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Predicting vehicular emissions in high spatial resolution using pervasively measured
 transportation data and microscopic emissions model

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21 Abstract

Air pollution related to traffic emissions pose an especially significant problem in cities; this 22 23 is due to it's adverse impact on human health and well-being. Previous studies which have 24 aimed to quantify emissions from the transportation sector have been limited by either 25 simulated or coarsely resolved traffic volume data. Emissions inventories form the basis of 26 urban pollution models, therefore in this study, Global Positioning System (GPS) trajectory 27 data from a taxi fleet of over 15,000 vehicles were analyzed with the aim of predicting air 28 pollution emissions for Singapore. This novel approach enabled the quantification of 29 instantaneous drive cycle parameters in high spatio-temporal resolution, which provided the 30 basis for a microscopic emissions model. Carbon dioxide (CO_2), nitrogen oxides (NO_x), 31 volatile organic compounds (VOCs) and particulate matter (PM) emissions were thus 32 estimated. Highly localized areas of elevated emissions levels were identified, with a spatio-33 temporal precision not possible with previously used methods for estimating emissions. 34 Relatively higher emissions areas were mainly concentrated in a few districts that were the

35 Singapore Downtown Core area, to the north of the central urban region and to the east of it. 36 Daily emissions quantified for the total motor vehicle population of Singapore were found to 37 be comparable to another emissions dataset. Results demonstrated that high-resolution spatio-38 temporal vehicle traces detected using GPS in large taxi fleets could be used to infer highly 39 localized areas of elevated acceleration and air pollution emissions in cities, and may become 40 a complement to traditional emission estimates, especially in emerging cities and countries where reliable fine-grained urban air quality data is not easily available. This is the first study 41 42 of its kind to investigate measured microscopic vehicle movement in tandem with 43 microscopic emissions modeling for a substantial study domain.

44

45 Keywords: air quality, transportation, emissions, microscopic emissions model, microscopic

- 46 vehicle movement.
- 47

48 **1. Introduction**

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With mass urbanization happening at an unprecedented scale, urban air quality is becoming an issue of global concern (WHO, 2014). Growth in populations, traffic, industrialization and energy usage have led to increased air pollution levels and subsequent public health effects at the urban, regional and global scale (Akimoto, 2003; Molina et al., 2004; Gurhar et al., 2010) The World Health Organization estimates that ambient air pollution leads to approximately 3.7 million premature deaths annually worldwide, with South-East Asia and the Western Pacific Regions having the largest air pollution-related health burden (WHO, 2014).

58

59 The adverse impact of air pollution exposure on human health is well documented in the 60 literature (WHO, 2014). Epidemiological studies have quantified the relationship between 61 adverse health effects and both long- and short-term exposure to air pollution (Bell et al., 62 2004; Jerrett et al., 2005; Laden et al., 2006; Lewtas, 2007; Krewski et al., 2009; Nyhan et al., 63 2014a; Nyhan et al., 2014b). In assessing the impact of air pollution on mortality in the 64 United States, Caiazzo et al. (2013) reported that the largest sector contributor of pollutant-65 related mortalities is road transportation, causing approximately 53,000 PM_{2.5}-related deaths 66 and approximately 5000 ozone-related deaths per year. These figures corresponded to 67 premature deaths from cardiovascular diseases and lung cancer due to long-term exposure to $PM_{2.5}$ (where $PM_{2.5}$ refers to the particulate matter fraction which is less than 2.5µm in 68 69 aerodynamic diameter).

70

71 Traditional methods for monitoring urban air quality employ discrete measurement stations 72 which sample atmospheric conditions at specific sites throughout a city. Networks vary both 73 in size and scale. The London Air Quality Network has over 50 sites classified as roadside, 74 background, suburban and industrial that are dispersed throughout the whole metropolitan 75 area (Laxen et al., 2003). Singapore, which is the focus of this study, has 14 high-grade 76 stations operated by the National Environment Agency, gathering data throughout the island 77 (NEA, 2015). Traditional approaches to monitoring air quality have several limitations, 78 including significant investment required to set up and maintain the measurement networks. 79 Furthermore, as air quality can exhibit large variations over a relatively small scales (Britter 80 and Hanna, 2003), sampling biases can be introduced which make the assessment of human 81 exposure and the sources of pollutants difficult (Vardoukalis et al., 2005). As a result of this,

82 municipal air quality monitoring is often supplemented by air quality models such as the 83 AERMOD modeling system (USEPA, 2009) and the ADMS Urban model (CERC, 2015) to 84 improve the spatial and temporal resolution of air pollution estimates. Sparsely located air 85 quality monitors are limited in their usefulness for accurately determining the locations of air 86 pollution sources. Therefore, air quality monitoring using distributed networks of sensors has 87 gained traction as sensors are becoming smaller, less expensive vet more reliable (Chong et 88 al., 2003; Burke et al., 2006; Cuff et al., 2008; Paulos et al., 2009; Kumar et al., 2015), 89 providing a wealth of high spatial resolution air quality information.

