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Sensitivity analysis of the near-road dispersion model RLINE - An evaluation at Detroit, Michigan

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ABSTRACT

The development of accurate and appropriate exposure metrics for health effect studies of traffic-related air pollutants (TRAPs) remains challenging and important given that traffic has become the dominant urban exposure source and that exposure estimates can affect estimates of associated health risk. Exposure estimates obtained using dispersion models can overcome many of the limitations of monitoring data, and such estimates have been used in several recent health studies. This study examines the sensitivity of exposure estimates produced by dispersion models to meteorological, emission and traffic allocation inputs, focusing on applications to health studies examining near-road exposures to TRAP. Daily average concentrations of CO and NO_x predicted using the Research Line source model (RLINE) and a spatially and temporally resolved mobile source emissions inventory are compared to ambient measurements at near-road monitoring sites in Detroit, MI, and are used to assess the potential for exposure measurement error in cohort and population-based studies. Sensitivity of exposure estimates is assessed by comparing nominal and alternative model inputs using statistical performance evaluation metrics and three sets of receptors. The analysis shows considerable sensitivity to meteorological inputs; generally the best performance was obtained using data specific to each monitoring site. An updated emission factor database provided some improvement, particularly at near-road sites, while the use of site-specific diurnal traffic allocations did not improve performance compared to simpler default profiles. Overall, this study highlights the need for appropriate inputs, especially meteorological inputs, to dispersion models aimed at estimating near-road concentrations of TRAPs. It also highlights the potential for systematic biases that might affect analyses that use concentration predictions as exposure measures in health studies.

1. Introduction

Exposure metrics used in health effect studies of traffic-related air pollutants (TRAPs) can affect estimates of health risk, such as the magnitude and confidence interval of odd-ratios in cohort and panel studies (Dionisio et al., 2015). While many approaches have been used, the development of accurate exposure metrics for these studies remains challenging (Batterman et al., 2014a; Jerrett et al., 2005). Studies requiring spatially-resolved exposure estimates cannot depend on central site air quality monitoring due to the local scale variation or spatial gradients of TRAP concentrations found near major roads (HEI, 2010) and the spatially sparse nature of ambient monitoring networks, including the lack of near-road monitoring sites. Considering active fine particulate matter ($PM_{2.5}$) monitors in US cities and surrounding suburbs, for example, Los Angeles has 11 monitoring sites, Washington DC has 4, and Detroit has 9 (US EPA, 2017a). Considering near-road monitoring stations, these cities have only one or two sites each, and a total of only 72 near-road sites operated across the US as of 2015 (Watkins and Baldauf, 2012a). Instead of central site monitoring, health studies have relied on exposure metrics derived using interpolation methods, geographic information system (GIS) variables, land use regression and other methods that incorporate variables such as the distance to nearby roads, traffic volume, vehicle mix, traffic intensity and population density (Batterman et al., 2014a; Jerrett et al., 2005). While useful for health effect analyses, these approaches have several limitations: most do not capture the temporal variability resulting from changes in meteorology, traffic patterns and emission factors; the ability to generalize to other environments and other pollutants is limited; and metrics expressed in terms other than concentration (e.g., proximity) can be difficult to interpret (Vette et al., 2013; Isakov et al., 2014).

Dispersion models can overcome many of the limitations of monitoring data and the exposure approaches noted above, and they have been used in a several recent health studies (Vette et al., 2013; Isakov et al., 2014; Bell et al., 2011; Lobdell et al., 2011; Wang et al., 2009, 2015; Wu et al., 2011; Beevers et al., 2012). Results of dispersion

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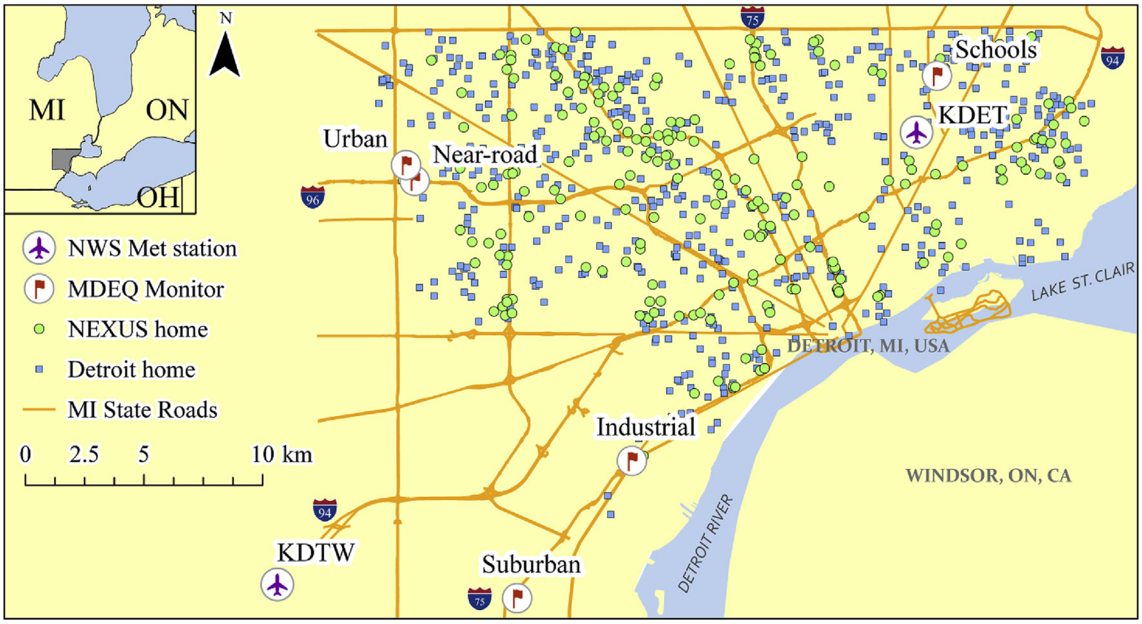

Fig. 1. The modeling domain, including National Weather Service (NWS) meteorological stations, Michigan Department of Environmental Quality (MDEQ) air pollution monitors, a subset of Michigan State Trunkline Highway System, locations of NEXUS receptors (representing 206 residences in the NEXUS cohort), location of Detroit receptors (representing a population-weighted sample of residences in Detroit, n = 543).

models, like other models, depend on the model inputs and parameters selected. Sensitivity analyses can reveal how a particular model responds to variations in input variables or internal parameters (Rao, 2005). While not providing a full measure of model uncertainty, sensitivity analyses reveal the relative amount of uncertainty associated with each model input, the robustness of the model with respect to changes in inputs and parameters, and critical model inputs, i.e., those that are uncertain and that cause large changes in model predictions (Rao, 2005; Vardoulakis et al., 2002).

