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Are we getting vehicle emissions estimation right?

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ABSTRACT

Simulation is a valuable prediction tool to evaluate the impact of climate change interventions prior to disruptive implementations that may yield unintended and unwanted consequences. Advances in agent-based simulation allow us to estimate the dynamic emissions produced by vehicles at a fine resolution, with each vehicle modelled individually. The scalability of these models allow decision-makers to evaluate large-scale scenarios. But how good are these models? In this paper, the authors apply a state-of-the-art emissions model in the Multi Agent Transport Simulation (MATSim) framework to simulate individual vehicle emissions. Simulation results are compared with real driving emissions tests, using a portable emissions measurement device on a light and heavy vehicle. Quantifying the gap between macro-level simulation and actual emissions, the paper contributes by showing that pollutants are significantly underestimated, especially for heavy vehicles. This confirms prior micro-scale studies and magnifies the detrimental impact of using uncorrected aggregated models to inform environmental policy affecting transport.

1. Introduction

This paper contributes by quantifying the gap between state-of-the-art simulation estimation at the city scale and actual emissions. The problem faced in the transport sector is that simulations, while efficiently evaluating costly scenarios without trial-and-error, often rely on laboratory or aggregate values, resulting in over or underestimating emissions. The emergence of Real Driving Emissions (RDE) tests, measured using PEMS equipment, resulted from precisely this knowledge that homologation results and actual emissions differ. The Volkswagen *Dieselgate* scandal (Chossière et al., 2017) popularised this difference, where vehicle manufacturers misled the public about real-world driving emissions.

While research has made much progress in measuring and understanding emissions at the very detailed and disaggregate vehicle level, the transport emission impacts on the macro-scale (city or region) are not as well understood. One reason is that most macro-scale emission estimates rely on aggregated fuel consumption or average travel speed and traffic situation models. Consequently, aggregate models lose their spatiotemporal granularity. One can therefore not ask more precise questions like *"where exactly in the city are the high carbon monoxide concentrations?"* or *"which neighbourhoods are affected, and how severely, with the introduction of low-emission zones?"*

Advances in activity-based and agent-based simulation now allow us to model more comprehensive scenarios at a higher, more detailed resolution. The literature agrees that agent-based transport models provide better travel time estimations than their trip-based counterparts. In this paper, the authors report simulation results of a leading agent-based transport model and compare the estimated emissions with onboard PEMS equipment capturing real-world driving conditions in Gauteng, South Africa. Instead of

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comparing different modelling approaches, this paper aims to quantify the gap between a state-of-the-art agent-based model and the actual emissions measured at the vehicle level.

This paper contributes to the field of transport simulation in two ways. Firstly, the scale of its focus. Much emissions research focuses on detailed dynamics and driver behaviour using well-controlled experiments with a reasonably small (spatial) extent. In this paper, the authors focus on applying a macro-scale model, using a 60 km+ urban route that more realistically captures the length of a typical urban commute (in South Africa), capturing various road types. The second contribution is concomitant: quantifying the variation and the gap between the simulation and empirical emissions for two vehicle types, three drivers and different road types.

Computational constraints force large-scale models to make simplifying assumptions and aggregations, and we tend to find that plausible and acceptable. This paper aims to quantify the price we pay for these simplifications when estimating emissions.

The remainder of the article is structured as follows. The next section reviews the literature regarding transport emissions measurement and simulation. Section 3 describes the simulation model applied to a Gauteng case study in South Africa. We present the PEMS experimental setup in Section 4. Section 5 discusses the simulation and PEMS test results, after which the conclusion in Section 6 introduces topics for future work arising from this paper.

2. Literature review

With increased urbanisation and the associated pressure on mobility, Low Emission Zones (LEZs) have been implemented extensively (and with great success) across Europe to combat the rise in traffic emissions in densely populated city centres. In the UK, London's Ultra Low Emission Zone (ULEZ) supports the country's legal commitment to reduce emissions to net-zero by 2050 (World Economic Forum, 2020b). The ULEZ has seen CO_2 emissions fall by 12 300 tonnes since 2016. The zone expanded in 2021 to include residential areas housing 3.8-million people, which could prevent hospitalisations over 30 years, saving the country's health service £5-billion (World Economic Forum, 2020a). Ježek et al. (2018) demonstrate, using simulation in their Central-European case study that removing 10% of the highest polluting vehicles in LEZs reduces the total black carbon and NO_x emissions from traffic by 39% and 33%, respectively. But all the results reported in literature are based on estimates that rely on a variety of underlying models.

Simulation is a valuable tool for evaluating interventions and anticipating their outcomes without time and cost constraints of implementation. While attractive, simulation models frequently deviate from reality as they are mere abstractions of reality. Dey et al. (2019) calculate the variation in damage costs of emissions and give an example of the consequence of over or underestimating emission inventories on its relevant application in Ireland. The cost of these inaccurate estimates was €40-million.

In this section, two main topics are reviewed. Firstly, the empirical measurement of vehicle (exhaust) emissions. Secondly, the use of simulation to estimate environmental impacts of transport on larger scale scenarios.

2.1. *Empirical transport emissions*

Onboard PEMS instrumentation is deployed to record the movement, geographical position and exhaust emissions of a vehicle driven over a real-world test route. PEMS record these measurements by taking emitted gas samples from the vehicle's exhaust. Engine output can be computed at each sampling instance using the test vehicle's specifications. This enables the prediction of instantaneous fuel consumption and exhaust emissions (Wyatt et al., 2014).

PEMS measurements include all sources of variability absent in most lab tests, e.g. driver behaviour, the impact of environmental conditions and traffic and variable vehicle operating conditions (López-Martínez et al., 2017). Additionally, with PEMS tests, the researcher can study a *distribution* of emissions measured across multiple trips, which is more comprehensive than point values from static measurements or averaged trip travel times. Simulation models can produce similar distributions from ensemble runs, making PEMS tests the ideal validation method.

Past studies demonstrate the use cases for PEMS as a validation method for instantaneous fuel consumption and emission models. Frey et al. (2003) evaluate three instantaneous fuel consumption and emission models (EcoGest, CMEM and ADVISOR). They validated their estimated emissions against the results from 824 one-way runs (over 100 driving hours) with onboard PEMS equipment on a 4.6 km test route in North Carolina, USA. They found that, except for the fuel consumption and CO_2 emissions, which can be accurately predicted, these models are limited in their ability to predict the short-term variation in NO_x, CO and HC emissions.