90

91 The availability of large transportation and mobility datasets from sensors, Global Positioning 92 System (GPS)-enabled devices, along with improvements in methods and computational 93 facilities for analyzing these have led to advancements in the field of urban computing 94 research in recent times. So-called opportunistic sensing which is the use of data that is 95 collected for one purpose but can be reused for another one (Campbell et al., 2008), has 96 proved useful in many research studies. Examples include using various anonymized or 97 aggregated spatio-temporal datasets created by different aspects of human activity, such as 98 cell phone data (Gonzales et al, 2008; Sobolevsky et al, 2013; Hoteit et al, 2014; Kung et al, 99 2014; Pei et al, 2014; Grauwin et al, 2014) or vehicle GPS traces (Kang et al, 2013). One 100 such example of opportunistically utilizing vehicle GPS traces is a recent study by Santi et 101 al., (2014) where the economic and environmental benefits of vehicle pooling in New York 102 were quantified based on the analyses of a taxi GPS dataset consisting of 150 million trips.

103

104 Emissions from on-road motor vehicles constitute one of the largest contributions to air 105 pollutants such as carbon monoxide, nitrogen dioxide, ozone, selected volatile organic 106 compounds and fine particulates (Molina and Molina, 2004), and also represent a factor in the 107 spatial variability of air quality in urban areas (Fecht et al., 2016). Vehicle emissions have 108 typically been estimated with the use of either measured (through loop detectors or similar) or 109 modeled (using a transport simulator) traffic data. Based on this information, emission factors 110 are commonly used to convert traffic loads into emissions (NARSTO, 2005). Emission 111 factors vary from location to location, and depend on the vehicle model and road conditions 112 (Zhang and Morawska, 2002; North et al., 2006). The application of emission factors to 113 traffic loads is unable to account for real driving conditions as they happen on the road 114 (Samuel et al., 2002). Thus, as an alternative, different vehicles models with different load 115 factors are often used as probes, whose emissions (and eventually the emission of nearby

116 vehicles) are measured on the road (Canagaranta et al., 2004; Shorter et al., 2005). The 117 aforementioned approaches do not allow the high resolution spatiotemporal mapping of 118 emissions as they do not take into account the 'drive cycle' which is the description of a 119 vehicle's velocity over time. The drive cycle allows the precise determination of consumption 120 and hence emissions (Mantazeri et al., 2003; Int Panis et al., 2006). In the widely used 121 MOBILE Model (USEPA, 2012), only 14 different drive cycles are used; however, these are 122 only expressed as average speed. Many studies have examined the impact of different vehicle 123 modes (idling, moving and accelerating) on the release of pollutants. In a study by Frey et al., 124 (2003) average emissions were observed to be five times greater during periods of 125 acceleration for hydrocarbons and carbon dioxide, and reached ten times as much for nitric 126 oxide and carbon monoxide compared with levels found in an idling vehicle. Similarly, 127 ultrafine particulates released whilst a vehicle is accelerating have also been shown to 128 increase significantly (Fruin et al., 2008). Hence, there is a need for the use of more detailed drive cycles, including velocity and acceleration parameters resolved in high spatial and 129 130 temporal resolution, in modeling emissions from transportation.

131

132 Many studies have led to the development of models that consider variations in speed and are 133 appropriate for instantaneous emission modeling. These include the Comprehensive Modal 134 Emissions Model developed at the University of California (An et al., 1997; Barth et al., 135 2006) and others (e.g. Rakha et al., 2004; Pelkmans et al., 2004; El-Sgawarby et al., 2005). 136 Along with this, significant effort has been devoted to the use of micro-simulation methods 137 for transportation modeling on road networks, for representing real-time, behavior-based 138 policies (e.g. Ben-Akiva et al., 1997; Hu and Mahmassani, 1997; Liu et al., 2006). Individual 139 driver behavior and individual vehicle's real-time space-time trajectories are explicitly 140 represented through traffic micro-simulation models and these produce detailed vehicle 141 operation, instantaneous speed and acceleration of vehicles that are necessary for microscopic 142 emissions models. A review by Fontes et al., (2015) examined combining various micro-143 simulation tools for assessing the impacts of road traffic on the environment, and identified 144 best practices which would aim to minimize errors in combining these. Int Panis et al., (2006) 145 presented a methodology for making instantaneous emission modeling compatible with 146 traffic micro-simulation models. In particular, the emissions caused by acceleration and 147 deceleration of vehicles were modeled based on microscopic traffic simulation model 148 integrated with an instantaneous emission model. The functions developed by Int Panis et al., 149 (2006) were incorporated into a study addressing optimum mitigation strategies for urban

transportation emissions by Osorio and Nanduri (2015) where a combination of macroscopicand microscopic traffic simulators and emissions models were employed.

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153 Recent developments in the field of vehicle emissions have seen the uptake of cell phones 154 and their built in sensors as on-board diagnostic systems - using the data gathered from the 155 GPS and accelerometer to monitor the drive cycle and hence consumption and emissions 156 (Thiagarajan et al., 2009). These approaches have been mostly confined to single or small 157 numbers of vehicles. In this study, however, it is intended to extend an emissions model to a 158 large vehicle fleet using GPS data collected. Intelligent Speed Adaption (ISA) systems are 159 technologies which incorporate GPS navigation to apply speed limits to cars on specific road 160 areas. Systems for monitoring and controlling vehicle velocities include ISA systems (Duynstee et al., 2001; Int Panis et al., 2006). These could also be used for reducing 161 162 emissions and fuel consumption on road networks, but require fine-grained emissions 163 predictions based on real-time GPS data.

