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# Linking an activity-based travel demand model with traffic emission and dispersion models: Transport's contribution to air pollution in Toronto

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ABSTRACT

This paper describes the development of an integrated approach for assessing ambient air quality and population exposure as a result of road passenger transportation in large urban areas. A microsimulation activity-based travel demand model for the Greater Toronto Area – the Travel Activity Scheduler for Household Agents – is extended with capabilities for modelling and mapping of traffic emissions and atmospheric dispersion. Hourly link-based emissions and zone-based soak emissions were estimated. In addition, hourly roadway emissions were dispersed at a high spatial resolution and the resulting ambient air concentrations were linked with individual time-activity patterns derived from the model to assess person-level daily exposure. The method results in an explicit representation of the temporal and spatial variation in emissions, ambient air quality, and population exposure.



## 1. Introduction

The growing complexity of travel demand patterns, as well as residential and firm location processes, adds to the challenge of reducing greenhouse gas (GHG) emissions and achieving more sustainable development patterns thus creating additional pressure on policy appraisal. Globally, this challenge has motivated the development of integrated urban models (IUM) as well as activity-based travel demand models as techniques for assessing the impacts of land-use and transportation changes. Despite significant efforts in developing IUM and activity-based models, they still lack the capability of fully synthesising air quality impacts. Indeed, there are few examples where these models have been extended with capabilities for simultaneous evaluation of emissions, air quality and exposure as a result of land-use and transport policy scenarios.

This paper presents an integrative process whereby models of travel demand, vehicle emissions and dispersion, which have traditionally evolved separately, are incorporated under a unified modelling framework. For this purpose, Travel Activity Scheduler for Household Agents (TASHA), an activity-based travel demand model for the Greater Toronto Area (GTA) developed at the University of Toronto (Miller and Roorda, 2003), is linked with models for vehicle emissions, meteorology, and air dispersion. This paper builds upon earlier work linking TASHA with Mobile6.2C, the Canadian version of the US Environmental Protection Agency (USEPA) emission factor (EF) model (Hatzopoulou et al., 2007, 2008). The resulting air pollutant concentrations are linked with time-activity patterns of individuals simulated within TASHA in order to derive daily exposure for Toronto residents. This approach is mainly concerned with exploiting the broad range of detailed travel information generated by activity-based travel demand models for the purpose of refining the modelling of transport-induced air pollution and assessing population exposure.

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## 2. Materials and methods

The contribution of household travel to air pollution in the GTA was estimated through the modelling framework illustrated in Fig. 1. First, output from TASHA is used to calculate vehicle emissions for start, hot soak, and running conditions. Only link-based exhaust emissions of nitrogen oxides ($NO_x$) are then input into CALPUFF, a puff-based Gaussian dispersion model driven by its meteorological pre-processor, CALMET. The resulting concentrations are compared with data from air pollution monitoring stations. Finally, population exposure to air pollution is assessed by tracking individuals throughout their daily activities using output from TASHA and CALPUFF.

Exhaust emissions of $NO_x$, carbon monoxide (CO), volatile organic compounds (VOC), and carbon dioxide ($CO_2$), as well as evaporative emissions of VOC were modelled for light-duty vehicles in the GTA using vehicle activity data generated by TASHA and emission factors (EFs) generated by Mobile6.2C, the Canadian version of the USEPA Mobile6.2 (US Environment Protection Agency, 2003). Emission modelling involves two main components; the development of hourly link-based exhaust, and start emissions for the GTA; and the estimation of hourly evaporative emissions for each traffic analysis zone (TAZ) (Fig. 2). Emissions are derived using 2001 travel activity data.

### 2.1. Link-based exhaust emissions

Using a version of Mobile6.2C loaded with input distributions specific for the GTA (Hatzopoulou et al., 2007), EF look-up tables for running emissions of $NO_x$, CO, VOC, and $CO_2$ were generated as a function of speed, roadway type, and time of day. A total of 60 speed-roadway type scenarios were modelled for each pollutant and time of day. Speed categories amount to 15 and include: 2.5 miles per hour (mph), 5 mph, 7.5 mph, and 10 to $\geqslant$65 mph in 5 mph increments. Roadway type categories amount to four and include: freeway, arterial, local, and ramp. Look-up tables for start EFs were generated as a function of different soak durations (preceding a start) thus differentiating cold and hot starts.

The output of an EMME/2 (INRO, 1998) traffic assignment comprising speeds and volumes on each network link by time of day was then linked with the EF look-up tables in order to obtain total emissions (EF in g/mi multiplied by vehicle miles travelled). For each hour a total of four running EFs were associated with every road segment thus representing the four pollutants (VOC, CO, $NO_x$, and $CO_2$). Note that speeds obtained by EMME/2 were not post-processed. While research into