Considering only a small road section might not convey the full capability of the simulation to predict pollutant emissions accurately at the city or regional level. To address this, the authors of this paper use a 61.7 km test route with different road types.

2.1.1. *Accounting for inconsistencies*

Real-world NO_x emissions often exceed estimates obtained by laboratory-based approval processes (RAC, 2020) or traffic emission models. O'Driscoll et al. (2016) use 39 Euro-6 diesel passenger cars to study the variance in NO_x emissions over a test route comprising urban and motorway sections. Their results show that the average NO_x emissions range from 1 to 22 times the Euro-6 limit. They attribute these high levels of emissions to an increased number of acceleration events.

The exclusion of road grade in emission models is also considered a viable cause for inconsistencies in emission estimates. Wyatt et al. (2014) verify this by finding that failing to account for even a relatively modest road grade in micro-scale emissions modelling could potentially result in highly inaccurate estimates of real-world emissions. Therefore, they propose a LiDAR (Light Detection and Ranging) – GIS (Geographic Information System) methodology for estimating road grade. The addition of the LiDAR-GIS data improved the CO_2 predictions of the PHEM instantaneous emissions model. Onboard PEMS measurements from 48 conducted trips were used to validate the simulation results. They found that the improved PHEM model accounted, on average, for 93% of the CO_2 emissions on the 4.3 km urban test route.

But like PEMS, LiDAR equipment is prohibitively expensive for widespread use in tests, limiting its application to specialised and focused experiments. Scaling the road grade estimation, using LiDAR, to a city scale so it can be incorporated in macro-level transport models is not practical. Estimating road grade from more ubiquitous and accessible data sources like Volunteered Geographic Information (VGI) services, such as *OpenStreetMap*, and Shuttle Radar Topology Mission (SRTM) elevation data is still quite new (Gerber and Joubert, 2022).

2.2. Simulated transport emissions

When emission models like Comprehensive Modal Emissions Model (CMEM) and Passenger car and Heavy duty vehicle Emission Model (PHEM) are validated through RDE tests, using PEMS, they become useful in large-scale applications like air emission inventorying (Bang et al., 2017) and, consequently, input to air quality studies.

Project Autonomous and Connected vehicles for CleaneR Air (ACCRA) in the UK (Rushton et al., 2018) demonstrates the usefulness of emissions modelling to develop high-resolution emission maps – a necessary input for air quality dispersion models and the ACCRA decision-making engine for generating geofenced air quality zones in Leeds, UK.

Many urban zones in the UK struggle to comply with the mandated reductions in type approval limit values for tailpipe NO_x emissions of new vehicles. Department for Environment, Food and Rural Affairs (DEFRA) predicts that areas of Leeds will not meet the binding EU annual mean limit value for NO_2 until beyond 2030. The city council in Leeds wanted to investigate the impact of geofencing and zero-emission vehicle operation as a local intervention to cut emissions on highly-affected road links. Project ACCRA counters the unrealistic emission reduction policies suggested by DEFRA with its model, utilising computational fluid dynamics and dispersion (emissions) modelling, allowing local authorities control over air quality areas in their jurisdiction. This project demonstrates the value of emission models for large-scale environmental studies on a regional level. For its scalability, the model pays the price of losing spatiotemporal granularity as it aggregates to emission zones instead of estimating at the vehicular level and dynamic traffic conditions.

A study in St. Petersburg by Lozhkina and Lozhkin (2015) evaluated the Russian road transport-related street pollution model. They confirmed its effectiveness to estimate local air pollution and proceeded by comparing it to COPERT, the most widely used emissions model in Europe (ERMES, 2021). COPERT showed promising results, considering its foreign application, with 3%–15% underestimations of emission rates. The "top-down" computational model of COPERT is based on statistical information about the vehicle fleet structure. This approach is applicable, for instance, when determining the total annual emissions of pollutants from motor vehicles on a region or a country scale. However, detailed information about the vehicle fleet is often lost in these aggregate approaches.

2.2.1. Limitation of aggregate approaches

Transport modelling and calculation of the related fuel consumption and emissions form the basis of quantifying and aggregating emissions from mobility (Nocera et al., 2018). This relates to the two-step process of simulating emissions: combining the traffic and emissions model (Nocera et al., 2017).

Linton et al. (2015) review different aggregate approaches to model emissions. Among these is system dynamics modelling (Feng et al., 2013) which estimates emissions based on fuel consumption, calculated by coupling the vehicle fleet, driven by socio-economic factors, with a transport sub-module. Further, techno-economic and integrated assessment models (Falcão et al., 2017; Loulou and Labriet, 2007) also estimate macro-scale emissions. They rely on the same premise of fuel consumption and socio-economic factors to calculate emissions. However, the emission calculations do not include the effect of different road types, the vehicle's engine size or Euro emissions rating. Most importantly, the models are typically not behaviourally sensitive to evaluate individuals' response to interventions.

Europe and the US have (primarily) adopted the use of average speed and traffic-situation models for emissions modelling (ERMES, 2021). However, these models all rely on the traffic models they are combined with, and traditionally this is the four step, trip-based model (McNally, 2007).

Rasouli and Timmermans (2013) identify shortfalls in the four-step model that fuelled the development and use of activity and agent-based models of travel demand:

(a) a need for consistency among sub-models makes the four-step model lack integrity;
(b) the erroneous assumption that the four steps are independent;
(c) the aggregate nature of the model, both in time and space; and
(d) the lacking behavioural realism evident in agent-based and behavioural models.

In line with macrosimulation tools, MATSim can aggregate emissions to a regional scale, but has the advantage of including the agent-specific properties: *individuality, autonomy, interactivity* and *adaptability* in a single model (Macal, 2016) – an advantage that MATSim holds above emission models that rely on the traditional four step model. Each person (or vehicle) can be modelled individually with each individual, data permitting, having its own attributes.

2.2.2. MATSim

The agent-based MATSim model simulates traffic emissions at a high resolution with its dynamic traffic assignment capability, allowing the modeller to study individual vehicle emissions. Because of its computational efficiency, it can still deal with large-scale scenarios while the modeller can aggregate individual vehicles' emissions to any desired regional scale. The review of Li et al. (2021) identified MATSim as the dominant agent-based model in its ability to be integrated with other urban mobility simulation tools. The review specifically reported on emission savings when investigating autonomous vehicles.