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165 The purpose of this study is to use data routinely captured by existing transportation networks 166 and vehicle fleets to predict vehicular emissions in high spatial resolution. For this, GPS 167 measurements gathered by a large taxi fleet in Singapore would be analyzed. Parameters 168 representative of vehicle drive cycles would then be characterized in high spatial and 169 temporal resolution at points throughout the road network. A microscopic emissions model 170 would be implemented to predict the emissions of carbon dioxide (CO₂), nitrogen oxide 171 (NO_x), volatile organic compounds (VOCs) and particulate matter (PM) throughout the study 172 domain, where particulate matter here refers to total suspended particles. Highly localized 173 areas of elevated emissions would thereby be identified, with a higher spatiotemporal 174 precision than commonly used methods. This is the first study to implement a microscopic 175 emissions model using measured microscopic vehicle trajectory data for an entire urban 176 region.

178	2. Methodology
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181	2.1. Overview of methodology
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183	In order to develop an emissions inventory, GPS trajectory data from 15,236 taxis were
184	analyzed. From this, the instantaneous parameters of velocity and accelleration were derived
185	and used as inputs for a microscopic emissions model. Emissions of CO ₂ , NO _x , VOCs and
186	PM were predicted across the road network of Singapore using this model. An analyses was
187	completed which compares the taxi data used to the overall traffic on the road network in
188	Singapore. Following this, emissions from the remainder of the total motor vehicle
189	population of Singapore were also estimated. The results were compared to emissions
190	estimates produced to those attained from the National Aeronautical and Space Agency
191	(Streets and Lu, 2012).
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194	2.2. Study domain and GPS data processing
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211 The GPS trace data was utilized to infer both the location of each vehicle, its velocity and its 212 acceleration. In applying a data cleaning process to the dataset, erroneous GPS points which 213 fell outside the boundary of Singapore or which have an unreasonable distance from its 214 previous location at a given time interval (distance/time ≤ 150 km/h) were eliminated. The 215 instantaneous velocities of vehicles were determined based on the time and distance between 216 geo-referenced points. The data was filtered so as to only examine changes in velocity that 217 occurred over short temporal ranges, where two consecutive data points were separated by no more than 5 seconds as intervals greater than this are unable to depict the microstructure of 218 219 the acceleration profile. A secondary filtering process was applied to the data to remove 220 errors attributed to GPS measurements, as these may be affected by the multi-path effect 221 within urban canyons (Parkinson, 1996). An outlier filter was used that removed all the acceleration values that exceeded 10 ms⁻² as these values are generally not attainable in an 222 223 average car. The normative driving cycle, used to homologate vehicles emissions are characterized by a maximum acceleration of 1.5 ms^{-2} for FTP-72 and 4 ms^{-2} for LA92 224 225 (Guzella and Sciarreta, 2005; Metric Mind Corporation, 2012), therefore sampling points with an acceleration value between 0.5 and 10 m s⁻² were used in this study. 226

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229 2.3. Comparison of taxi fleet and total traffic

230 By applying the above filters, the distribution of the sampling intervals of the 15,236 taxis, 231 indicate that only 7.71% of the logged data has a sampling interval of less than 5 seconds as 232 well as a valid acceleration value. This indicates that the majority of vehicles demonstrate 233 intermittent data logging at intervals greater than 5s. The spatial distribution of the valid 234 samples was correlated with a co-efficient of determination of 0.75 to the spatial distribution 235 of the raw vehicle-GPS points. In order to examine the spatial distributions of GPS points, the 236 city was divided into road links. The valid accelerations of all the vehicles were then 237 attributed to one of the road links based on their latitude and longitude data, and were 238 projected onto a map of Singapore.

239

Aslam et al., (2012) demonstrated that vehicular GPS taxi network data can be used to infer general traffic patterns in Singapore. Aslam et al., (2012) used data from the same taxi fleet as used herein this study. Measured traffic data (i.e. counts of vehicles on road links per time intervals) were obtained through loop count data from the Land Transport Authority (LTA) of Singapore. By examining the fraction of road segments the taxi fleet covers during workdays,

245 it was concluded that 700 taxis were sufficient to cover 70% of the roads for the majority of 246 the day's 1-hour time windows, with the exception of those in the middle of the night when 247 vehicle numbers are sparse. Further to this, Aslam et al., (2012) also observed that 2000 taxis 248 were sufficient to cover 90% of the total loop detector locations during a period of 15 minutes 249 in the morning (from 08:00~08:15) on all workdays. Similarly, we compared our taxi fleet 250 data to measured traffic data obtained from loop detectors operated by Singapore's LTA for 251 the same time period as our study. To achieve this, the taxi data was synchronized with the 252 loop detector data, which was aggregated every 15 minutes. The time series of GPS points for 253 taxis were first matched to road links and then segments on the road network of Singapore. 254 The number of taxis on road segments where loop detectors are located, were counted every 255 15 minutes. These counts were then compared to the loop counts which were regarded as the 256 ground truth for traffic conditions. Figure 1 shows the taxi and loop detector count data for 15 257 randomly selected Singapore road segments. The taxi distribution tended to underestimate the 258 loop distribution and this underestimation was variable across road segments. On each road 259 link, a bias was observed which varied throughout the day, however this bias was relatively 260 consistent across days.