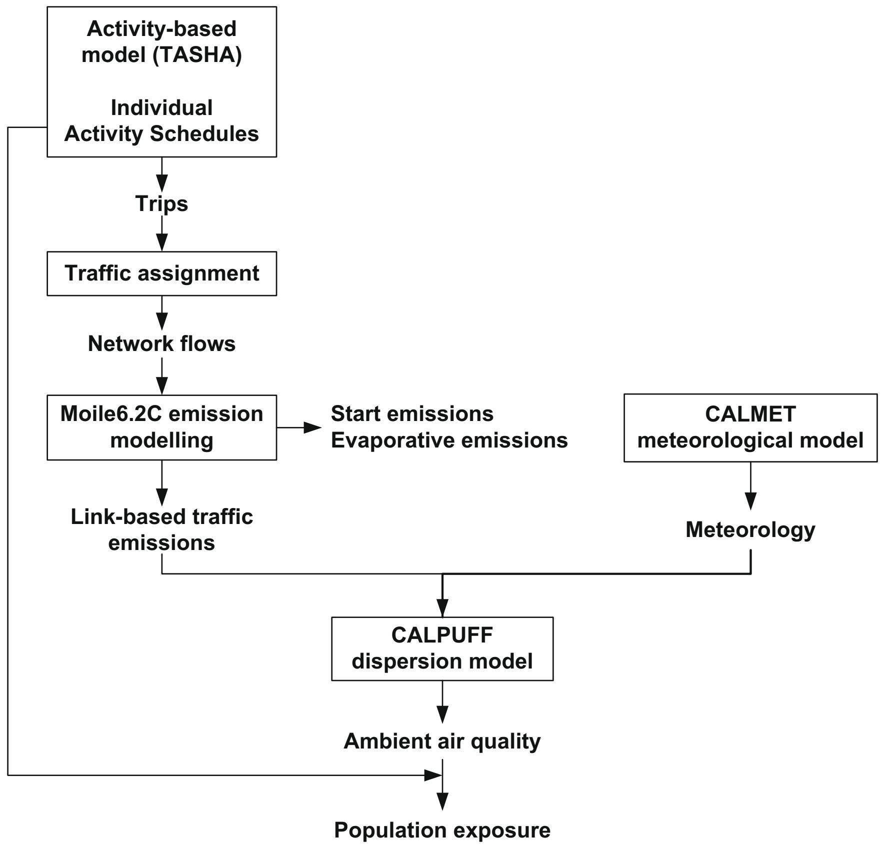


**Fig. 1.** Study methodology.

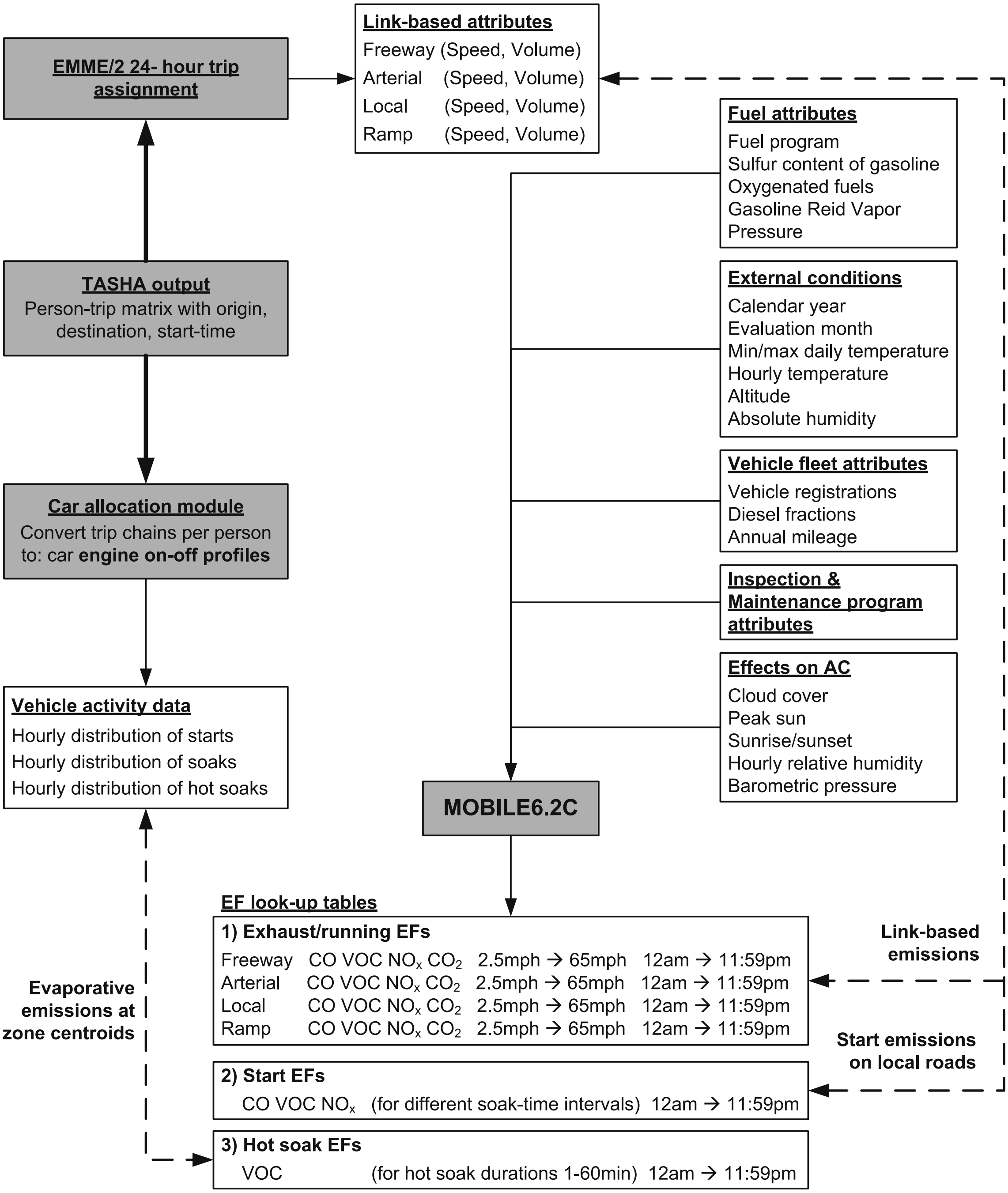


**Fig. 2.** Methodology for emission modelling.

different types of speed post-processors has shown that they generally reduce speeds generated by the travel demand model in already congested situations (thus increasing emissions) (Dowling and Skabardonis, 1993; Helali and Hutchinson, 1994); different post-processors have had dissimilar impacts on mobile emission inventories (Bai et al., 2007) thus stressing the need for further research into the most appropriate post-processing method for computing on-road emission inventories. The current version of EMME/2 used for the GTA uses a modified Bureau of Public Roads (BPR) function that better handles over-saturated travel times (Miller, 2004). Validation of the outputs versus measured travel times indicated that the EMME/2 times are generally reasonably close to observed times within the GTA.