Initially, MATSim mainly focused on accurately modelling traffic dynamics and travel behaviour and was therefore coupled with external emissions models. One example is from Tampa, Florida, in which Gurram et al. (2019) combine the MATSim dynamic traffic assignment model with the MOVES mobile source emissions estimator and the R-LINE dispersion model, and estimate the individual-level exposure to the population, both spatially and temporally. In their research, however, no mention is made of checking the accuracy of these models, either individually, or jointly.

But MATSim developers also embedded emissions functionality as a tight coupling with the simulation core. Hülsmann et al. (2011) developed an emissions modelling framework when they linked MATSim's transport model with traffic situations in the Handbook Emission Factors for Road Transport (HBEFA). They tested this approach and reported that the simulated average travel times approximate the average travel times derived from driving cycles appropriately. Agarwal and Kickhöfer (2015) apply their emissions modelling approach in a real-world application in Munich, Germany. Their study investigates the effect of congestion optimisation on emissions levels and vice versa. This while also considering heterogeneity in individual attributes and choice behaviour — elements lost in large-scale, aggregate approaches.

MATSim's emissions modelling framework has been applied to evaluate various emission reduction scenarios. Pukhova et al. (2021) test policies for emission reduction from passenger aviation in Germany. Kaddoura et al. (2021) apply the framework for their decarbonisation study of Berlin and Kickhöfer et al. (2018) test optimal emission pricing strategies that would result in reaching set policy targets regarding greenhouse gas emissions in Munich. Gräbe and Joubert (2021) showed that MATSim is behaviourally sensitive to emissions-specific interventions and triggers like restricted vehicle access based on the vehicle's emissions class, for example.

Both MATSim and the individual emissions models, like HBEFA, are reputable in their own right. Consequently, they are frequently used to estimate the effect that transport interventions will have on the overall state of emissions. Yet, the emission estimations of these agent-based models have, to the authors' knowledge, not been validated or compared with empirical emission measurements. And it is this gap in the literature where this paper aims to contribute.

3. Simulation model

Following on Li et al. (2021), this paper uses MATSim as a reliable activity-based transport model to simulate detailed vehicle movement on a large city-scale. Is the coupling of MATSim with HBEFA even relevant to a South African case study? In the absence of any South African specific reference data, the authors are compelled to look for international alternatives. The HBEFA database is both publicly accessible at a very reasonable price and the emission concepts are aligned and easily transferrable to the vehicle fleet in South Africa (Joubert and Gräbe, 2021). And since the MATSim coupling with the HBEFA database is an open source software contribution, its use is an attractive first attempt at modelling emissions in a state-of-the-art manner.

The point of departure is a calibrated four-step model of Robinson and Venter (2019), a trip-based *Saturn* transport model that was developed for the South African National Road Agency Limited (SANRAL) in 2016. It is the dominant and most recent model that covers the entire province of Gauteng in South Africa. Gauteng is the economic centre of the country with a population of approximately 16.1-million inhabitants across three metropoles (Johannesburg, Ekurhuleni and Tshwane/Pretoria) and two district municipalities (Sedibeng and West Rand).

Why start from a trip-based model? Two reasons. Firstly, many current macro-level emission models rely on trip-based transport models in one way or another. Secondly, both Fourie (2010) and Gao et al. (2010) show that if you convert a trip-based model directly into an activity-based or, more specifically, an agent-based model, the latter not only provides a richer result set that can be analysed at a more disaggregate level, it also estimates travel time distributions more accurately than its trip-based counter-part. The more accurate travel time distributions is a result of the dynamic traffic assignment approaches that allows more realistic travel phenomena like spill-backs.

Joubert and Gräbe (2021) describe in more detail how the Gauteng trip-based model is converted. Each trip in the commuter origin–destination matrix is converted into a single agent (person) having a home-work-home activity chain. Similarly, agents are generated for the business-trips matrix, as well as the heavy vehicles (commercial traffic) matrices.

For the road network, this paper relies on VGI data provided by *OpenStreetMap*. Each link in the network carries attributes about the number of lanes, allowed free speed, and flow capacities. From these attributes, we can derive the most suitable urban road classification that aligns with the HBEFA database, for example *access* roads, *local* or *distribution* roads, *trunk* roads, city or national *motorway* links. While road type can be inferred from the *OpenStreetMap* data, road grade cannot. Digital elevation models and digital terrain models often rely on available SRTM but given its general granularity of 30 m × 30 m, it remains challenging to accurately estimate road grade on large networks (Gerber and Joubert, 2022; Hugo, 2021). While MATSim is able to handle three-dimensional coordinates for its road network, and has shown to be behaviourally sensitive to road grade (Joubert, 2017), the functionality has not been extended to the emissions contribution.

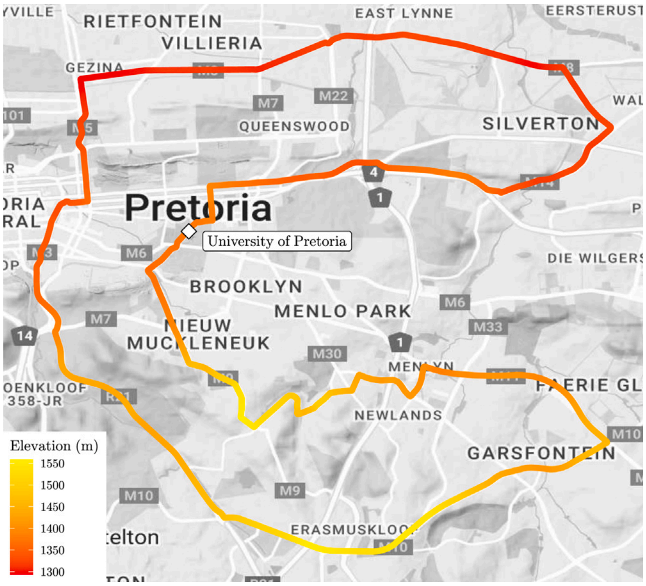


Fig. 1. The C-route (61.7 km) starting and ending at the University of Pretoria's Hatfield campus, approximate location is 28.228°E, 25.752°S.

Given the initial plans as travel demand, containing precise descriptions of the agent's activity chain, the activity locations and durations, the trips connecting two activities, including travel modes and routes, MATSim executes every agent's plan in its queue-based mobility simulation (Gao et al., 2010). Since the model is derived directly from a calibrated trip-based model, no additional calibration is done at this point.