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Figure 1. Distribution of traffic volumes (i.e. number of vehicles per road segment) on 15 randomly selected road segments for the 23rd February 2011. The x-axis includes 15 road segments including a point for every 15 minutes during the 24-hour day. The y-axis represents the percentage of traffic at that location and time. The taxi distribution (in blue) underestimates the loop distribution (in green) and the underestimation is variable.

For inferring general traffic patterns, an artificial neural network model was employed, as has 269 270 been used in another study for predicting traffic volumes on road links (Moretti et al., 2015). 271 The model utilized was a simple corrective model for inferring vehicle distribution as 272 detected by loop detectors from vehicle distribution as determined by the taxi fleet. A 2-layer 273 feed-forward network was implemented, with a tan-sigmoid transfer function in the hidden 274 layer and linear transfer function in the output layer. The model was run for 500 road 275 segments. In determining the performance of the model, a linear regression between modeled 276 traffic volume and the corresponding targets of measured traffic volume was conducted. 277 Figure 2 shows the results of learning for trained model for a sample of data points. As there is a strong association between the modeled and measured traffic volumes, this demonstrates 278 279 that the taxi fleet data may be used to predict general traffic on specific road segments, and 280 the results were similar across the road network of Singapore.



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Figure 2. Results of the feed-forward artificial neural network model implementation. Regression plot of a partial set of modeled traffic volumes versus corresponding measured traffic volume for the (a) training phase ($R^2=96\%$), (b) validation phase ($R^2=93\%$), (c) tesing

286 phase ($R^2=92\%$) and (d) overall model ($R^2=94\%$). A sub-sample of points are presented for 287 clarity.

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289 2.4. Microscopic emissions model

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A microscopic emissions model was implemented and this computed the instantaneous air pollution emissions associated with CO_2 , NO_x , VOCs and PM. The emissions model was based on a model developed by Int Panis et al., (2006), and has been adopted by Osorio and Nanduri (2015). The model utilizes instantaneous velocity and accelerations derived from the GPS dataset to compute emissions. The emission rate at a given time-instant *t* is given in the following equation:

297
$$ER_n^k(t) = max[E_{0n}^k, f_{1n_1}^k + f_{2n}^k v_n(t) + f_{3n}^k v_n(t)^2 + f_{4n}^k a_n(t) + f_{5n}^k a_n(t)^2 + f_{6n}^k v_n(t) a_n(t)], \quad (1)$$

where k is the pollutant type, i.e. $k \in \{CO_2, NO_x, VOC, PM\}, v_n(t)$ is the instantaneous 298 299 speed of vehicle n at time t (in m/s), $ER_n^k(t)$ is the instantaneous emissions rate of pollutant k (in g/s), $a_n(t)$ is the instantaneous acceleration of vehicle n at time t (in m/s²), E_{0n}^k is the 300 lower limit of emission rate for each pollutant type (in g/s), and f_{1n}^k , f_{2n}^k , f_{3n}^k , f_{4n}^k , f_{5n}^k and 301 f_{6n}^k are the emission rate constants specific to each vehicle and pollutant type. Equation (1) 302 303 holds for CO₂ and PM emissions. For NO_x and VOC emissions, the emissions rate 304 coefficients differ depending on whether the vehicle is in acceleration or deceleration mode. 305 If $a_n(t) \ge -0.5 m/s$, then

$$306 \qquad ER_n^k(t) = max[E_{0n}^k, f_{1n_1}^k + f_{2n}^k v_n(t) + f_{3n}^k v_n(t)^2 + f_{4(1)n}^k a_n(t) + f_{5(1)n}^k a_n(t)^2 + f_{6(1)n}^k v_n(t) a_n(t)], (2)$$

307 Otherwise, if
$$a_n(t) < -0.5 m/s$$
, then

$$308 \qquad ER_n^k(t) = max[E_{0n}^k, f_{1n_1}^k + f_{2n}^k v_n(t) + f_{3n}^k v_n(t)^2 + f_{4(2)n}^k a_n(t) + f_{5(2)n}^k a_n(t)^2 + f_{6(2)n}^k v_n(t) a_n(t)], (3)$$

The lower limit of the emissions rate E_0 is fixed to zero for all pollutant types and vehicle types. The emission rate constants (e.g., f_1 , f_2 , etc.) are specified for each pollutant type and vehicle type, and were determined from emissions measurements of on-road instrumented vehicles. These were determined for the car, heavy duty vehicle (HDV, diesel) and bus (diesel) categories. A table describing these emission rate constants are described in Int Panis et al., (2006).