Results of dispersion models can be sensitive to model inputs and parameters. For example, all dispersion models require meteorological data, which fundamentally influence dispersion calculations (Vardoulakis et al., 2002; Dhyani and Sharma, 2017; Gulia et al., 2015; Salizzoni et al., 2012). Ideally, these data use on-site or local observations (Salizzoni et al., 2012). However, local meteorological datasets are typically limited, e.g., of the 72 near-road monitoring sites in the USA, only 6 have a National Weather Service (NWS) meteorological station within 5 km, and the average distance to the nearest station is 18.5 km (US EPA, 2015). Previous sensitivity studies using industrial emissions, e.g., mercury and hexavalent chromium, attributed 16–25% variability in results to changes in meteorological inputs (Hodgson et al., 2007; Sax and Isakov, 2003). However, with regards to TRAPs in urban areas, such sensitivity studies are limited. As a second example, emission data used in dispersion models depend on traffic activity (e.g., number of vehicles, vehicle mix, vehicle speed and acceleration), which in turn depends on commuting and work schedules, construction activity, weather and many other factors (Batterman, 2015). Typically, emission rates are derived using simplified and default allocations to obtain hourly and daily estimates from annual average data. Again, local information regarding traffic volume and mix is recommended, but such inputs are rarely available.

This study examined the sensitivity of exposure estimates for health applications produced by dispersion models to meteorological, emission and traffic allocation inputs. The analysis used the Research Line source model (RLINE), a research-grade dispersion model specifically designed for near-road applications (Snyder et al., 2013), to predict daily average concentrations of two common TRAP, oxides of nitrogen (NO_x) and carbon monoxide (CO). These concentrations were compared to measurements at near-road monitoring sites in Detroit, MI, and were used to assess the potential for exposure measurement error in cohort and population-based studies. $PM_{2.5}$ was also measured at near-road monitoring stations in Detroit; however, previous analyses (Milando and Batterman, 2018) showed that background levels of $PM_{2.5}$ were high (> 85% of total), thus the sensitivity of $PM_{2.5}$ to changes in mobile source modeling was not examined.

2. Methods

The sensitivity of dispersion model-based exposure estimates was determined by comparing baseline (or "nominal") and alternative inputs for meteorological, emission, and traffic allocation parameters. This work builds on a previous operational evaluation of RLINE (Milando and Batterman, 2018), which covers in detail the methods by which emissions from point and mobile sources in Detroit, MI were modeled (only the RLINE mobile source modeling is described below). Model predictions using nominal and alternative inputs were compared to observed monitoring data, and exposure estimates using nominal and alternative inputs were compared for a "vulnerable" and general population in Detroit, MI. Differences in predicted concentrations due to varying model inputs were assessed using metrics recommended for air quality model evaluation (Hanna and Chang, 2012; Chang and Hanna, 2004), and in the application are translated to possible health impacts using health impact assessment techniques.

2.1. Monitored data

The Detroit area contains five US Environmental Protection Agency (EPA) Air Quality System (AQS) monitoring stations located near high traffic roads (Fig. 1). These include: the "suburban" Allen Park site 190 m southeast of Interstate 75 (I-75; annual average daily traffic (AADT) of 89,800 (MDOT, 2014b)); the "industrial" Dearborn site (150 m northwest of I-75; AADT = 105,800); the "schools" or East 7 Mile site (390 m east of MI-97; AADT = 9500); and the "near-road" and "urban" Eliza Howell sites (respectively 10 and 100 m north of I-96, AADT = 152,000). Air quality data for 2011 to 2014 were obtained from the US EPA AQS Datamart (US EPA, 2016). Over the study, these sites used several types of monitoring instruments that differed in sensitivity and possibly other aspects, thus, analyses at each site are separated by instrument type (US EPA, 2017b). NO_x at the near-road and urban sites was monitored using gas-phase chemiluminescence and Ecotech 9814B monitors ("IGpCHEM") from October 2011 through December 2013, and using Thermo Environmental Instruments Model 42C instrumental chemiluminescence ("ICHEM") in 2014. NO_x at the schools site was measured using a Thermo Environmental Instruments Model 42C and by ICHEM. CO was monitored at the near-road site by instrumental gas filter correlation using an Ecotech 9830 monitor ("EC9830T") from October through December of 2011, and a Thermo Model 48C monitor using instrumental non-dispersive infrared ("INDiI") through 2014. CO at the urban site was measured using Thermo Environmental Instruments Model 48C and by INDiI, and at the suburban site using an instrumental gas filter correlation analyzer ("IGFC"). CO at the industrial site was measured using a Teledyne API T300 using IGFC. For comparison to model predictions, NO and NO_2 measurements in ppb were converted to NO_x concentrations using the average observed ratio ($1\,\mu g\,m^{-3}$ $NO_x = 0.5495$ ppb NO_x); CO comparisons were made in ppb. Measurements below method detection limits (MDLs) were omitted. Daily averages were calculated from hourly data.