The procedure for start emissions is slightly different as they are assumed to occur only on local roads and only in the direction of the centroid of a traffic analysis zone (TAZ) to a link node. The rationale behind this is that local roads in that same direction carry vehicles that have just started a trip and are leaving their origin to reach the road network. Start emissions are expected to occur at the start position but also during this short period when the vehicle is on a local road.

### 2.2. Zone-based evaporative emissions

Hot soak emissions reflect evaporative emissions that occur while the engine is off and are mostly composed of VOC. As such they entail the development of soak duration distributions. Earlier research has recognized the importance of developing regional and zone-specific soak-time durations (Nair and Bhat, 2000). The benefit of using GTA-specific soak distributions was also demonstrated in an earlier study whereby EFs derived from Mobile6.2 default inputs and GTA-specific inputs were compared (Hatzopoulou et al., 2007).

Soak durations were generated using output from TASHA. Indeed, TASHA microsimulates a 24-h schedule formation process for residents of the GTA and outputs a list of individual trips (and associated trip chains) per household. Each trip is attached with an origin, destination, start and end times. This clearly allows for the estimation of the amount of time a vehicle is off and hence to extract a hot soak duration and the duration for the rest of the soak. Note that the hot soak duration spans from a minimum of one second (instantaneously after the engine is off) to a maximum of one hour, after which the engine attains ambient temperature. The emissions are highest immediately after the engine is shut down and decrease over time, reaching a baseline level in about an hour (US Environment Protection Agency, 2001).

While TASHA predicts the mode for each conducted trip, it does not attempt to allocate the different cars owned by a household to specific trips. For the purpose of extracting distributions on an individual vehicle basis; there is a need to attach specific household cars to person-trips in order to convert the list of person-trips into a list of vehicle-trips. For this purpose, a car allocation model was developed and applied to the TASHA output thus generating a list of trip chains for each car. The car allocation model attempts to decide "which car" was used for "which trip" by "which individual". The model was developed in an object-oriented platform using the Python programming language. It allocates cars on the basis of entire trip chains. Based on the number of cars in the household, a pool of cars is developed, containing the household cars as distinct elements. When an individual starts a trip chain, he/she will request a car from the car pool and when that individual finishes the trip chain, the car will be released. Throughout the day; cars are requested and released until the end of the day where the car pool is re-populated for each household (Hatzopoulou et al., 2007). Soak durations are also of importance to the estimation of start emissions.

Hot soak durations for each vehicle were linked with hot soak EFs generated by Mobile6.2C in order to estimate total emissions. Hot soak emissions were allocated to zone centroids as they are considered to be the point of departure and end of trips.

### 2.3. Air quality modelling

Understanding vehicle-induced emissions alone is not sufficient to understanding the problem of air pollution in an urban area. For this purpose, the TASHA-Mobile6.2C interface was also linked with an air quality model. At this stage, only link-based emissions are dispersed, future research will look at the dispersion of evaporative VOC emissions from TAZs as area sources. Among the range of pollutants for which emissions were estimated, $NO_x$ were selected for dispersion modelling due to their central role in the generation of tropospheric ozone ($O_3$). In the City of Toronto, transportation is responsible for around 73% of $NO_x$ emissions (ICF International, 2007).

The CALMET/CALPUFF system (Scire et al., 2000a,b) was selected for air quality modelling especially due to its non-steady-state, puff-based formulation which allows the model to capture the effect of low wind speeds and stagnation events that often occur in Toronto during the summer; ability to capture near-field and far-field impacts; ability to capture the effect of Lake Ontario on the generation of land/sea breezes; ability to handle individual roadway links as emission sources taking away the need to allocate emissions to gridcells (which generally runs the risk of underestimating emission density); and ability to handle an extremely large number of individual sources.

The CALMET meteorological domain has an area of $252 \times 252$ km. It includes the GTA, the City of Hamilton as well as most of Lake Ontario, Lake Simcoe, the Niagara Escarpment, and Nottawasaga Bay (Fig. 3). Vertically, the domain consists of 10 levels, up to 3000 m. Terrain elevation data, land cover data, hourly meteorological data for six stations within the modelling domain, and three dimensional hourly meteorological data obtained from the Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) mesoscale model MM5 (Grell et al., 1994) were processed in order to develop a meteorological scenario for 2001.

CALMET was run in a diagnostic wind field module which uses a two step approach to the computation of wind fields. In the first step, an initial guess field (using MM5 data) is adjusted for terrain effects thus producing Step 1 winds. Step 1 winds are then refined through the introduction and processing of observational data thus resulting in the Step 2 or final wind field. The weight given to surface observations versus the Step1 wind field is an extremely important factor. A high weight given to a surface station would force winds to follow the wind vector recorded at the station thereby wiping out terrain effects. In addition, MM5 data can capture sea and land breezes which may not be captured by surface stations. Surface stations are believed to accurately represent "microenvironments" and therefore care was taken when weighing observations.