For each pollutant, the expected total emissions (in g) in the specified vehicle network during the simulation period were computed by:

317
$$E[TE^k] = \sum_{l \in L} E[TE_l^k], \qquad (4)$$

318 where *L* is the set of all road links in the network, and $E[TE_l^k]$ denotes the total emissions (in 319 g) of pollutant *k* on link *l*. The latter term in Equation (4) is approximated by:

319 g) of pollutant k on link l. The latter term in Equation (4) is approximated by:

 $320 E[TE_l^k] = E[ER^{k,l}]E[T_l]\lambda_l\Delta T, (5)$

where $E[ER^{k,l}]$ denotes the expected emissions rate (in g/s) for link *l* and pollutant type *k*, $E[T_l]$ is the travel time on link *l*, λ_l is the arrival rate of vehicles to link *l* and ΔT is the total simulation time. For a given link *l* and pollutant type *k*, the term $\lambda_l \Delta T$ approximated the expected total demand over the time period of interest, while $E[ER^{k,l}]E[T_l]$ approximated the expected emissions per vehicle. The emissions computed for each road link were projected onto a map of Singapore.

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Emissions for the total motor vehicle population, represented by general traffic patterns, across the road network of Singapore were quantified. Emissions were estimated on a daily basis according to Equation (5). In this scenario however, the arrival rates of vehicles to each road link, λ_l , were predicted using the traffic model described in Section 2.3. Daily emissions were calculated for each of five days of data available, and the mean of these five days was then compared to mean daily emissions estimated by Streets and Lu, (2012).

334

335 2.5. Vehicle fleet composition

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337 The emissions model took into consideration the estimated composition of the vehicle fleet of 338 Singapore. This was based on information collected by the Land Transport Authority of 339 Singapore (LTA, 2015). The data-set yielded counts of the various categories of motor 340 vehicles within the overall transportation fleet i.e. Cars, Taxis, Motorcycles, Goods and Other 341 Vehicles, and Buses, and these categories were further stratified by type of fuel used i.e. 342 petrol, diesel, petrol-electric, petrol-CNG, CNG and electric for each of the respective 343 categories of vehicle type. Data for the year 2011 were used as this corresponded to our 344 vehicle data-set (see Table 1 for details).

Table 1. Motor vehicle population in Singapore by category and type of fuel used for the year
2011. Figures exclude tax exempted vehicles for off-the-road use (RU plates).

nuue tax exempted	venicies for on-the	-ioad use (ito plates).
Cars	Petrol	596,947
	Diesel	346
	Petrol-Electric	3,786
	Petrol-CNG	2,642
	CNG	-
	Electric	2
	Total	603,723
Taxis	Petrol	279
	Diesel	23,880
	Petrol-Electric	56
	Petrol-CNG	2,836
	CNG	-
	Electric	
	Total	27,051
Motorcycles	Petrol	145,672
	Electric	8
	Total	145,680
Goods & Other	Petrol	9,058
Vehicles	Diesel	136,076
	Petrol-Electric	1
	Petrol-CNG	14
	CNG	8
	Electric	1
	Diesel-Electric	-
	Total	145,158
Buses	Petrol	194
	Diesel	16,433
	Petrol-Electric	-
	Petrol-CNG	8
	CNG	14
	Electric	3
	Total	16,652

348

349 3. Results350351

352 3.1. Spatial distribution of accelerations and predicted emissions

353

354 Figure 3 shows counts of all valid acceleration data on each link on the road network. Higher 355 counts of valid accelerations were concentrated in the Singapore Downtown Core area, at 356 Changi International Airport and some parts of Jurong, Bishan and Yishun. As demonstrated 357 in Section 3.3., the taxi data may be used to predict general traffic on road segments, 358 therefore counts of valid accelerations were proportional to the distribution of vehicles in the 359 city, and proportional to the number of accelerations of each road link. Valid accelerations on 360 each road link were utilized for the emissions model. However, areas such as the Singapore 361 Downtown Core area and the vicinity of Changi International Airport which were 362 characterized by a relatively higher number of sample points of acceleration than other areas. 363 This may indicate a bias in the dataset.

364

The spatial distributions of vehicle emissions computed for each road link in Singapore are shown in Figure 4. With regards emissions related to specific parameters, we can see that for all of CO_2 , NO_x , VOC and PM, elevated levels were identified in a concentrated number of locations in the Singapore Downtown Core area, south of Newton and in Geylang. Elevated levels were also identified in the area surrounding Changi International Airport, Bishan and Jurong West.

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Figure 3. Spatial distribution of the number of valid accelerations in Singapore on the 23rd
February 2011. Locations where relatively higher numbers of valid accelerations are
observed in the vicinity of the Singapore Downtown Core area and the Changi International
Airport in the east.









386

Figure 4. Spatial distributions of predicted daily emissions from the vehicle fleet for each road link for the parameters of (a) CO_2 (tonnes/day), (b) NO_x (tonnes/day), (c) VOC (g/day), and (d) PM (g/day) in Singapore on the 23rd February 2011. Locations of relatively highemissions, are observed in the Singapore Downtown Core area in the south-center of Singapore and in other locations throughout the island.

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The locations where predicted emissions were relatively higher across Singapore can be 394 395 identified for the four pollution parameters of CO₂, NO_x, VOC and PM. In terms of CO₂ 396 emissions, the areas which were identified as having relatively higher CO₂ output from the 397 vehicle fleet. Marina South and Raffles Place in the Downtown Core area, the Harbour Front 398 area, Jurong East, Clementi, Sin Ming and an area close to the Seletar Reservoir in Yishun 399 were identified. In the east of Singapore, the area between Tampines and Changi International 400 Airport was identified as having relatively higher CO₂ emissions than other areas. The Bukit 401 Timah Road - Whitley Road Intersection was selected as having relatively higher CO₂ 402 emissions as were the busy areas Novena, Newton, Somerset, Dhoby Ghaut (north) and 403 Farrer Park which are located north of the central region of Singapore.