2.2. Meteorology

Meteorological data were obtained at the five AQS sites, two local National Weather Service (NWS) stations located 33 km apart (Detroit City Airport or KDET; Detroit Metro Airport or KDTW; see Fig. S1 for wind roses) (NWS, 2016), and the Pontiac, MI radiosonde site (approximately 45 km north of Detroit) (NOAA, 2016) (Fig. 1). The NWS data include the meteorological parameters needed by the AERMET meteorological data preprocessor (Cimorelli et al., 2005) (See Table S1 for list of parameters) to develop the "surface" (SFC) meteorology files used by RLINE, whereas the AQS sites collect only basic parameters, e.g., surface wind speed and direction. The NWS data at KDET was designated as nominal due to its central location and presumed representativeness (Isakov et al., 2014). Three sets of alternative meteorological inputs were developed: SFC files using NWS data at KDTW; AQS-site-specific meteorology supplemented with KDET data (on-site/KDET); and site-specific meteorology supplemented with KDTW data (on-site/KDTW). SFC files generated using AERMET and the NWS data were confirmed to be similar or identical to those distributed by the Michigan Department of Environmental Quality (MDEQ) for air quality modeling purposes (Japan Meteorological Agency, 2017). Differences between nominal and alternative wind-speed and direction were evaluated using the circular correlation coefficient (Jammalamadaka and Sengupta, 2001). Hours missing any required parameter were excluded. The SFC files were mostly complete, e.g., only 6–15% of all hours were missing, with most of the missing hours occurring at night-time (see Table S2).

2.3. Emission inventory, emission factors, and time allocation factors

A spatially- and temporally-resolved link-based emission inventory consisting of 9701 links provided emission factors which were used to generated RLINE predictions for dispersion of NO_x and CO from all but the smallest (local) roads in Detroit (Snyder et al., 2014; Milando and Batterman, 2018; MDOT, 2014a). As described elsewhere (Milando and Batterman, 2018), the original inventory was updated with more recent traffic volume data from the Michigan Trunkline Highway System (MDOT, 2014a). The nominal emission factors (g vehicle^{-1} mile^{-1}) were derived using the Motor Vehicle Emission Simulator (MOVES) version 2010 (US EPA, 2014) and Detroit-specific data for 2010. Other MOVES inputs included temperature (grouped in 11 bins from 0 to 100 °F in 10° increments) and barometric pressure (using defaults similar to local conditions) (SEMCOG, 2011). Following previous work (Snyder et al., 2014; Decker et al., 1996), emission factors for running exhaust and running evaporative modes were calculated. The emissions inventory was updated to create alternative inputs using MOVES 2014a (US EPA, 2014) and 2015 inputs for the 3-country area (Wayne, Macomb and Oakland counties) provided by the Southeast Michigan Council of Governments (SEMCOG). The updated inventory reflects changes from 2010 to 2015, as well as differences between fleets in the 3-country area as compared to Detroit (which occupies most of Wayne County). The sum of the link-based emissions inventory for Detroit represented 66 and 71% of the CO and NO_x emissions, respectively, of 2011 National Emission Inventory (NEI) on-road emissions for Wayne County (Table S3).

Hourly vehicle volume estimates were derived for each link of the emissions inventory from annual average daily traffic (AADT) estimates adjusted by temporal allocation factors (TAFs), e.g., for month-of-year, day-of-week and hour-of-day adjustments (Snyder et al., 2014). For the alternative cases, Detroit-specific TAFs separated commercial and non-commercial vehicles and are based on 2009 to 2012 data monitored at 13 permanent counting stations in southeast Michigan (Batterman et al., 2015). Importantly, these "local" TAFs distinguish the morning and afternoon commuting ("rush hour") volume peaks for passenger vehicles from the mid-day peak for commercial vehicles. A profile that merged commercial and non-commercial fleets in Detroit was also used as alternative. The nominal profile of default US TAFs for a combined commercial and non-commercial fleet was generated from previous work (Batterman, 2015).

2.4. Receptor sets

Three sets of receptors were used. The first placed receptors at the near-road monitoring sites in the study domain (n = 5; Fig. 1). The second and third sets respectively represent location of a vulnerable school-age population and the general population. The second set used 206 receptors that represented residences of children with asthma participating in the NEXUS study (called "NEXUS" receptors; 6 receptors outside the modeled domain were excluded) (Vette et al., 2013). Approximately two-thirds of these children lived within 200 m of roads with AADT > 75,000 (e.g., interstate highways) at the time of enrollment into NEXUS, thus, this set oversamples near-road locations. The third set was designed to be representative of residences in Detroit. This set, called "Detroit," was created by randomly selecting (with replacement) 1000 of the 2010 Census blocks in Detroit, which resulted in 543 unique blocks. Receptors were placed at the building footprint-centroid of the highest occupancy parcel in each selected block (Urban, 2014; US Census Bureau, 2015a).

Distances to the nearest "major" road, i.e., AADT > 10,000 (a conservative cut-point for distinguishing high trafficked roads), were calculated for receptors in sets 2 and 3 (Fig. S2). For the NEXUS receptors, 61% were within 200 m, 20% within 200–400 m, and 19% beyond 400 m; for the Detroit receptors, these three groups contained 57, 29 and 13% of the population-weighted receptors, respectively. The differences between receptor sets 2 and 3 reflect the design of the NEXUS study which selected households that were near major roads (< 200 m) as well as comparison households that were further away (> 350 m), however, differences are somewhat diminished since many NEXUS children moved during the study period. We also calculated the number of major roads within 500 m of each receptor. For the NEXUS receptors, 10% of receptors had no major roads within 500 m, 66% had 1–10 major roads within 500 m, and 23% had more than 10 major roads within 500 m; for Detroit receptors, the corresponding percentages are 7, 74 and 17%, respectively. Thus, not only are NEXUS receptors closer to major roads, they are also closer to more major roads than the general Detroit population.