In light of the importance of wind fields to the transport of pollutants, wind vectors generated by CALMET were validated against surface observations. For this purpose, time series files for hourly wind speeds and directions for 2001 were extracted

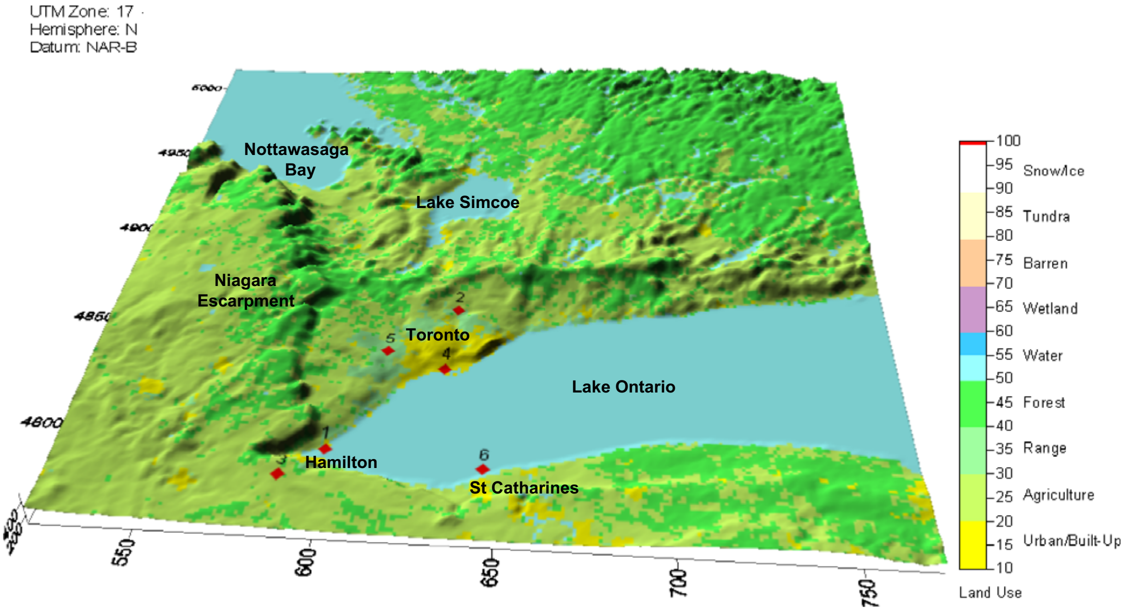


**Fig. 3.** 3D terrain overlaid by land-use for the modelling domain. *Note*: Map features surface meteorological stations – (1) Burlington, (2) Buttonville, (3) Hamilton airport, (4) Toronto Island Airport, (5) Toronto Pearson International Airport, (6) Port Weller.

at different locations. In general, CALMET captured well the most frequent winds in the GTA (Westerly, Southwesterly, and Northwesterly). Northern winds were somehow under-represented by the model especially the Northern wind gusts which occur in the winter season. Overall, CALMET predicted lower wind speeds and under-represented winds higher than 10 m/s. In an application of CALMET to wind resource assessment and forecasting, Klausmann and Scire (2005) compared annual windroses for CALMET and observed winds at Nantucket Airport. A similar observation was made: overall wind directions and speeds are well captured by the model but the frequency of high wind speeds is higher among measured data.

Following the generation of three dimensional meteorological data for the modelling domain, the CALMET output file was used to drive the CALPUFF dispersion. Meteorological data and link-based emissions were used to estimate base-case 2001 pollutant concentrations. Individual road segments in the City of Toronto were input into CALPUFF as area sources (based on road widths) thus generating a total of 15,000 areas sources. For each area source, information on the effective height, base elevation, and initial vertical dispersion coefficient ($\sigma_z$) were input. The latter ($\sigma_z$) takes into account traffic-induced mixing near the roadway as well as canyon effects, to a certain extent. Values for $\sigma_z$ around 3 m (and up to 30 m) are commonly used for traffic dispersion modelling. A value of 3 m for $\sigma_z$ on all roadways was used in the current study, except in downtown Toronto where a value of 10 m was used.

Recall that emissions were estimated solely for private autos (excluding, buses, trucks, and other commercial vehicles). As such, the concentrations resulting from a dispersion of these emissions are expected to reflect the contribution of light-duty vehicles to air pollution. In the GTA and especially in the City of Toronto, road transportation contributes to a significant fraction of total emissions and private autos constitute the majority of road emissions (ICF International, 2007). As such, an assessment of the contribution of private autos to air pollution can provide valuable information on air quality patterns.

CALPUFF was run for selected days in 2001. Due to the considerable number of emission sources, a large amount of puffs are emitted in the domain at every time step. A single day of meteorology and emissions takes 190 h of run time with gridded receptors covering the domain and located 1 km apart (62,500 receptors). In order to reduce computing time, a set of discrete receptors was used for most runs (while gridded receptors were used for selected runs); each receptor representing the centroid of a TAZ. This assumes that $NO_x$ levels are uniform within each TAZ. Within downtown Toronto and a large portion of the City of Toronto, the size of the TAZs is smaller or slightly larger than the spatial resolution of the model thus making this assumption acceptable. In addition, a population distribution within each TAZ is not available in TASHA; both zonal population and employment are located at the centroid.

## 3. Results

Typical model output for exhaust and evaporative emissions in the City of Toronto is presented in Fig. 4. Both types of emissions were estimated on an hourly basis for each link and TAZ. Clearly, the highest emitting links are major highways. While the peaks in exhaust emissions correspond with the peaks in daily travel, evaporative emissions follow a different pattern. They peak subsequently to the peaks in traffic and are highest following the evening peak period when most vehicles are undergoing a hot soak.