404

405 Relatively higher levels of NO_x emissions were predicted in the Downtown Core Area such 406 as in Chinatown, Outram Park, Clarke Quay and Raffles Place. The Chin Swee Tunnel -407 Havelock Road intersection area was also identified. North of Dhoby Ghaut, City Hall, on the

408 Central Expressway side of Fort Canning Park and Little India were areas where relatively 409 higher NO_x emissions were predicted. Connected to these, Somerset and Orchard were areas 410 with relatively higher NO_x emissions. The Moulmein Flyover, the Jalan Bukit Merah - Lower 411 Delta Road Intersection (located west of the Downtown Core area), the Kallang-Paya Lebar 412 Expressway (KPE) - Nicoll Highway Intersection (located east of the Downtown Core area), 413 and further east, an area in the vicinity of Changi International Airport was also identified. 414 For VOC emissions, the areas of elevated emissions were observed to be centrally located 415 with a few areas scattered in other parts of Singapore. Located centrally were Orchard Road, 416 the River Valley Road - Zion Road Intersection, Outram Park, Marina South, Suntec City and 417 Little India. Moving east from the urban central region - Selegie, Lavender, Kallang, 418 Geylang, and further east, the Layang Avenue - Pasir Ris Drive 1 Intersection and the Pan 419 Island Expressway (PIE) - Tampines Expressway (TPE) Intersection near Changi 420 International Airport were identified as hotspots for VOC emissions. North-east of the central 421 region was Tao Payoh and further north was Sin Ming (Yishun area). Westwards from the 422 Downtown Core areas were Bukit Merah, the Hollande Road - Farrer Road Intersection. 423 Further west was Clementi, Jurong East and Bukit Batok. In the north-west of Singapore, 424 Choa Chu Kang was observed to have relatively higher levels of VOC.

425

426 For PM emissions, all the areas of relatively highest predicted emissions were concentrated in 427 the Downtown Core area with some areas identified to the east of it. The areas identified 428 included the areas of Outram Park, Chinatown, Raffles Place and Clarke Quay. South of these 429 the Tajang Pagar area near Keppel Road was chosen and slightly north of these, the Havelock 430 Road - Outram Road Intersection. River Place near the Chin Swee Tunnel and the Central 431 Expressway side of Fort Canning Park were identified. On the east of the Downtown Core 432 area were Bugis, Beach Road and Geylang. On the west side of the Downtown Core area; the 433 Jalan Bukit Merah - Lower Delta Road Intersection was included in the selection of areas 434 determined to have increased PM emissions relative to the rest of the island. Other areas were 435 the extent of Orchard Road, Farrer Park and Balestier.

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438 3.2. Comparison of predicted emissions for the total motor vehicle population

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Total emissions of each pollutant parameter for the vehicle fleet studied were computed for each day and the means determined are presented in Table 2. The mean daily CO_2 and NO_x

emissions determined were respectively representative of 7.9% (\pm 3%) and 7.6% (\pm 1.4%) of emissions estimates for the total motor vehicle population of Singapore (including the previously calculated vehicle fleet emissions). For VOC and PM, the proportions were smaller, whereas the total daily emissions computed were approximately 3.2% (\pm 1.7%) and 3.5% (\pm 1.6%) (respectively) of total motor vehicle population emissions (see Table 2 for details).

448

449 Daily emissions from the total motor vehicle population were then computed for one week 450 and compared to other transportation emissions estimated by Streets and Lu (2012) (see Table 451 3). The overall emissions levels computed for the entire fleet were comparable to those 452 attained from Streets and Lu (2012). Whereas our analyses predicted mean daily emissions 453 from the entire motor vehicle population to be 27656 (\pm 3049) tonnes for CO₂, Streets and Lu 454 computed 24417 tonnes/day. Therefore, the relative difference in emissions was found to be 455 15% ($\pm 1.7\%$). For NO_x we determined total daily emissions to be 155 (± 33.1) tonnes/day 456 while Streets and Lu computed 121 tonnes/day, and this corresponded to a relative difference 457 of 24% (±4.9%). A larger disparity was observed in the case of VOC. We predicted total 458 emissions to be 9.7 (±2.6) tonnes/day whereas Streets and Lu determined a value of 21.6 459 tonnes/day. This is equivalent to a relative difference of -49% (±12.3%). Finally, for PM we 460 computed 8.5 (±3.4) tonnes/day while Streets and Lu predicted 14.1 tonnes/day. Similar to 461 VOC, we calculated a relatively lower value to Streets and Lu by 39% (±15.5%), but 462 exhibiting a larger uncertainty.

463

Table 2. Modeled emissions for the taxi fleet and the proportion of modeled taxi emissions in

the estimated total motor vehicle population emissions, for each of four air pollutantparameters.