2.5. Model evaluation and sensitivity analysis

Model predictions and monitoring observations were compared in an operational evaluation intended to assess model performance for specific applications (Milando and Batterman, 2018), e.g., daily exposure measures in health studies. A daily period also is motivated wind direction variability that renders evaluations at the hourly level “almost fruitless” (Chang and Hanna, 2004). Previous RLINE evaluations have provided diagnostic evaluations using short-term (e.g., hourly) analyses (Snyder et al., 2013; Venkatram et al., 2013; Heist et al., 2013). Comparisons and sensitivity analyses were conducted by pollutant, wind direction, monitoring site, season and day-of-week. Wind direction was determined for wind speeds exceeding 1 m/s, and labeled at each monitoring site as “downwind” if within 30° of perpendicular of the nearest major road and as “parallel” for directions within ± 15° of parallel (Venkatram et al., 2013). For each analysis, daily average concentrations were calculated if a minimum of 6 h of valid model-observation pairs existed, e.g., for comparisons of daily averages during downwind conditions, 6 h of downwind data on a specific day were required for the daily average to be calculated.

The performance evaluation emphasized four metrics that are widely used for dispersion modeling and for which performance criteria have been suggested (Chang and Hanna, 2004): percent of modeled values within a factor of 2 of observed values (F2); Spearman ranked correlation coefficient (R_{SP}); fractional bias (FB); and geometric variance (V_G). The ratio between the natural logarithm of the reducible component of V_G and total V_G (the product of the systematic and random components) was used to estimate the percentage of reducible model errors (% Red). The sensitivity analyses used these metrics to contrast performance of nominal and alternative nominal model inputs.

Given the number of comparisons in the analysis (by site, pollutant, input, and metric), several rules were used to identify potentially meaningful differences and produce a summary measure. Each metric was compared to its “best” value (i.e., 1.00 for R_{SP} and V_G, 0.00 for FB and % Red), and symbols were used to show whether an alternative model input improved model performance (●), gave results that were among those that improved results (‘ ~ ’), did not conclusively improve model performance (‘ ’), or diminished performance from nominal (○). Only comparisons with at least one $R_{SP} \geq 0.1$ were considered. Only potentially meaningful changes were distinguished; changes in R_{SP} and other metrics had to exceed a chosen threshold of 0.05; this threshold was selected to balance sensitivity and avoid false indications. Comparisons of 2010 (nominal) and 2015 emission factors, and comparisons of the US default TAF (nominal) to the two alternative TAFs (Detroit-specific with commercial and non-commercial traffic separated, and combined) used the above comparison scheme. Comparisons of the four sets meteorological inputs were more complex. We checked whether on-site/KDET meteorology provided the best results (denoted as “on-site/KDET highest?”); whether KDET data provided better results than KDTW data when using NWS data alone or in conjunction with on-site data (“KDET > KDTW?”), and if on-site data generally improved results over NWS data alone (“on-site > NWS?”).

2.6. Application

To demonstrate the possible effect of model inputs on health outcomes in an epidemiological study, we estimated NO_x-attributable health impacts for two sets of meteorology and receptor sets 2 (NEXUS) and 3 (Detroit). Daily NO_x concentrations at the NEXUS and residential receptor sets were calculated using KDET and KDTW meteorology for 2011, commercial and non-commercial traffic allocation factors and 2015 emission factors. Every 12th day of the year was analyzed due to the large computation burden of modeling hourly data using 9701 sources and 754 receptors. Outcomes considered included childhood asthma exacerbations (defined as one or more asthma-related symptoms for children ages 6–14), emergency department (ED) visits for asthma (children ages 0–17), and hospitalizations for asthma (ages 0–64). Baseline data used in these estimates included current asthma hospitalizations and ED visits in Detroit (DeGuire et al., 2016; Batterman et al., Unpublished results), an incidence rate of 0.412 cases per person-day for asthma exacerbations (6–14 years) (Batterman et al., Unpublished results), the prevalence of asthma in Wayne County (AIM, 2014), and 2010 Census population data (US Census Bureau, 2015b). Concentration-response coefficients used log-linear and logistic models (Linn et al., 2000; Ito et al., 2007; Yang et al., 2005; Schildcrout et al., 2006). Predicted health outcomes for the two sets of meteorological inputs and two sets of receptors were compared using the non-parametric paired Wilcoxon signed rank test and descriptive statistics.

3. Results

At four of the monitoring sites (all but the industrial site), both NO_x and CO predictions met recommended performance criteria (Hanna and Chang, 2012; Chang and Hanna, 2004), specifically, F2 ≥ 50%, $V_G \leq 1.6$, and mean bias ≤ 30% (not considered in this work). These criteria were not met at the industrial site, where performance was poor (e.g., $R_{SP} < 0.1$). While close to I-75 (150 m), CO levels at this site may be affected by many factors that are incompletely known and/or modeled, including emissions from three adjacent and active rail lines and nearby industry (e.g., refining, cement, salt, steel, coke, sludge incineration). In addition, both I-75 and a major arterial (Fort St.) at the site become elevated to cross the rail lines and the River Rouge. For these reasons, this site was excluded from further analysis.

3.1. Sensitivity to meteorological inputs

Comparisons of RLINE predictions were sensitive to the selection of the meteorological inputs (Table 1). Generally, the best match to monitored data was obtained using on-site/KDET meteorology. For example, for NO_x at the near-road and urban sites, on-site/KDET meteorology gave the highest R_{SP} (0.57–0.74), among the lowest bias, and the lowest V_G. The best performing case (NO_x monitored at the near-road site using the IGpCHEM instrument) also had the lowest % Red with the on-site/KDET data. While the schools site performed better with the NWS data, R_{SP} was low (0.40–0.43 with KDTW data, compared to 0.32 for KDET data). Comparing the NWS data both with and without the on-site data, KDET obtained better performance in most cases. CO results were similar, e.g., on-site/KDET data attained among the highest R_{SP} at near-road and urban sites, the best performing case (near-road site, EC9830T method) had the only improvement seen in % Red (although higher bias), and V_G was generally lowered. At sites more distant from roads, performance trends for CO were less clear and often comparable for the four meteorological datasets due to the variation and overlap of R_{SP} and FB across the sites, while V_G and % Red were very similar at most sites.