The Gauteng model includes two additional agents, each representing a *probe vehicle* similar to what will be used for the empirical PEMS test. The first is a petrol-powered light passenger vehicle with a Euro-5 emissions classification. The second is a rigid-body, diesel-powered heavy goods vehicle with a Euro-III emissions classification. While all other agents are allowed to reroute and find their own way and route to travel between consecutive activities, the two probe vehicles are assigned a fixed route that coincides exactly with the actual route travelled when conducting the RDE tests with the onboard PEMS equipment. The circular C-shaped test route (Fig. 1) was constructed in a way to be close to 60 km in length and consist of a near-equal share of freeway, urban and suburban road types which should realise the different HBEFA traffic states, namely: "freeflow", "heavy", "saturated" and "stop & go" (Kickhöfer, 2016).

During the mobility simulation, all agents execute their daily plans on the network. Over multiple iterations, all agents except the probe vehicles are allowed to adjust their activity timing and route choice so as to maximise their utility. The co-evolutionary mechanism in MATSim stabilises over a number of iterations. The simulation is set up to perform 50 ensemble runs to account for the inherent variability in the simulation model as agents autonomously adjust their plans.

As agents navigate through the network in the mobility simulation, the event-based infrastructure records every instance when a vehicle enters and leaves a link. Each event notes the vehicle and the time stamp. The travel time and level of congestion is recorded, as is the type of vehicle. This then allows the simulation to look up and report the estimated emissions from the HBEFA database. As a result, the emissions is calculate on a per vehicle per link basis and can be aggregated to any required level.

4. Real Driving Emissions

The literature confirms that PEMS tests are useful for validating traffic emission models. Including all sources of variability absent in most lab tests and enabling the researcher to study a distribution of emissions measured across multiple test trips, the authors of this paper utilise PEMS equipment in their local, South African context. RDE tests are conducted with a PEMS unit to establish a standard against which MATSim's emission estimates for light and heavy vehicles are compared.

4.1. Field test setup

The PEMS unit is mounted on two vehicles from the University of Pretoria (UP)'s fleet. The unit measures instantaneous emissions for various pollutants at a rate of 1 Hz. Multiple trips are conducted with each test vehicle to account for the variability associated with driver behaviour and varying traffic conditions. Each trip conducted follows the same predetermined route that starts and ends at UP's Hatfield campus in Gauteng (Fig. 1). The 61.7 km long C-shaped route includes residential, local, secondary, primary and freeway road sections.

Equipment

The SEMTECH DS+ PEMS unit is mounted according to the same setup as described in the public data set (Joubert and Gräbe, 2022). For the light vehicle, the main analysis and control units are placed on the back seat and connected to the exhaust flow module using a heated line. The following is a concise explanation adapted from Joubert and Gräbe (2022):

> "Spatial data is captured using a Garmin Global Positioning System (GPS) module integrated with the PEMS unit. A weather probe is also integrated into the unit and provides ambient readings… The PEMS unit has an integrated In-vehicle Control Module (ICM) that allows the driver to record event markers (flags) during a field test. The ICM also connects to and records the vehicle's Onboard Diagnostics (OBDII) port while driving…
>
> Exhaust gasses pass through the 4-inch (±100 mm) Exhaust Flow Meter (EFM) tube, responsible for measuring the raw exhaust mass flows…. The EFM operates under Bernoulli's principle using averaging pitot tubes and employing five dual-stage, differential pressure transducers. The gas analyser unit houses the analytical devices for the gaseous measurements of CO, CO_2, NO, and NO_2."

After installation, the unit is calibrated to ensure correct pollutant concentration span. The unit is then

> "…switched over from shore power to its dedicated power source: a 13 V Lithium Iron Phosphate (LiFePO4) battery with a 108 Ah capacity. The purpose of the power source independent of the vehicle's battery is not to place an additional burden on the vehicle's alternator to charge and power the DS+, potentially affecting fuel consumption and emissions.
>
> The (co)driver places a data marker in the field test recording, using the In-vehicle Control Module (ICM) unit, and the driver starts the vehicle".

Passenger car

The test vehicle representing the passenger car vehicle class is a 1.5-litre Ford Figo. The light vehicle has a Euro-5 emissions rating. It takes approximately 90 min to complete one trip along the C-route in typical urban traffic conditions. Three different drivers completed ten field trips each. The thirty field trips were conducted during the period 27 July to 8 September 2021.

Heavy goods vehicle

The test vehicle used for the heavy vehicle class is the RRV – a rigid-body research vehicle based on an Isuzu FTR850 AMT. The heavy goods vehicle has a 7.8-litre, common-rail diesel engine with a Euro-III emissions rating (Isuzu, 2021). The RRV takes approximately 110 min to complete one trip along the C-route in typical urban traffic conditions. The field trips for the RRV were conducted during the period 2 February to 11 March 2021.

5. Results

The PEMS emission data set is publicly available (Joubert, 2022). Elevation data from the Global Positioning System (GPS) unit fitted with the PEMS equipment provides additional insights when plotted together with the cumulative emissions. Fig. 2(a) shows the rate at which the cumulative CO_2 emissions are generated as the test vehicles and their simulated counterparts travel along the C-route. Fig. 2(b) considers a particular part of the test route: the first 10 km along which cold-start emissions would occur. The field test containing such an event is usually (only) the first test of a day.

The purpose of this second graph is to illustrate that the current emission model's omission of cold-start emissions does not drastically affect its ability to predict the cumulative emissions for both vehicle types. HBEFA does not provide any cold-start emissions for heavy vehicle categories; only for cars and light commercial vehicles (LCVs).

The MATSim model shows negligible variance in the emission results from 50 ensemble runs. Hence, these cumulative emissions are only plotted as a single (black) line.