	Modeled Emissions Taxi Fleet	Proportion of Modeled Taxi Emissions in the Total Motor Vehicle Population Emissions
	(tonnes/day)	%
	Mean (SD)	Mean (SD)
CO ₂	2176.6 (1023.5)	7.9 (3.0)
NO _x	11.9 (2.8)	7.6 (1.4)
VOC	0.3 (0.2)	3.2 (1.7)
PM	0.3 (0.2)	3.5 (1.6)

- 470 Table 3. Comparison of the mean daily emissions predicted for the total motor vehicle
- 471 population of Singapore to estimated ground transportation emissions attained from Streets472 and Lu (2012).

	Predicted Total Motor Vehicle Population Emissions (tonnes/day)	Streets and Lu (2012) (tonnes/day)		
	Mean (SD)	Mean	Range of Ratios	Average difference (SD) (%)
CO ₂	27656 (3049)	24417	(1.1-1.3)	15.1 (1.7)
NO _x	155.2 (33.1)	121	(1.0-1.6)	24.1 (4.9)
VOC	9.7 (2.6)	21.6	(0.4-0.7)	-49.3 (12.3)
PM	8.5 (3.4)	14.1	(0.4-0.8)	-38.7 (15.5)

477 **4. Discussion**

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- 479

480 Recent advances in urban computing and the availability of large transportation GPS datasets 481 have presented new opportunities for real-time transportation and emissions modeling. 482 Transportation and emissions modeling conducted in previous studies have been limited by 483 coarsely resolved predicted or measured traffic information. In this study, we analyzed GPS 484 traces from a fleet of over 15,000 vehicles in Singapore with the aim of using this 485 information to make predictions of emissions in high spatial resolution throughout the study 486 domain. The instantaneous velocities and accelerations of vehicles, which were extracted in 487 high spatial and temporal resolution, were inputted into a microscopic emissions model. The air pollution emissions of CO₂, NO_x, VOC and PM were thus quantified. The spatial 488 489 distributions of the emissions were examined and this enabled highly localized areas of 490 elevated emission levels to be identified. The study demonstrated how instantaneous drive 491 cycles can be used to predict vehicular pollutant emissions and this forms an important 492 component of the urban emissions inventory.

493

494 An analyses demonstrated that the taxi data could be used to predict overall traffic volumes 495 on road segments throughout the road network. Emissions from the taxi fleet and then the 496 total motor vehicle population were therefore predicted for the study domain of Singapore. 497 The subsequent emissions levels computed for the entire motor vehicle population was 498 comparable to those attained from Streets and Lu (2012). Whereas the modeled values are in 499 the same order of magnitude for each pollutant parameter, the results likely varied due to the 500 different emissions modeling methods employed. Further to this, in the case of Streets and Lu 501 (2012) estimates of emissions from the transportation sector are from the year 2012, while 502 our data are representative of one week of data for the year 2011. Predicted emissions 503 computed for CO₂ and NO_x were higher than VOC and PM. The reason for this is that the 504 emissions function parameters used are higher for CO₂ and NO_x. CO₂ and PM emission 505 estimates are more sensitive to vehicle velocities than VOC and NO_x which are more 506 sensitive to accellerations (Int Panis et al., 2006).

507

508 This paper presents a novel methodology for making instantaneous emission modeling 509 compatible with microscopic traffic patterns (measured on a second by second basis). 510 Previous studies have focused on the microscopic traffic simulation coupled with

511 microscopic emissions modeling (Int Panis et al., 2006) or a combination of macroscopic and 512 microscopic traffic simulation combined with microscopic emissions modeling (Osorio and 513 Nanduri, 2015). However, to the authors knowledge, a study investigating measured 514 microscopic vehicle movement (measured on a second by second basis using GPS) in tandem 515 with microscopic emissions modeling has not been completed successfully for a substantially 516 sized vehicle fleet and study domain, rather have been limited to small ad hoc deployments.

517

518 The methodology described in this study has the potential to inform environmental policy 519 related to transportation in urban areas. With the framework proposed, where appropriate data 520 is available, responsive and adaptive strategies could be implemented should the emissions 521 model be applied using real-time GPS data. The methodology described demonstrated the 522 potential for linking GPS measured vehicle movements directly with microscopic emissions 523 models (based on the instantaneous driving speed and acceleration) for quantifying traffic 524 emissions. Although the computation of emissions is clearly a useful application, it is in the 525 implementation and evaluation of real-time, technology-based environmental policies related 526 to transportation where its application would be most beneficial. Technologies for monitoring 527 and controlling vehicle velocities include Intelligent Speed Adaption (ISA) systems 528 (Duynstee et al., 2001; Int Panis et al., 2006). ISA systems are electronic systems installed in 529 vehicles, which utilize GPS navigation to evaluate the vehicle location and apply appropriate 530 speed limits on specific road segments ISA systems combined with an appropriate real-time 531 emissions model could be utilized for minimizing emissions and fuel consumption in urban 532 road networks in the future.

533

534 Environment related transportation policies such as restricting vehicles in a city-center zone 535 or restricting odd/even number plates in urban regions have been adopted in a number of 536 cities in recent years (Fensterer et al., 2014; Holman et al., 2015). Whereas these have helped 537 in the reduction of congestion and pollution levels in urban centers, more beneficial 538 approaches may be based on the detection of the specific, fixed positions where emissions 539 take place, rather than in substantial urban regions. With the dynamic fine grain emissions 540 inventory presented in this study, it may become feasible to target air pollution emissions 541 mitigation efforts in a far more direct manner. The health and economic benefits of reducing 542 air pollution emissions across various sectors including transportation, thereby improving air 543 quality, has been quantified in many reports. For example, the US EPA computed the costs 544 for the implementation of the 1990 Clean Air Act to be about 65 million dollars, with a

potential benefit reaching 2 trillion dollars from 1990 to 2020, potentially avoiding
approximately 230,000 premature deaths in 2020 (USEPA, 2011).