Analyses by wind direction, weekday and season, while not definitive, again suggested that best performance was attained using on-site/KDET meteorology (Table S5–S10). For NO_x, weekday results largely mirrored results discussed earlier, but for Saturday and Sunday results, on-site/KDET only produced the highest R_{SP} at the near-road site (IGpCHEM instrument). By season, only the near-road site followed the overall trend. Interestingly, results by wind direction show better performance using KDTW rather than KDET meteorology at the near-road site. This site is at the western part of the study area and, unlike the other monitoring sites, is about the same distance to KDTW (20 km) and to KDET (22 km). Nevertheless, both NWS datasets gave relatively high R_{SP} at this site (0.57–0.70; IGpCHEM monitor). For CO, missing data hampered analyses, but on-site/KDET sometimes improved performance, e.g., this dataset obtained the highest R_{SP} at the near-road (EC9308T method) and urban sites during weekdays and during downwind conditions, and during winter, the near-road site (EC9830T) had lower bias and V_G using on-site/KDET. However, the other CO results were inconsistent, e.g., on-site/KDET meteorology increased bias and V_G during downwind conditions at the near-road and urban sites, and parallel winds lowered R_{SP} at the urban site. Changes at the

Table 1
Summary of sensitivity analysis for meteorology inputs, showing results of performance evaluation for NOx and CO for three comparisons. Symbols: ● = improved/supporting, ○ = diminished/contrary, ~ = comparable, ‘ ’ = indeterminate (sets overlap by more than the minimum of 0.05 and 50% of the smaller within-set range). (See Table S4 for underlying data.)

Metric	Supporting argument	NO_x						CO		
		Schools ICHEM	Near-road ICHEM	Near-road IGpCHEM	Urban ICHEM	Urban IGpCHEM	Suburban IGFC	Near-road EC9830T	Near-road INDiI	Urban INDiI
R_{SP}	On-site/KDET highest?	○	~	●	~	~	○	~	~	~
	KDET > KDTW?		●	●	●	●	●	●	●	●
	On-site > NWS?	○		●		●	○			
FB	|On-site/KDET| lowest?	○	●	○	●	●	~	○	●	●
	|KDET| < |KDTW|?									
	|On-site| < |NWS|?	○		○				○		
V_G	On-site/KDET lowest?	~	●	~	~	~	~	○	~	~
	KDET < KDTW?						●			
	On-site < NWS?	○	●	●	●	●	●	○	●	●
% Red	On-site/KDET lowest?	○	○	●	○	○	○	●	○	○
	KDET < KDTW?							●		
	On-site < NWS?	●	○		○	○	○	●	○	○

suburban mostly fell below the significance threshold (e.g., 0.05 for R_{SP}).

3.2. Emission factors

The updated (2015) emission factors mostly did not change R_{SP} for NO_x, though FB and V_G were lowered (i.e., improved) in three cases (at the near-road/ICHEM and urban sites; Table 2). CO showed similar but less consistent effects. Results for downwind and parallel winds suggested improvements for NO_x using the updated emission factors, e.g., R_{SP} increased and bias decreased at the near-road/ICHEM and urban sites, V_G increased at the same sites, and % Red decreased at the near-road/IGpCHEM site. For CO, the updated dataset did not change R_{SP} for downwind and parallel winds, but % Red was lowered at the near-road/EC9830T site, and bias and V_G were lowered at the other sites.

Day-of-week analyses for NO_x showed that the updated emission factors improved R_{SP}, bias and V_G on weekdays (all sites) and Saturdays and Sundays (most sites) (Table S11–S16). Day-of-week analysis for CO gave similar trends, e.g., the updated emission factors lowered bias and V_G at the near-road/INDiI site across all day types. Seasonal trends were less consistent. For NO_x, the updated emission factors improved R_{SP} at the near-road and urban/IGpCHEM sites, and lowered bias and V_G at the urban site in winter; effects in other seasons were less consistent. For CO, investigations were hampered by missing data, but results with the updated inventory showed some improvements, e.g., in winter and fall, % Red decreased at the near-road site, and bias and V_G were lowered in most cases, and in spring and summer, bias and V_G were lowered at the near-road/INDiI and industrial sites.

3.3. Temporal allocation factors

The three sets of TAFs yielded few differences above significance thresholds in either NO_x and CO predictions. Thus, the Detroit-specific TAFs that separated commercial and non-commercial traffic did not perform better than the simpler and default TAFs. Given the large changes in the hourly profiles, this lack of sensitivity to the TAFs is surprising. It might result from the use of daily averages in the evaluation, which could mask hourly changes, or other compensating errors.

3.4. Exposure estimates

Predictions of daily average NO_x concentrations using the KDET and KDTW meteorology respectively at the NEXUS receptors averaged 12.5 and 15.6 $\mu g\,m^{-3}$, higher than those at the Detroit receptors (8.3 and 11.1 $\mu g\,m^{-3}$), reflecting locational differences between the receptor sets, and in particular, the proximity of many NEXUS participants to major roads (Table 3).

Scatterplots of daily NO_x predictions comparing predictions using KDET and KDTW meteorology for receptor sets 2 (NEXUS) and 3 (Detroit receptors) show high correlation ($R_{SP} > 0.85$) on most days (Fig. 2). Somewhat lower correlations on a few days (e.g., for 8/28/2011, NEXUS $R_{SP} = 0.81$ and Detroit $R_{SP} = 0.79$) were due to relatively large changes at a subset of receptors located across the area; otherwise no systematic spatial or other pattern was observed on these days. The most striking observation, however, of this comparison are the large day-to-day shifts in the bias between predictions using KDET and KDTW meteorology. Of the 30 days modeled, predictions using KDTW meteorology were biased upwards on 16 days, downwards on 3 days (4/6/

Table 2
Summary of sensitivity analysis for emission factor inputs, comparing results of performance evaluation for nominal (2010) and alternative (2015) emission inventory. Symbols: ● = improved/supporting, ○ = diminished/contrary, ~ = (comparable).