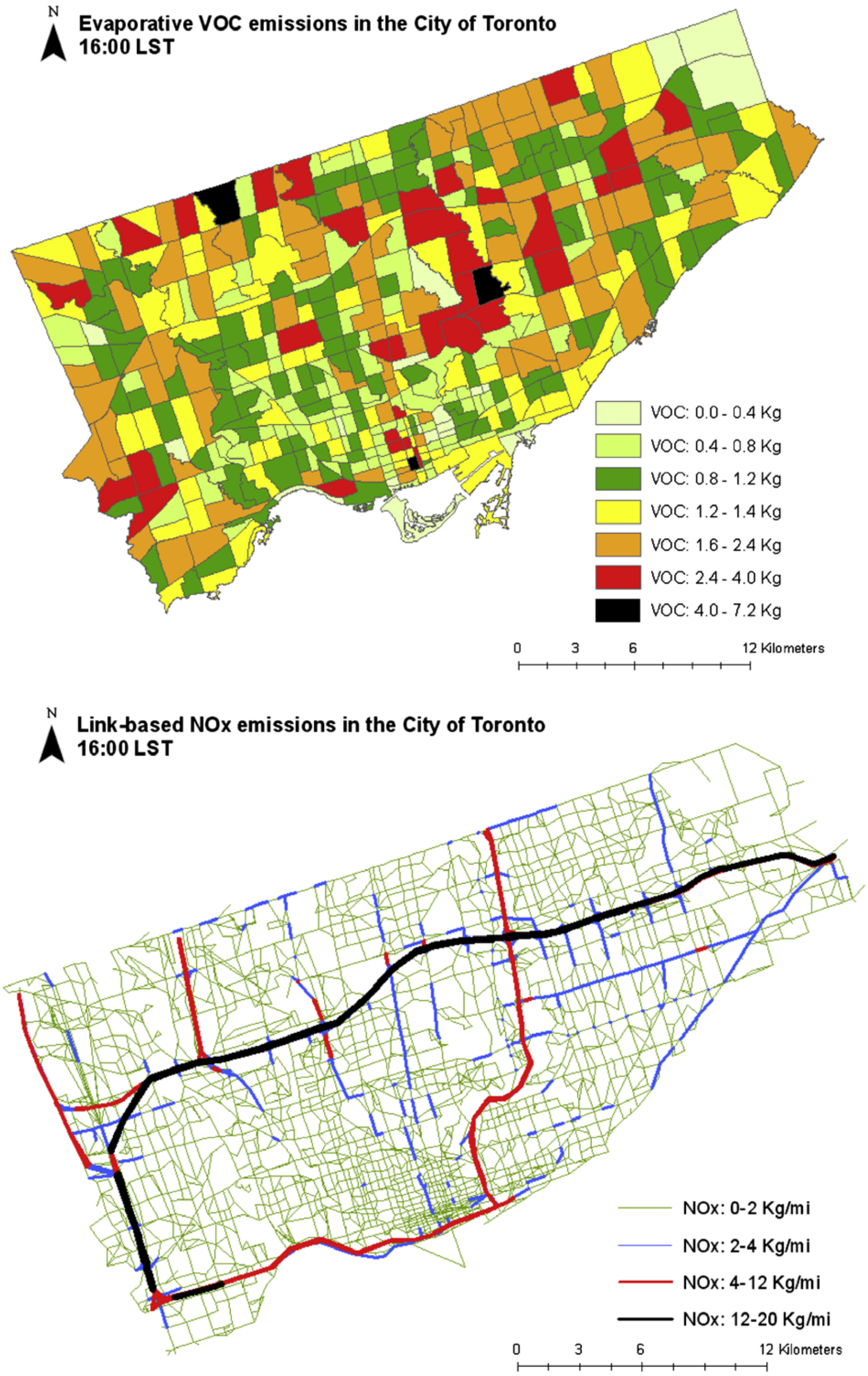


**Fig. 4.** Evaporative and exhaust emissions in the City of Toronto (weekday, 4:00 PM).

Hourly gridded concentration contours within the City of Toronto are presented in Fig. 5 for June 21, 2001. The peaks in concentrations within the City correspond to the peaks in travel and emissions. Peak period concentrations are quickly dispersed away from the sources. Note that the meteorological conditions on June 21, 2001 (partial cloud coverage and moderate winds) were favourable for good mixing of pollutants and dispersion. This situation may not be generalized, whereby specific meteorological conditions may cause stagnation and accumulation of pollutants in the City thus causing the peaks in pollution to follow the peaks in travel.