547

548 For the first time, the data collected allow us to see an emission inventory not as something 549 static which only changes from one road segment to the other, but which has more detailed 550 characteristics with spatiotemporal variation. This enables a better estimate of the impact of 551 pollution on the urban population which also exhibits variable spatial and temporal 552 distribution profiles over the course of the day (Nyhan et al., forthcoming). The advantage of 553 the proposed method is that by interrogating and interpreting easily accessible data from 554 existing fleets (such as vehicle or bus services), considerable information regarding air 555 pollution emissions can be obtained at a low cost and minimal effort in cities. Such a system 556 can be applied in other cities, perhaps through government encouragement to make 557 transportation GPS data available. This information may be of considerable value in 558 determining the most appropriate locations of where to take action to reducing emissions and 559 subsequently air pollution concentration levels in cities. This type of data could also be used 560 to compute fine-grained fuel consumption patterns from the transportation sector.

561

562 This approach we adopted for predicting emissions has some limitations. In the development 563 of the emissions model functions, Int Panis et al., (2006) primarily used measurements made 564 in urban traffic (with low speeds) for determining functional forms and the variables in the 565 emissions equations used in this study. This is considered sufficient for the purposes of 566 evaluating the effects of speed management in urban networks. It is possible that the emission 567 functions for highway traffic (at higher speeds) differ for those of urban traffic and the traffic 568 on highways was insufficiently represented in the functions used. The emissions model did 569 not allow for the specific model or age of the vehicles to be considered in computations 570 either. Some additional measures would also be needed to verify the quality of the 571 acceleration data obtained from GPS traces. There are inherent inaccuracies associated with 572 GPS measurements, which however are compensated by the large volume of data collected. 573 There is a necessity to connect the movements of the subset of vehicles with the movement of 574 all the vehicles in the city. For this, calibrations parameters could be applied based on the 575 sampling of the available vehicles versus the total number of vehicles. Finally, additional 576 work would be needed to link the emissions predicted for various parameters to local 577 measured air pollution concentration levels. A future study by these authors will therefore

examine the relationship between predicted emissions using the methodology describedherein this study, and measured or modeled values of air pollution concentrations.

580

This methodology described in this paper may be replicated in a number of cities worldwide, as GPS traces from vehicles become increasingly available. Vehicle fleet operators can do a major public service by providing GPS data for research, in particular for predicting emissions and other information relevant to environmental health from it. This information may be used for designing air pollution intervention strategies (long-term, short-term, responsive and adaptive) for the protection of human health and well-being.

587

588

589 **5. Conclusions**

590

591 Through analyzing GPS data from a large transportation fleet in Singapore, fine grained 592 emissions were estimated in high spatial resolution. The emissions model was based on the 593 inputs of velocity and acceleration parameters extracted from the data. Air pollution 594 emissions related to CO₂, NO_x, VOC and PM were thereby quantified. The spatial 595 distributions of the emissions were investigated thereby enabling highly localized areas of 596 relatively higher emissions levels to be identified. This study also shows how the 597 instantaneous drive cycles can be applied in the estimation of the overall emissions from the 598 transportation sector within the study area.

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*List of Tables*Table 1. Motor vehicle population in Singapore by category and type of fuel used for the year
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Figure 1. Distribution of traffic volumes (i.e. number of vehicles per road segment) on 15 randomly selected road segments for the 23rd February 2011. The x-axis includes 15 road segments including a point for every 15 minutes during the 24-hour day. The y-axis represents the percentage of traffic at that location and time. The taxi distribution (in blue) underestimates the loop distribution (in green) and the underestimation is variable.

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Figure 2. Results of the feed-forward artificial neural network model implementation. Regression plot of a partial set of modeled traffic volumes versus corresponding measured traffic volume for the (a) training phase ($R^2=96\%$), (b) validation phase ($R^2=93\%$), (c) tesing phase ($R^2=92\%$) and (d) overall model ($R^2=94\%$). A sub-sample of points are presented for clarity.

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Figure 3. Spatial distribution of the number of valid accelerations in Singapore on the 23rd
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Figure 4. Spatial distributions of predicted daily emissions from the vehicle fleet for each road link for the parameters of (a) CO_2 (tonnes/day), (b) NO_x (tonnes/day), (c) VOC (g/day), and (d) PM (g/day) in Singapore on the 23rd February 2011. Locations of relatively high-

- 909 emissions, are observed in the Singapore Downtown Core area in the south-center of
- 910 Singapore and in other locations throughout the island.

Highlights

We present a novel method for predicting air pollution emissions using transport data Study uses measured microscopic transport data and a microscopic emissions model GPS data from over 15000 vehicles were analyzed to quantify speeds and accelerations CO₂, NO_x, VOCs and PM were modeled in high spatio-temporal resolution Highly localized areas of elevated emissions were identified