Metric	Supporting argument	NO_x						CO		
		Schools ICHEM	Near-road ICHEM	Near-road IGpCHEM	Urban ICHEM	Urban IGpCHEM	Suburban IGFC	Near-road EC9830T	Near-road INDiI	Urban INDiI
R_{SP}	2015 inventory highest?	~	~	~	~	~	~	~	~	○
FB	2015 inventory lowest?	~	●	○	●	●	~	○	●	~
V_G	2015 inventory lowest?	~	●	~	●	●	~	○	●	~
% Red	2015 inventory lowest?	~	○	●	○	○	~	●	○	○

Table 3
Annual (2011) average NO_x concentrations (μg m^{-3}) predicted at NEXUS and Detroit receptors using KDET and KDTW meteorology.

NWS station	NEXUS	Detroit
KDET	12.5	8.3
KDTW	15.6	11.1

2011, 5/12/2011, 9/21/2011), and similar on the remaining 11 days. These results, which include weekdays and weekends, are attributable solely to the meteorological inputs. (Stratification by season, day type and other factors was not attempted due to the limited sample size.) These changes appear to be driven by wind speed and stability effects, and receptors clustered within about 100 m of M-10 and I-94 were especially affected (Fig. S3). These large changes were unexpected since daily averages and meteorological parameters at the two NWS sites were highly correlated (Table S17).

The positive prediction bias at the NEXUS and Detroit receptors was reflected in predicted health outcomes. The average attributable health impact differed significantly between KDET and KDTW on all but one of the 30 days modeled, and KDTW meteorology increased the frequency of adverse outcomes on most days, especially for the NEXUS cohort (Table S18). Similarly, when outcomes were pooled across receptors and days, differences in the average attributable cases at NEXUS receptors exceeded those for the Detroit receptors (Table 4).

4. Discussion

4.1. Meteorology

The sensitivity of RLINE results to meteorological inputs highlights the importance of appropriate input data. Some results tended to differ by site. For the sites nearest roads, on-site/KDET followed by KDET performed best, e.g., attaining the highest R_{SP}. At the suburban and urban sites, performance with KDET data also was better than with KDTW, but NWS data performed better than on-site. These sites are farther from major roads, and monitored concentrations likely result from multiple emission sources and not just traffic on the nearby road. In these cases, on-site meteorological measurements may be less representative for dispersion modeling than airport data, at least under some source and meteorological conditions, e.g., ground level emissions during calms, and NWS data may better represent the conditions affecting dispersion from roadways. Prior dispersion modeling in Detroit has judged both NWS sites to be representative, e.g., modeling of SO_2 emitted from mostly elevated point sources used KDTW (MDEQ, 2015),

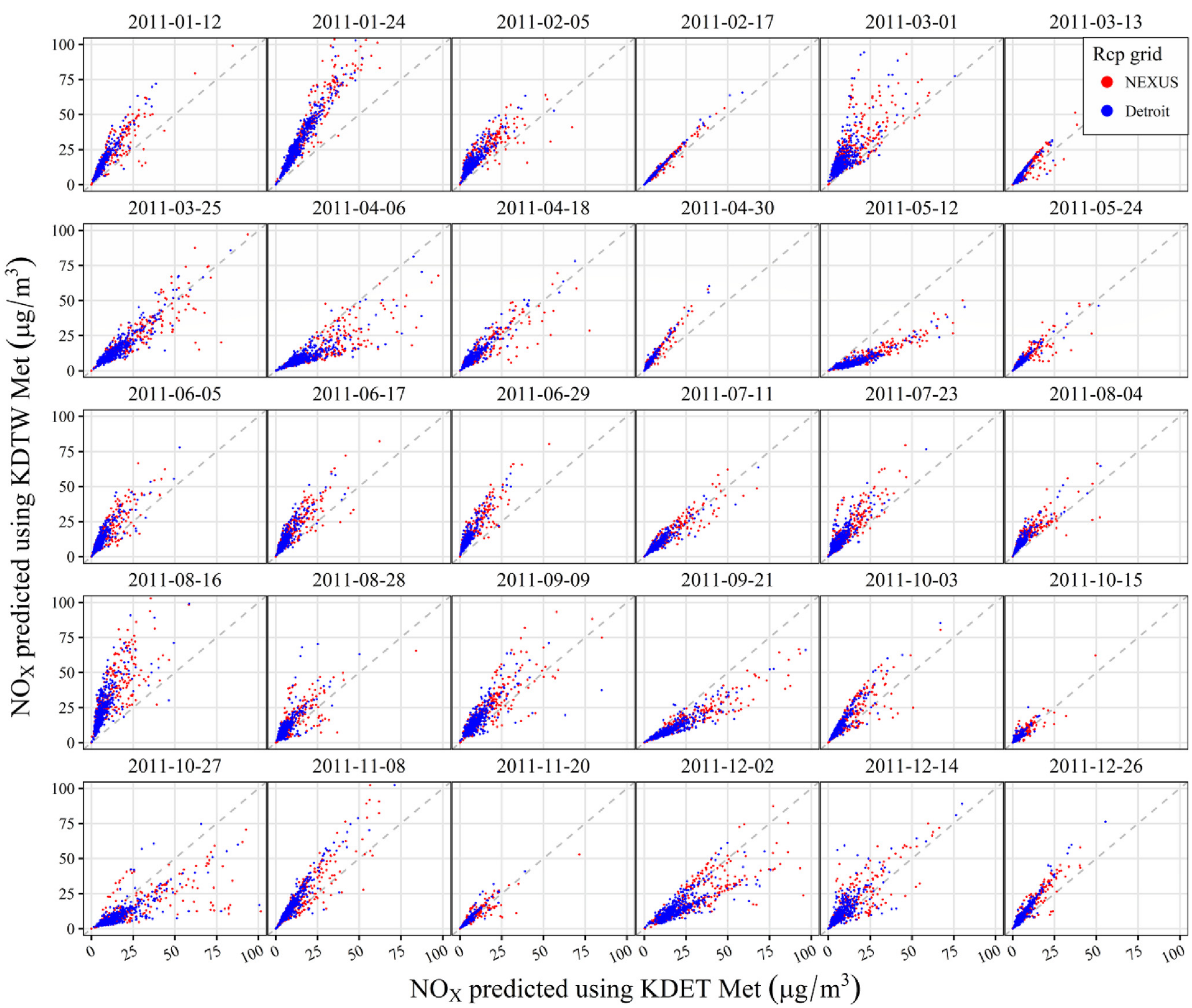

Fig. 2. Scatterplots of NOx predicted using KDET or KDTW meteorology at NEXUS (n = 206) and Detroit receptors (n = 543) by days. Each plot shows the 1:1 line and is truncated at 100 μg m^{-3}.