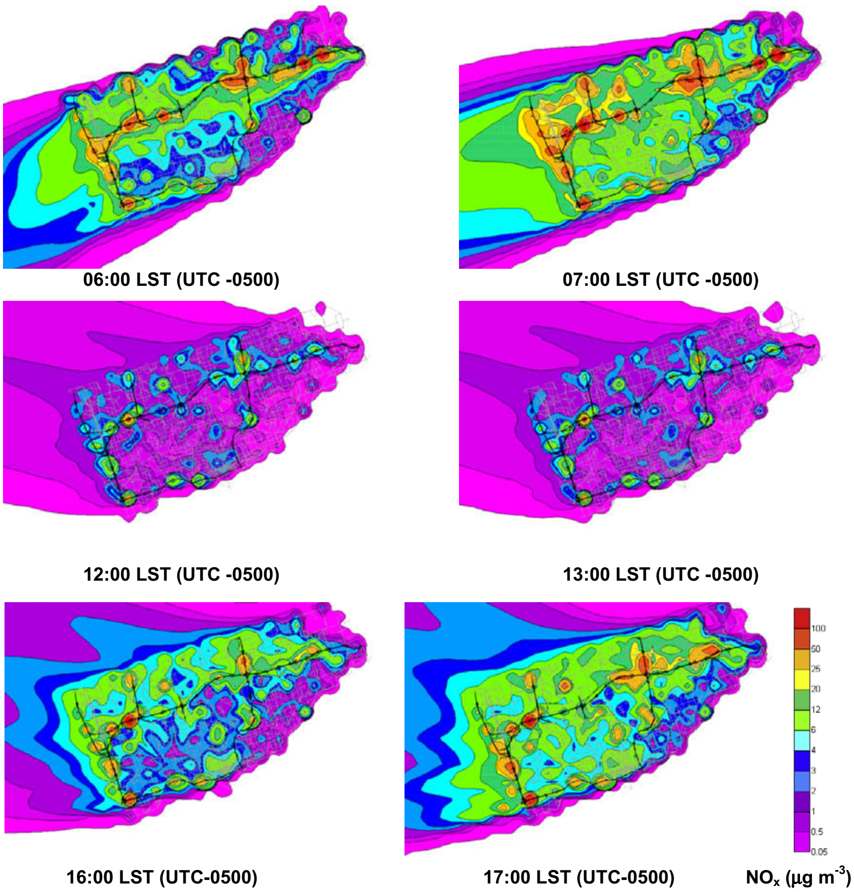


**Fig. 5.** Hourly gridded concentration contours in the City of Toronto (June 21, 2001).

Fig. 6 presents the concentrations at zone centroids for 7 and 8 PM and contrasts the results obtained for June 21 with the ones for July 17. While the peaks in $NO_x$ concentrations on June 21 follow the peaks in travel, the situation on July 17 is noticeably different. Due to the meteorological conditions that are unfavourable for mixing and dispersion of pollutants (very low wind speeds), the $NO_x$ emitted during the evening peak period have accumulated within the City thus causing levels in most parts of the City to be high. This is especially the case for the Northeast part of the City where $NO_x$ levels are in the range of 100 to more than 400 $\mu g\ m^{-3}$. The WHO hourly standard (200 $\mu g\ m^{-3}$) is clearly violated in several zones. Note that this is only taking into account the contribution of private autos.

Fig. 6 also overlays hourly population estimates in every zone. Recall that TASHA microsimulates activities and derives trips for individuals thus keeping track of the location for every individual within the GTA. As such, output from TASHA was used to extract the activities, durations, and locations for individuals in the GTA by time of day. By overlaying concentration levels per TAZ with the total number of people in that zone, one can derive the percentage of population exposed to air pollution levels higher than ambient air quality standards. Note however, that such an assessment is static because it assumes that in each hour, the population of every TAZ is fixed. In reality, individuals are moving within the urban area and often spending less than one hour at a single location. For this purpose, a more dynamic assessment of population exposure was also conducted using the same data but by processing the information at the individual level (cf. Section 4).

Observed $NO_x$ concentrations in the City of Toronto were obtained from four roadside monitoring stations managed by Environment Canada and compared with $NO_x$ concentrations predicted at the same locations. Fig. 7 illustrates the observed and predicted concentrations plotted as a function of time on July 17. Overall, the model captures reasonably well the general trend in $NO_x$ throughout the day except for the morning period where modelled $NO_x$ levels do not show the drop recorded at the monitoring stations. Indeed while inversion conditions are frequent at night and lead to accumulation of $NO_x$ which dissipate at sunrise; at this stage, the model does not capture these conditions since it is run for one day at a time. It is thus important to run the model for two or three consecutive days allowing for a warm-up. Also note that predicted concentrations are less than a factor of two of observations and this is primarily due to the fact that trucks and other commercial vehicle movements as well as other point sources of $NO_x$ in the City are not taken into account.

