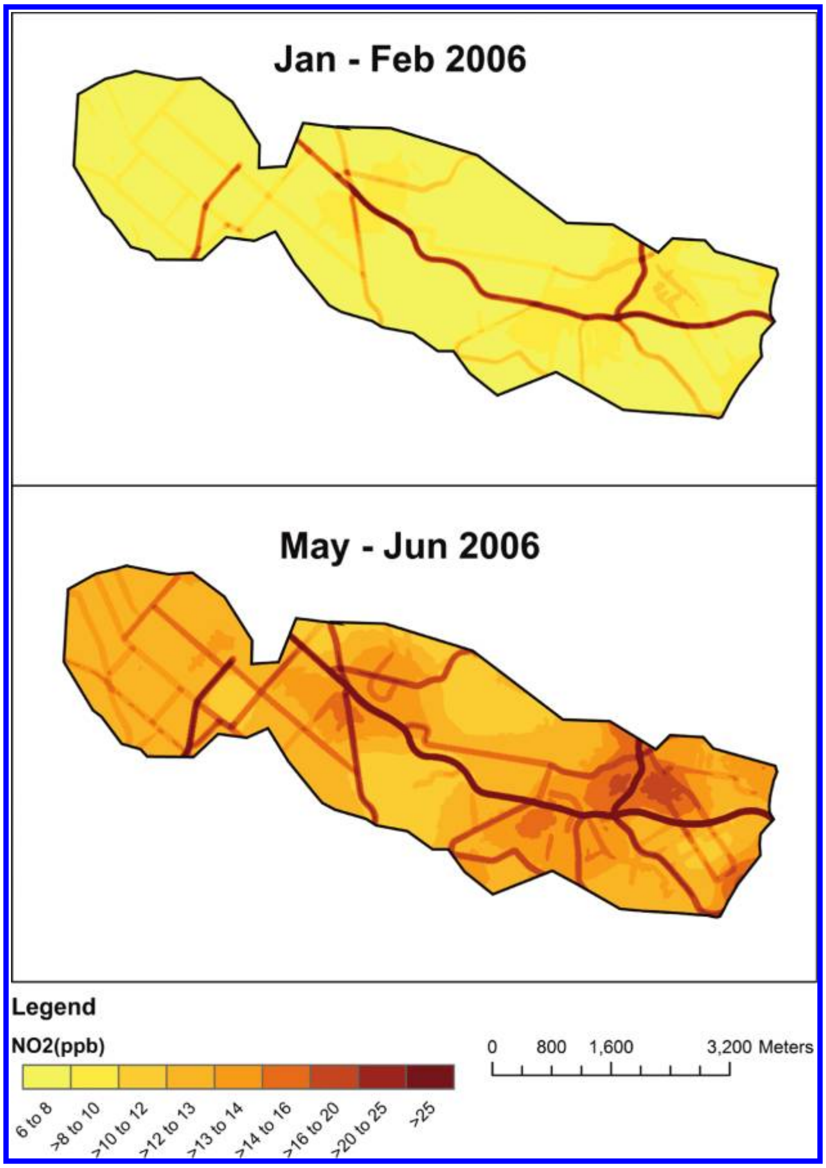

FIGURE 3. Maps estimating mean concentration of NO_2 (ppb) over a two month period during early and mid 2006.

close to roads. As well as being the central most monitor, CBW had a very low density of roads nearby, as well as low population density and proximity to commercial land use. It is difficult to be sure how significant the different positioning of the fixed site monitors had on the final results and whether it is important that a fixed site monitor strictly measure background levels. The intercept term in the model will always allow appropriate adjustment in the context of lower passive sampler readings to fixed site readings. The other interesting observation is that only one fixed site monitor was sufficient to produce the optimal model. It may be that the differences in pollution levels across the three years seen in Figure 1 were not significant enough to require the inclusion of data from all four monitors. More research is need however to determine the optimal positioning of fixed site monitors and the number of monitors needed for larger study areas.

The predictive model used in this study may have been improved further if passive samplers had been deployed during the first half of 2006 and 2007. However, the incorporation of data over three years, which allowed the inclusion of information from the passive samplers that were deployed in early 2008, and the inclusion of data from four fixed site monitors as if they were passive samplers for the first half of 2006 and 2007, have helped overcome this data limitation. This is reflected in the validation of the LUR model against the fifth fixed site monitor (not used in development of the model) where it performed well in predicting temporal variation in NO_2.

Traffic density within 50 m was a strong individual predictor of NO_2 concentrations in this study area. All LUR models used to predict spatial variability of NO_2 have found that measures related to traffic, including traffic volume, density, or intensity, distance to roadways, length of roads within certain buffers, road type, or road vehicle emissions, have contributed to the predictive capability of NO_2 (*1, 23*). In our study, other traffic related variables such as weighted road density and distance to major road were tested but were found not to be as good a predictor as traffic density (*12*). However, the buffer distance for traffic density that was significant in this model (up to 150 m) is smaller than the buffer distance (>300 m) identified in some previous studies (*24*−*27*). This may be due to the fact that the main roads in this study had relatively light traffic (predominantly light vehicles and less than 100 000 vpd) compared with those included in other studies. Further application of this method is recommended to give a clearer picture of how well it performs in different study areas.

This mixed effects regression model combining data on traffic and population density with data from a central fixed site monitor provides a reliable and accurate solution for epidemiological studies where spatiotemporal exposure data are required. We have demonstrated that it is possible to estimate average pollutant levels, in this case NO_2, for time periods much shorter than used in previous LUR models. The utility of our spatiotemporal model lies in the ability to estimate air pollutant concentrations for any two week period and at any point within a defined study area. The importance of this is evident in Figure 3, which demonstrates how greatly the levels in NO_2 can vary between different times of the year. For larger study areas, and/or where the only available temporal readings are some distance away, the mixed model approach is a better alternative than using a ratio method to adjust annual LUR predictions because sites with missing values do not need to be dropped. A disadvantage of our approach is the necessity to measure NO_2 throughout the study period. Given that it is not always practical to deploy fixed site monitors for many studies, an alternative approach may be to deploy one or more passive samplers every two weeks throughout the year thus providing the temporal readings required for this model. We suggest that the spatiotemporal technique outlined in this paper provides a more valid air pollution estimate for epidemiological studies where the exposure period is less than a year and/or where exposure periods differ between individuals.

Acknowledgments

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Supporting Information Available

Map of study area, table of traffic and land use variables tested, summary statistics of NO_2 passive sampler readings (parts per billion) by year, and plots of predicted NO_2 versus observed NO_2 for LUR model compared to just using nearest fixed site monitor. This material is available free of charge via the Internet at http://pubs.acs.org.

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