Table 4
Average attributable cases made using KDET and KDTW meteorology at NEXUS and Detroit receptors for various NO_x related health outcomes. All differences were significant (Wilcoxon signed rank test CI of 95%).

Health outcome	Units	Age group	NEXUS		Detroit	
			KDET mean cases	KDTW mean cases	KDET mean cases	KDTW mean cases
Asthma ED visit	per 10,000	0–17	0.81×10^{-1}	1.01×10^{-1}	4.96×10^{-2}	6.56×10^{-2}
Hospitalization due to asthma	per 10,000	0–64	2.00×10^{-3}	2.50×10^{-3}	1.21×10^{-3}	1.61×10^{-3}
Asthma exacerbation	per 10,000	6–14	1.40×10^{2}	1.73×10^{2}	0.87×10^{2}	1.15×10^{2}

while TRAP modeling used KDET (Batterman et al., 2014b). As noted, individual meteorological parameters, e.g., wind speed or direction, typically are highly correlated between the nominal and alternative inputs, although some differences were identified, especially at the suburban site (Table S17). However, the combined effect of different meteorological datasets is best determined by sensitivity analyses examining pollutant predictions.

Application to the NEXUS and Detroit receptors receptor sets showed that meteorological datasets obtained at NWS stations 18 km or more apart can make large differences in daily concentration predictions on some days, which supports findings from comparisons at the monitoring sites. Both NWS are at airports, and the surrounding terrain is flat and mostly urban, commercial, wooded, or agricultural. The differences in predicted concentrations likely result from changes in atmospheric stability that alters near-road concentration gradients, possibly due to very stable conditions which can cause the highest concentrations (Snyder et al., 2013). This suggests the possibility of significant exposure measurement error if the meteorological data are not representative, e.g., measured at a distant site. Moreover, errors may be higher for more vulnerable populations, as portrayed by the NEXUS receptors for children who lived close to major roads.

Due to siting and instrumentation limitations, relatively few air quality monitoring sites, including the near-road sites, measure all of the meteorological parameters required for research or regulatory-grade dispersion modeling. Thus, local measurements were blended together with NWS (or other) observations. While this approach is workable, incorporated in the AERMET processor, and generally obtained the best performance in the Detroit application, a full set of local measurements (e.g., including parameters given in Table S1) may be preferable for obtaining wind fields that are the most representative of near-road environments. This option, which could not be fully tested in Detroit, leads to a recommendation to collect a full set of local meteorological measurements for dispersion modeling when practicable (including ground cover, surface roughness, and other factors that affect the spatial variation in wind fields). This reinforces long standing model guidance that recognizes the increased heat flux and surface roughness in urban areas and the general need for multiple monitoring sites in large urban areas (Salizzoni et al., 2012; US EPA, 2000). However, no specific guidance is yet provided for near-road modeling. For larger roads in urban settings, such modeling involves winds, emissions and pollutant dispersion transitioning from the road "microenvironment," defined by large paved areas (e.g., portions of the right-of-way for I-96 in Detroit exceeds 150 m in width as each traffic direction includes three local and three express lanes, a two lane service road, multiple shoulders, and some vegetated buffers), to the adjacent populated "microenvironment," which can be mostly suburban in nature, dominated by buildings and trees and with relatively fewer flat paved surfaces. Guidance defining the most representative meteorological data for traffic-related emissions in such settings, which differs from the general urban environment, would improve near-road predictions.

4.2. Emission factors

The performance analysis suggested that RLINE performed slightly better using the alternative emission factors as compared to the nominal ones. The alternative inputs substantially changed emission factors for several vehicle classes, e.g., overall emissions from light duty gas vehicle (LDGV) and heavy duty diesel vehicle (HDDV) classes decreased by 48 and 30% for NO_x, and by 30 and 23% respectively for CO; changes at certain speeds and temperatures could be larger (Table S19–S20). To help interpret these changes as well as traffic activity estimates, which are frequently reduced to vehicle counts (see next section), emission factor differences among vehicle classes can be expressed as passenger car equivalents (PCEs) (Batterman et al., 2015; Watkins and Baldauf, 2012b). As examples, using LDGV emissions as a base: NO_x emissions from a single HDDV represent 12 to 63 PCEs; CO emissions represent only 0.2 to 1.3 PCEs; and both NO_x and CO PCEs increase at lower speeds and colder temperatures (Table S21). The large changes in NO_x emission factors suggest that emission estimates can be very sensitive to the estimated traffic activity (e.g., commercial traffic counts), especially during cold weather and congestion when speeds are lower and the PCEs are high. The temperature and pressure dependence of MOVES-generated emission factors might partially mask modeled differences in predicted concentrations obtained using different emission factor sets, although the post-processing steps taken (e.g., creating temperature-specific emission factors) may mitigate this effect. Alternatively, emission factors also depend on the fleet mix. Our fleet mix estimates for commercial vehicles (which are mostly diesel) in Detroit range from 3 to 5% on most roads to 9% on portions of major roads, e.g., I-75 and I-94 (Table S22). Considering a NO_x PCE of 20 and 5% HDDVs, emissions from HDDVs and LDVs are comparable, which shows the need to obtain accurate traffic activity data.