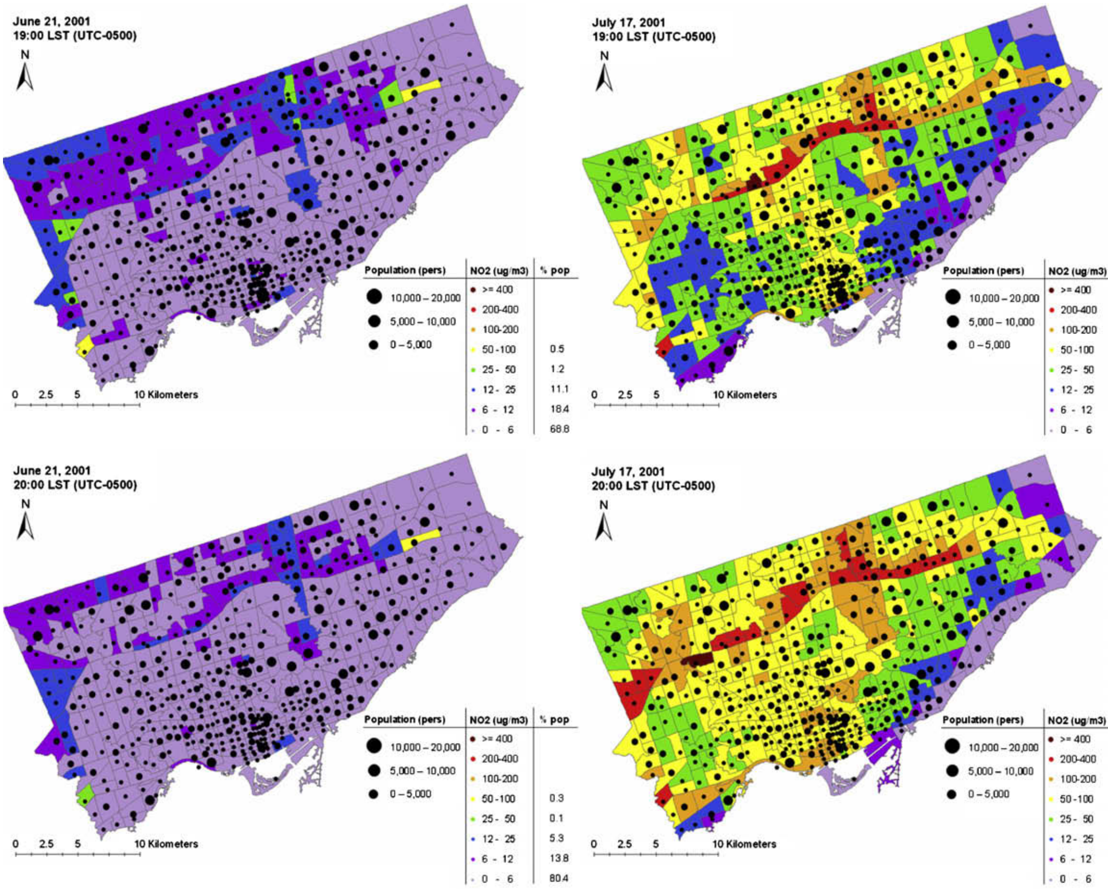


**Fig. 6.** Concentrations at zone centroids at 19:00 and 20:00 LST (June 21 and July 17, 2001).

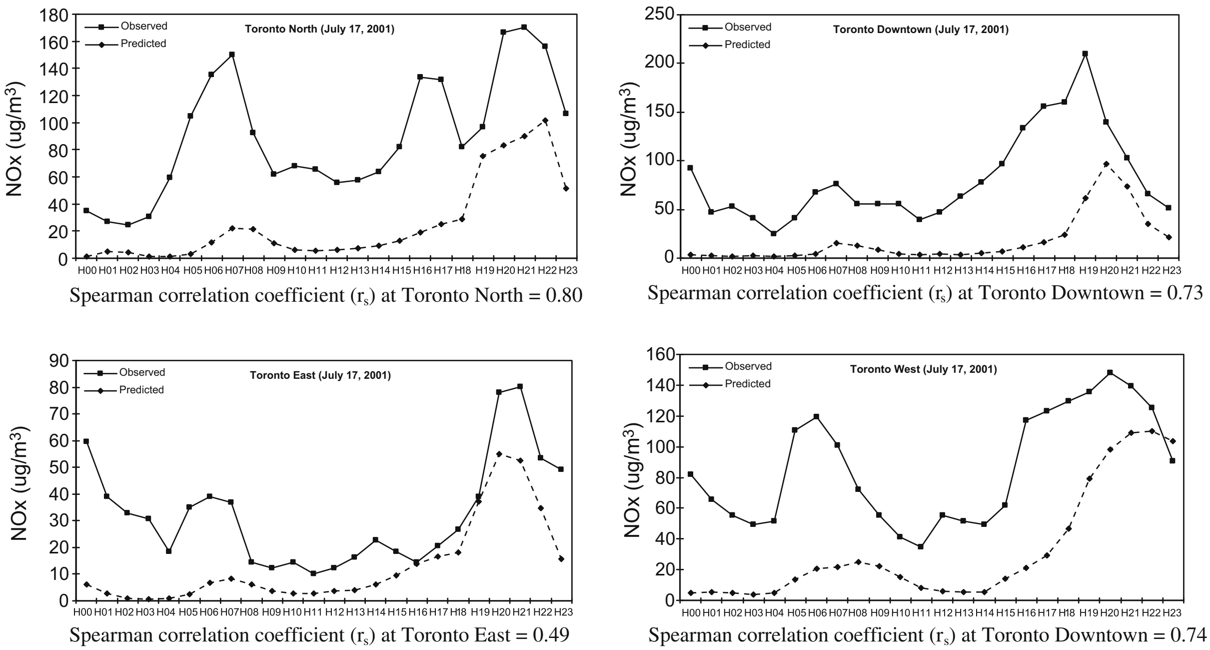


**Fig. 7.** Evolution of hourly $NO_x$ concentrations at the four monitoring locations in the City of Toronto. *Note*: Observed are $NO_x$ concentrations measured at monitoring stations and predicted afre estimated $NO_x$ concentrations reflecting the contribution of light-duty vehicles.

## 4. The simulation of population exposure

Using hourly concentration distributions at the 463 TAZs making-up the City of Toronto and individual activity locations predicted by TASHA, population exposure profiles were constructed. For each individual, the daily exposure is a function of the time spent at every location and the $NO_x$ level; it is the sum of partial exposures in different TAZs and at different times

$$E = \sum_i T_i * C_i \tag{1}$$

where $E$ is total personal exposure, it is the average concentration for the integration period, $T_i$ is time fraction spent in $i$th TAZ and $C_i$ is hourly concentration in $i$th TAZ.

Two major assumptions associated with this exercise are important:

- The indoor $NO_x$ exposure level is assumed to be the same as the calculated outdoor $NO_x$ concentration. This approximation is considered valid from a policy perspective because there is often an interest in identifying people who engage in activities located in polluted areas. In a 2006 study conducted in Toronto, associations between personal exposures and fixed-site ambient measurements were established using personal exposure device data; the authors found strong personal-ambient correlations for $NO_2$ suggesting that ambient $NO_2$ levels may be used as surrogates of personal exposure to $NO_2$ (Kim et al., 2006).
- Exposure during travel is not taken into account. As such, individual daily average exposures are based on less than 24-h since they do not account for the time spent travelling. In-vehicle exposures are significantly different from ambient air concentrations and future research will look into incorporating the results of in-vehicle versus ambient air pollutant levels.