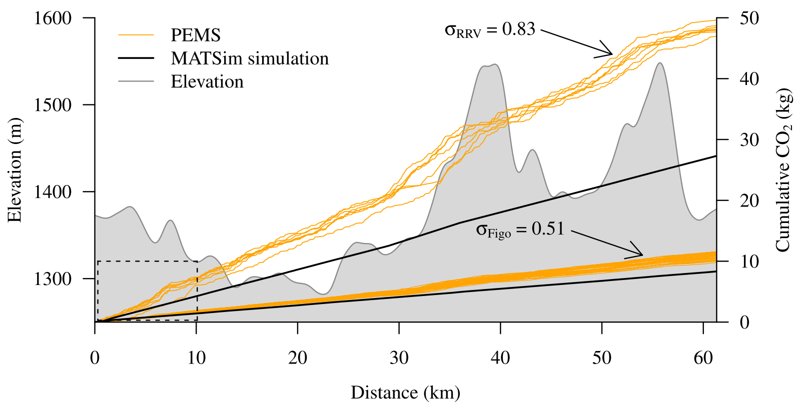
Table 1 contains the mean pollutant totals obtained from the PEMS trips compared to MATSim's estimation. The published OEM data is shown as it compares to the (true) measured and simulated values. Shaded cells indicate the highest of the compared values. The MATSim emission model accounts for 77% and 57% of the greenhouse gas, CO_2, measured by the PEMS test on the 61.7 km long C-route for the light and heavy vehicle, respectively. In fact, the model accurately predicts CO_2 of the Ford Figo within 2% of the value stated by the OEM (132 g/km).

The observed (true) CO emissions are 1.7 times *higher* than the simulation. This raises concern when considering how much the local estimations of this odourless, colourless and poisonous gas (CO) might be off on a regional scale.

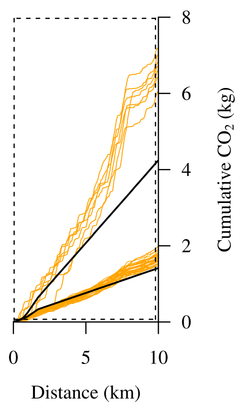
In all but one case, OEM data severely underestimates RDE for both vehicle types. This is consistent with the findings from O'Driscoll et al. (2016) and Chossière et al. (2017). The task at hand remains to investigate *where* and *why* the simulation could be over- or underestimating the true emissions measured by PEMS.

5.1. Travel time

Both Fourie (2010) and Gao et al. (2010) show that agent-based models derived from trip-based models provide more accurate travel time distributions. What we do not know is how well these distribution comparisons would fare when performing trip-by-trip comparisons. Fig. 3 shows the variation in travel times between the different drivers, vehicle types and between the simulated trips and the field test trips. Part of the differences in the total pollutants can certainly be attributed to the difference in travel time. But even so, averaging travel times and traffic conditions still fails to capture the large variation that is evident in real driving emissions.



(a) Elevation profile with the heavy and light vehicle's cumulative CO_2 emissions.



(b) Emissions along the first 10km of the test route.

Fig. 2. Cumulative CO_2 emissions along the C-route.

Table 1
C-route emissions comparison between the Ford Figo and RRV's PEMS trip data, their simulated counterparts in MATSim and the applicable OEM emissions data as reference (see Ford (2020), Isuzu (2021), DieselNet (2021) and Joubert and Gräbe (2022)).

Vehicle	Pollutant (g)				
	CO	CO_2	NO	NO_2	NO_x
Light vehicle					
PEMS: Ford Figo	41.2	10 824	5.8	0.1	5.9
MATSim	24.7	8 324	0.5	0.0	0.5
OEM data[a]	≤61.9	8 171	–	–	≤3.71
Heavy vehicle					
PEMS: RRV	120.8	48 191	403.4	17.6	421.0
MATSim	71.8	27 308	0.5	10.9	11.4
OEM data[a]	≤58.81	18 570	–	–	≤48.28

[a]Based on the per-km emission rates and Euro emission standards as published by Ford (2020) and Isuzu (2021). DieselNet (2021) is used as reference for emission standards. The Ford Figo falls under the category *M* (passenger car) and the RRV, weighing ± 10 740 kg (Joubert and Gräbe, 2022), is classified as an *N2*-category vehicle, having a total mass of between 3.5 and 12 tonnes.

5.2. Cold-start events

The authors found outlier trip data in some of the cumulative emission plots. An initial portion of these outlier trips' data contain "cold-start" emissions. Cold-start emissions occur when the engine functions below its normal operating temperature. After driving the vehicle for some time, the engine coolant temperature increases and stabilises at the normal operating temperature (usually at or above 70 °C). In the PEMS tests, only the first trip of a given day exhibits cold-start emissions.

HBEFA does not provide any cold-start emission factors for vehicle categories other than passenger cars and light commercial vehicles (LCVs), resulting in the current model not being able to account for these emissions of Heavy Goods Vehicles (HGVs). This may cause inaccuracies in the estimated cumulative emissions during the initial portion (about five minutes) of the C-route trip. The exact extent of these inaccuracies remains unknown.

One way to overcome the lack of cold start emission factors for HGVs is to impute the missing data. A recent study by Gable et al. (2022) simulates emissions for different HGV sizes. To do this, MATSim would require additional detail about the vehicle's Euro class to ensure the correct HBEFA lookup but this level of detail was beyond their scope. To deal with the missing (average) cold emission factors for heavy vehicles, Gable et al. (2022) reconstruct an existing HBEFA database to implement their use case in MATSim's `freight` contribution.

5.3. Road type comparison

Road grade and traffic conditions affect the engine's RPM at different speeds and idle and moving time over various sections along the route. This causes fluctuating demand on the engine, which results in different instantaneous mass emission rates. Three