Uncertainty in mobile source emission inventories can arise from many sources, e.g., the representation of the road network geometry, uncertainty in traffic activity (e.g., vehicle-kilometers traveled or VKT, volume, vehicle type and age, speed, acceleration, and the number of cold starts), and uncertainty in emission factors estimates for engine exhaust noted above (Fujita et al., 2012; Wang et al., 2008; Li et al., 2009). These factors can vary temporally and spatially. Other notable factors include a lack of traffic counts and on-road emission measurements, and discrepancies between fleet classifications and VKT needed by models and the available statistical summaries (Snyder et al., 2014; Zheng et al., 2009). Because fleet mix and VKT data usually are collected and aggregated at the county level, data may not be representative of the city or the roads of interest. As noted above, even modest changes in the commercial fraction of traffic may significantly affect emissions since, for NO_x, one HDDV can emit the equivalent of many passenger cars. This may be especially important in Detroit given the considerable through-traffic of commercial vehicles (mostly HDDVs) crossing the Ambassador Bridge to or from Canada via along I-75 and I-94, which may have the effect of increasing the HDDV fraction among these roads and boosting NO_x emissions. NO_x also may have been underestimated since the simplified emission factors averaged out higher emissions from cold starts. While possibly less important for mobile source inventories when aggregated to the annual average and city-wide level, these issues may be important for estimating spatially- and temporally resolved exposures.

4.3. Temporal allocation factors

The three sets of TAFs yielded few differences above significance thresholds in either NO_x and CO predictions. Thus, the alternative Detroit-specific TAFs that separated commercial and non-commercial traffic did not perform better than the nominal TAFs. This result was unanticipated, especially for NO_x, given the differences between commercial and non-commercial vehicles, and the differences seen in the simplified analyses (discussed previously). The fairly large hour-to-hour differences in TAFs at the hourly level may be "washed out" at the daily level or just not observable given other errors and uncertainties. In addition, the local TAFs were based on only the larger Detroit area roads equipped with permanent traffic monitoring recorders. Smaller roads can account for a sizable fraction of TRAP emissions, e.g., based on the Detroit link-based inventory (Snyder et al., 2014), the smaller (non-trunkline) roads accounted for 60% of total VKT in 2010. Our calculations show VKT for all vehicles and commercial vehicles increasing by 1 and 2% per year, similar to a recent SEMCOG report (SEMCOG, 2015). The use of local TAFs might improve modeling at the hourly level, which was beyond the present scope, as has been suggested elsewhere (Lindhjem et al., 2012).

4.4. Application

The large differences in predictions that occurred on a few days (see Fig. 2 and Fig. S3), while uncommon, can result from changes in atmospheric stability that alters the near-road concentration gradient. Thus, while KDTW and KDET obtain mostly similar measurements, the hours or days that differ can cause potentially large impacts on the estimated health impacts. This possibility may increase when meteorological data are obtained at a distant site or is not representative of local conditions. In the present application, predicted exposures differed significantly using the two NWS datasets, and the differences were magnified for the vulnerable population (Table 4). Thus, effects due to exposure measurement errors may be magnified among sensitive populations, as seen in the NEXUS sample.

4.5. Comparison to literature

The sensitivity of dispersion model results and model-based exposure estimates to input data has been explored, however, in applications with limited generalizability. A city-scale study ($189\,km^2$) that used the Atmospheric Dispersion Modeling System (ADMS) to simulate industrial mercury emissions in northwestern England showed that varying meteorological inputs (e.g., meteorological station, release point temperature) changed population-weighted exposures by up to 16% (Hodgson et al., 2007). Meteorological inputs also produced the largest variability (compared to other inputs) in exposures in a study using ADMS to simulate traffic-related emissions of PM_{10} (Gulliver and Briggs, 2005). A local-scale study ($8\,km^2$) that used AERMOD and the Industrial Source Complex Short Term model (ISCT3) to simulate hexavalent chromium emissions from a shipbuilding facility in California showed similar dependence (25% variation) on meteorological inputs (Sax and Isakov, 2003). The variations owing to meteorological data in these studies on non-TRAP pollutants were similar to results found in this work. An assessment of airport and local meteorological data used in urban canyon models found that use of local data improved results (Vardoulakis et al., 2002). However, with reference to the present application, these applications have neither studied traffic-related pollutants, which are of concern in urban areas, used recent roadway dispersion models, nor commented on the potential influence on sensitive near-road communities.

4.6. Limitations and uncertainty

Several limitations and uncertainties are noted. Predictions did not include chemical transformations and cold start emissions. The summary comparisons of modeled and monitored concentrations used a chosen threshold (0.05) to denote differences in the performance measures, which does not imply statistical significance. The computational burden limited the number of days that could be simulated, and thus seasonal and day-of-week analyses were not attempted. Exposures and health outcomes were based on point estimates of the concentration-response coefficient, and consideration of the confidence intervals may dampen observed results. We did not consider statistical power, or how results might vary given different samples of Detroit receptors (e.g., a population-weighted sample). There was an issue with identifying the sampling instrument at certain sites, which was not resolved – however, the sampling method and detection limit for all were identified. Some sources of potential errors pertaining to near-road modeling may be important, but were not examined, e.g., geospatial errors in the road network linearization. The exposure results did not account for indoor/outdoor relationships or time-activity information, e.g., the time children spent at school. We had insufficient data to distinguish results by season.

5. Conclusions

The goal of this paper was to examine the sensitivity of dispersion model predictions of TRAP exposure to key model inputs. While data and computationally intensive, dispersion models and especially high fidelity models can provide great flexibility and theoretical strength, and can represent the spatial variability of TRAP concentrations at locations not measured by conventional and spatially sparse air quality monitoring networks. However, model estimates are sensitive to input data, and our applications highlighted the need for representative meteorological data to predict near-road exposures. In particular, several systematic biases can cause exposure measurement errors that could affect results and subsequent calculations, e.g., estimated health impacts. This leads to several recommendations: the need to develop guidance that defines appropriate meteorological data for dispersion modeling of the complex near-road environment (e.g., robust wind fields created by computational fluid dynamics models); the use of on-site (local) meteorological inputs in near-road dispersion modeling; and that air quality monitoring sites be equipped with meteorological instrumentation sufficient to obtain parameters needed by the AERMET meteorological pre-processer for generating the input files necessary to run RLINE and other dispersion models. Finally, to confirm and extend our results, additional operational performance evaluations and sensitivity analysis should be conducted across a range of urban settings.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.atmosenv.2018.03.009.

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