The frequency distribution of individual exposures (on July 17) for the City of Toronto residents is presented in Fig. 8. Assuming that all individuals spend the entire day at home, the distribution of exposures based on the home location was generated and presented on the same graph. Both distributions are similar except that the former (based on time-activity patterns) has less noise than the latter (based on the home location). The figure shows how the time-activity distribution "averages-out" the noise in the distribution based on the home location. This averaging is because the distribution based on the home location can take one of 463 different values corresponding to $NO_x$ levels in the 463 TAZs. In contrast, the distribution based on accumulated concentrations throughout the day has a wider range of values. One difference between the distributions is seen by looking at the ranges in the concentrations obtained whereby the highest daily concentration at any location is 74 $\mu g/m^3$ while the highest accumulated concentration by any individual is 81 $\mu g/m^3$. This means that certain individuals accumulate an average daily concentration higher than the highest daily average at any location. This is because they may happen to be at the worst time period in each location they visit. While this difference is attributed to a small percentage of the sample, it provides an example of the effect of moving people in the city.

The similarity in the two distributions raises the question as to whether the daily concentration at the home location can be used as a proxy for the daily individual exposure. In studying the associations between personal exposures (measured by personal exposure devices) and fixed-site ambient measurement in the City of Toronto, Kim et al. (2006) found relatively good correlations between concentrations at the home location (approximated by the concentration measured at the monitoring location closest to the home location) and personal exposure throughout the entire day. Fig. 9 illustrates the mean of the concentrations generated by accumulating time-activity patterns for all individuals plotted as a function of the daily concentration at the home location. It can be seen that individuals living in zones with low daily $NO_x$ concentrations accumulate

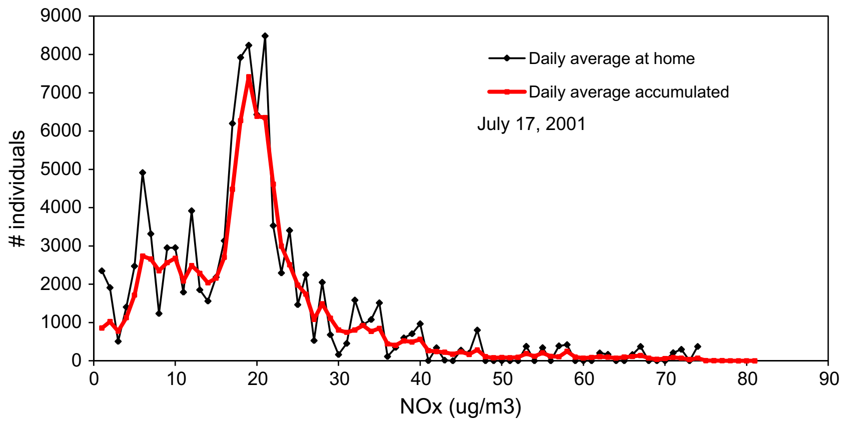


**Fig. 8.** Overlapping distributions of exposures based on home location and daily activity patterns.

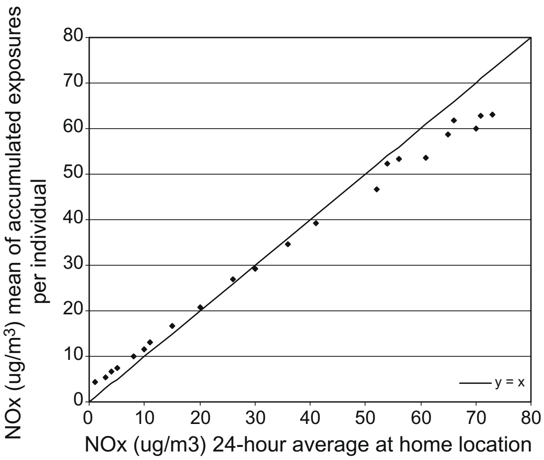


**Fig. 9.** Mean of distribution of exposures based on activity patterns as a function of daily concentration at the home location.

over the span of a day an average concentration higher than what they would have accumulated if they stayed at home (data points fall above the $y = x$ line). In contrast, individuals living in zones characterized by high daily concentrations accumulate in a day an average concentration that is lower than the daily average at the home location (data points fall below the $y = x$ line). Indeed, while it is recognized that air quality at the home location highly influences the total accumulated exposure, it is important to examine the "micro-data" especially for individuals at risk since they could be exposed to high concentrations throughout the day despite the fact that they may live in locations characterized by acceptable air quality. An additional attribute of TASHA that was not taken advantage of in this particular study, is the possibility of attaching socio-economic attributes to daily exposures. The car ownership variable differentiates the exposures of drivers and non-drivers thus allowing for the computation of equity measures. In addition, exposures can be linked with specific activities such as work, school, or shopping thus providing information on the activities in which individuals are exposed to the highest concentrations.

## 5. Conclusions

The study provides a comprehensive treatment of vehicle emissions by explicitly representing most variables affecting the level of emissions in addition to their spatial and temporal variation. The use of an activity-based travel demand model (TASHA) for the purpose of generating vehicle activity inputs rather than a conventional 4-stage model has enabled the achievement of more comprehensive emission results that account for the time of day. Indeed, TASHA models 24-h travel on a 5-min increment basis and provides a much better internal consistency across time periods than is the case for conventional models. In addition, by microsimulating individual trips and tours, TASHA provides information on vehicle engine on–off patterns thus allowing for the estimation of start and soak emissions. The treatment of individual link emissions as individual line sources within the dispersion model allows for improved spatial representation of $NO_x$ concentrations that does not resort to gridding. Indeed, a main drawback of many existing modelling approaches for large urban areas is the allocation of emissions to grid cells. This reliance on spatial surrogates runs the risk of underestimating emission density and hence pollutant concentrations along and in the vicinity of roadways.

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