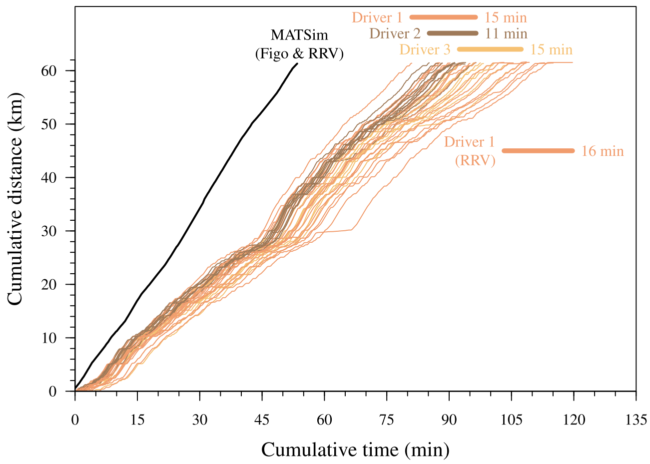
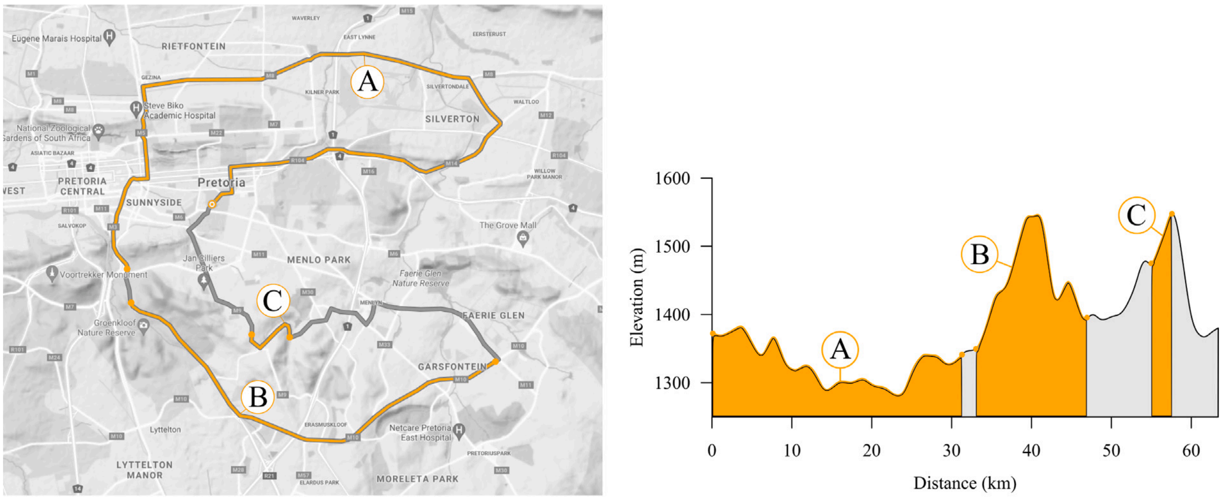


Fig. 3. Space–time diagram showing the difference between simulated and actual trip times. The horizontal bars indicate, for the different vehicle types and drivers, the time span across different field test trips. The variation over the different simulation runs in the ensemble was negligible.



(a) Road sections on map

(b) Road section elevation

Fig. 4. Different road sections used for pollutant comparison per vehicle type, where A = *Urban*, B = *Freeway* and C = *Steep (suburban)*.

road sections on the C-route are used to compare the total emissions generated between different road types (Fig. 4): ***urban***, located around the city centre, ***freeway***, with allowed speeds of 80–120 km/h and ***steep*** (suburban) sections, with lower speeds in "stop & go" traffic conditions. The purpose of this comparison is to show, irrespective of the cumulative emissions over the entire C-route, where RDE exceed the simulated emissions generated on different road types.

Table 2 shows the calculated proportion of pollutant emissions accounted for by MATSim's emission model. This emphasises the *factor* by which the simulation underestimates the actual emissions measured on the specific road section of the C-route. For example, when MATSim underestimates the light vehicle's CO_2 emissions on the urban road section, Table 2 indicates that the simulation only accounts for *0.75* (or 75%) of the observed (true) emissions.

Most notably is the underestimation of emissions on steep road sections, but more so, the drastic underestimation of NO_x pollutants. The simulation rarely captures more than 20% of the true emissions on steep sections and specifically for NO_x, rarely above 5%.

"Stop & go" traffic conditions increase the number of acceleration events, causing peaks in NO_x emissions. These emissions vary non-linearly with speed, making them hard to capture accurately. While MATSim deals much better with short road sections than its trip-based counterparts, it still underestimates quite dramatically. This is in line with Frey et al. (2003) who note that emission models have limited ability to estimate short-term variation in pollutant emissions.

Table 2
The proportion of PEMS emissions accounted for by MATSim on different road sections of the C-route.

Pollutant	Road type	Light vehicle		Heavy vehicle	
		PEMS emissions (g)	MATSim proportion	PEMS emissions (g)	MATSim proportion
CO_2	Urban	5500.67	*0.75*	22 789	*0.58*
	Freeway	2175.66	*0.83*	10 393	*0.60*
	Steep	501.29	*0.51*	3235	*0.25*
CO	Urban	18.89	*0.99*	61.97	*0.64*
	Freeway	10.72	*0.34*	16.24	*0.89*
	Steep	2.79	*0.09*	9.31	*0.18*
NO_x	Urban	2.59	*0.16*	201.44	*0.03*
	Freeway	1.48	*0.07*	91.00	*0.03*
	Steep	0.39	*0.0*	28.43	*0.01*

Note: higher proportion values close to 1.0 represents a better estimate.

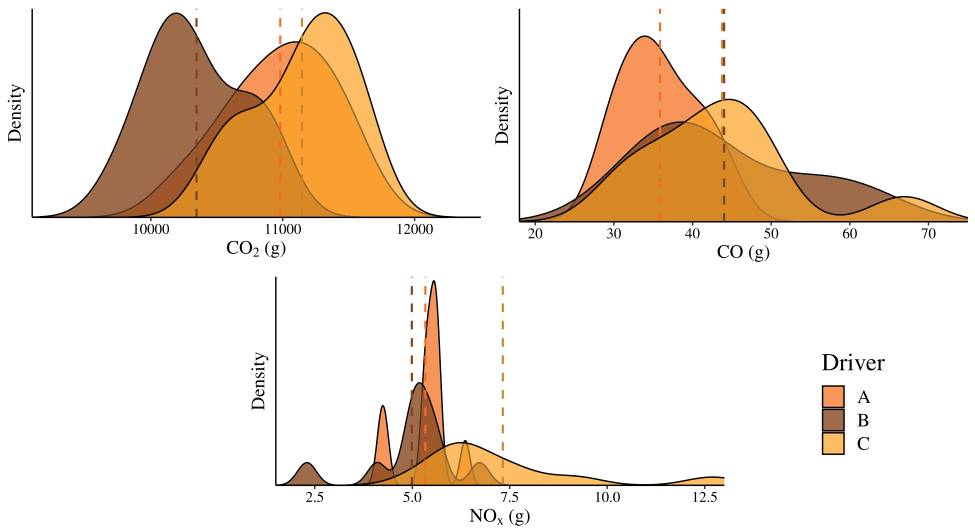


Fig. 5. Empirical probability density functions showing the total pollutants emitted by the Ford Figo, differentiated between drivers. Dashed lines indicate mean values per driver. Absolute density values are omitted and the focus should be on the relative position of the modes and the spread of the distributions.

5.4. Driver comparison

Accelerating, braking, and a vehicle's time spent idling effects fuel consumption and, ultimately, emissions. Indicators like (1) saturation flow, (2) emissions and (3) fuel consumption vary significantly between different drivers. Experienced drivers, for example, exhibit high saturation flow, meaning their braking and acceleration are gradual without abrupt stops or jolting pull-aways. This has a similar effect on the trailing vehicles, affecting the traffic flow rate. These drivers have lower fuel consumption and emissions than *aggressive* drivers. Zheng et al. (2017) find that *cautious* drivers have the lowest of the three indicators. The difference between claimed and actual emissions data is frequently attributed to driver behaviour.

While the individuality of persons can be uniquely captured in activity- and agent-based models, linking driver behaviour to each individual is outside the scope of this paper. Still, we compare the field trips of the different drivers to gain insight as one possible cause of emission variation. Due to a lack of trip data for the RRV (with only one qualified driver with a heavy vehicle licence), the authors only compare the drivers of the Ford Figo. Fig. 5 shows the smoothed empirical probability density functions for three different pollutants for the three drivers, all having performed ten trips on the C-route (±15 driving hours each). The absolute density values (y-axes) have little interpretable value and are omitted. Instead, the reader's attention is drawn to the position of the mode (peak) and the spread for the different distributions.

By solely examining driver C's emissions, he arguably fits the profile of an *aggressive* driver. This correlates with O'Driscoll et al. (2016) finding that NO_x emissions are delivered in peaks that coincide with acceleration. Meaning that an aggressive driver, frequently accelerating, would display higher NO_x emissions. The large spread of the density distribution underscores this inference. On the contrary, driver B shows low CO_2 and NO_x emissions, allowing one to infer that this would be a *cautious* driver when conducting field tests.

What is notable is not only the difference in mean pollutant values, but also the spread of the distributions. This is more pronounced for CO and NO_x than for CO_2. The results from this investigation also confirm the findings of Zheng et al. (2017). Driver behaviour influences vehicle emissions and is, therefore, an essential factor for future PEMS testing.

5.5. Discussion

The reported results show that state-of-the-art simulation underestimates actual vehicle pollutants. It is worth discussing the limitations of this paper's simulation implementation as these most certainly contribute to the gap. The first data limitation relates to the assumption that the road network is appropriately categorised. The VGI community of *OpenStreetMap* suggests specific tagging guidelines that may vary from one country to the next, and South Africa is one such country with its context-specific suggestions.[1] Two possible problems arise. The first is that volunteers are unaware of the guidelines or do not abide by the recommendations, resulting in erroneously tagged road segments. The second and more general problem is that the mapping from *OpenStreetMap* to HBEFA road types is not coherent. For example, some roads tagged as secondary in *OpenStreetMap* may be considered urban in HBEFA. In contrast, other secondary roads should be rural, especially in large multi-metropolitan areas like Gauteng where road ownership can be municipal, provincial or national. Improper road classification can result in erroneous emissions factors used in the simulation.

The second data limitation in the current simulation implementation is the lack of road grade. In line with Wyatt et al. (2014), this most certainly contributes to the gap between predicted and actual driving emissions. The MATSim simulation can deal with elevation in its road network, and MATSim can also cater for arbitrary attributes for each link, of which road grade might be one such attribute. The HBEFA database does contain emission factors for different road grades. But as noted in the review section, Gerber and Joubert (2022) show that inferring road grade from elevation data is not quite as simple and remains a topic for future work. Once that hurdle is overcome, the coupling of the two models must be actioned to allow for the road grade to influence emission factors.

This section should also briefly discuss two methodological discrepancies. The first relates to the traffic dynamics that contribute to the congestion state. The travel demand for MATSim represents the morning peak, and the simulated probe vehicles departed on their C-route trips at approximately 07:00. The PEMS field tests, however, only saw the first trip on any particular day starting at around 07:30 after completing all the calibration sequences. On a good day, the team conducted three trips, with the other two occurring throughout the day. We acknowledge that a day's second and third trips were not during the morning peak as was the case for their simulated counterparts. But because the trips occurred outside peak traffic, they were less likely to be affected by heavy congestion, resulting in lower actual emissions than what would have been the case during more congested traffic conditions. Consequently, it would render the reported results on the conservative side, and the gap may even be more extensive.

The second methodological issue relates to the number of drivers and the total number of field tests. This paper did not embark on defining individual driver behaviour through an explanatory model. Instead, the authors aimed to, as a minimum, account for the accepted phenomenon that driver behaviour contributes to emission variation. Still, the field tests' total distance was approximately 2 345 km, which compares favourably to the 3 790 km of Frey et al. (2003) and 206 km of Wyatt et al. (2014).

The presented simulated results may tempt the reader to conclude that disaggregate, agent-based simulations are inaccurate to the point of being untrustworthy; that would be wrong. Decision-makers desperately need macro-scale models to evaluate city or region-wide interventions' intended and potential unintended environmental consequences.

The proposed agent-based approach allows researchers to avoid the ecological fallacy that arises when decision-makers erroneously make policy choices for, say, a low-emission zone at the neighbourhood level when the decision-support relies on the inference that originates at the city or regional level. An activity-based simulation lets you model at the vehicle level and allows decision-makers to align their analyses and decisions to the same neighbourhood level. The individualistic nature of the model allows one to assign vehicle-specific attributes like the emissions concept. But here, we acknowledge that one can indeed commit the ecological fallacy. Individual vehicles received their emissions concept based on the probability distribution derived from Joubert and Gräbe (2021), which, in turn, used the national second-hand car market as a proxy for the overall fleet structure. Committing this fallacy does not affect any inference in this paper because the authors only compare two specific vehicles for which the emissions concept is known.

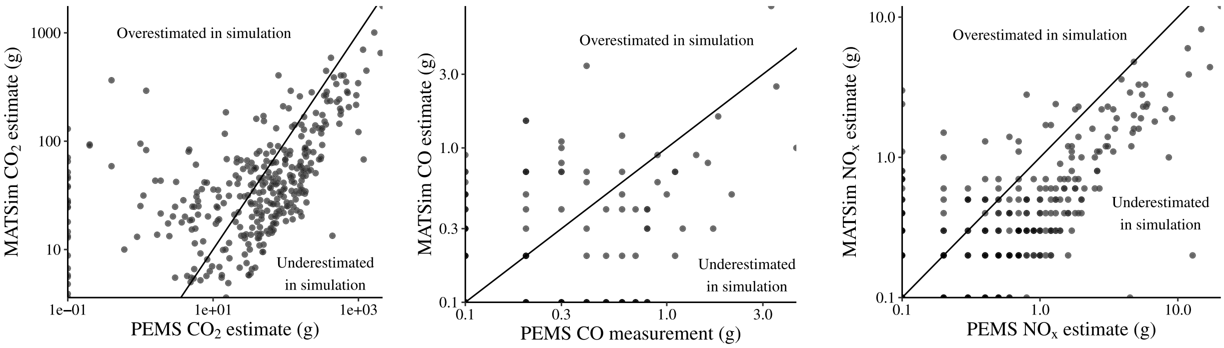
The granularity of activity-based and, in particular, agent-based emissions is a significant advantage, and it holds much benefit over aggregate, trip-based approaches. Whereas trip-based models assume a vehicle is simultaneously present across its entire trip, the spatiotemporal nature of MATSim allows the researchers to analyse the emission impact at the street, neighbourhood, or city level.

6. Conclusion

We rely on macro-scale transport models to evaluate the environmental impact of interventions like changes in vehicle technology and access restrictions for certain vehicle types. Discrepancies between emission models and real driving emissions have been studied at the micro-level. But the impact that model simplifications and model-coupling have at macro-level has, to our knowledge, not received much attention.

The activity-based MATSim model, coupled with HBEFA emission factors, is compared with empirical PEMS tests at a city scale. Compared to CO_2 emissions claimed by OEMs, MATSim does not do too badly as it is able to capture traffic dynamics more accurately. This is in line with literature where CO and NO_x are not predicted as accurately. Accurate PEMS measurements reveal that on specific road types, like steeper sections of the route, the simulation can underestimate NO_x by a factor of 100 for heavy

[1] https://wiki.openstreetmap.org/wiki/South_African_Tagging_Guidelines.



(a) CO_2 (b) CO (c) NO_x

Fig. 6. Individual link emissions estimated by MATSim compared to measured values from PEMS tests for the RRV.

vehicles. Granted, heavy vehicles do make up a smaller proportion of the road users, but their contribution to absolute NO_x is a factor of 60–100 higher than light vehicles.

Quantifying this gap between macro-level simulation and reality presents researchers with a starting point to improve the state of traffic emissions modelling. The authors provide the following topics for future work that aim to improve the current state of emission simulation. If one can compensate for the known variance in a simulation model, possible discrepancies can be anticipated and mitigated to produce emission models that accurately capture RDE.

6.1. Future work

Firstly, Wyatt et al. (2014) note that failing to account for road grade could potentially result in highly inaccurate estimates of real-world emissions, especially when performing micro-scale emissions modelling. This was confirmed in this paper. The emission factors extracted from HBEFA can be configured to compensate for road grade. Recent contributions (Hugo, 2021; Gerber and Joubert, 2022) reveal the complexity in accurately estimating road grade, especially in developing countries where a lack of detailed road network data persists. Also, elevation can be accommodated in MATSim's road network. Whether elevation can be accounted for in other aggregated macro-level models is less certain. What remains is to integrate the capabilities of both the transport and emissions models to account for road grade.

Secondly, data availability of detailed fleet compositions remain a challenge. The synthetic vehicle population of Gauteng's MATSim model provides detailed emission profiles for passenger cars only. The HGVs in the current paper's population are not modelled with distinct fuel types and emission concepts and therefore emission calculations reverts to averaged values. Applying the same refinement to the heavy vehicles as was done for light vehicles in the synthetic population would provide a more accurate estimation of emissions generation on a regional scale.

Thirdly, rigorous calibration procedures need to be developed. Calibrating against total emissions may yield temporary satisfaction to the modeller, but often at the expense of the spatial and temporal granularity that activity-based models allow. Fig. 6 provides a starting point.

Each point represents a single link in MATSim's C-route network. The point's y-value depicts the simulated emissions for a pollutant and the point's x-value the actual emissions measured during a single trip on that link. The variance can be analysed at a much more disaggregate level, opening the door for validation that goes beyond traffic counts or travel time distributions.

The goal of calibration should not be to merely get the numbers right by adjusting some abstract intermediary. It is essential that the calibration is behaviourally sound. And here, agent-based models again have a significant advantage. Since individuals are modelled, the calibration could aim to capture and use a latent variable at the individual like *driver behaviour*.

CRediT authorship contribution statement

Ruan J. Gräbe: Formal analysis, Validation, Visualisation, Investigation, Data curation, Writing – original draft. **Johan W. Joubert:** Conceptualisation, Funding acquisition, Methodology, Software, Supervision, Investigation, Resources, Data curation, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The data used in the paper was already published in a Data in Brief article (2022).

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References

Agarwal, A., Kickhöfer, B., 2015. Agent-based simultaneous optimization of congestion and air pollution: A real-world case study. Proc. Comput. Sci. 52, 914–919. http://dx.doi.org/10.1016/j.procs.2015.05.165.

Bang, H.Q., Khue, V.H.N., Tam, N.T., Lasko, K., 2017. Air pollution emission inventory and air quality modeling for can tho City, Mekong Delta, Vietnam. Air Qual. Atmos. Health 11 (1), 35–47. http://dx.doi.org/10.1007/s11869-017-0512-x.

Chossière, G.P., Malina, R., Ashok, A., Dedoussi, I.C., Eastham, S.D., Speth, R.L., Barrett, S.R., 2017. Public health impacts of excess NOx emissions from volkswagen diesel passenger vehicles in Germany. Environ. Res. Lett. 12 (3), 034014. http://dx.doi.org/10.1088/1748-9326/aa5987.

Dey, S., Caulfield, B., Ghosh, B., 2019. Modelling uncertainty of vehicular emissions inventory: A case study of Ireland. J. Cleaner Prod. 213, 1115–1126. http://dx.doi.org/10.1016/j.jclepro.2018.12.125.

DieselNet, 2021. Emission standards - EU: Cars and light trucks. URL https://dieselnet.com/standards/eu/ld.php [Accessed: 2021-11-17].

ERMES, 2021. European research on mobile emission sources. URL https://www.ermes-group.eu/web/leading_EU_models [Accessed: 2021-03-03].

Falcão, E.A.M., Teixeira, A.C.R., Sodré, J.R., 2017. Analysis of CO2 emissions and techno-economic feasibility of an electric commercial vehicle. Appl. Energy 193, 297–307. http://dx.doi.org/10.1016/j.apenergy.2017.02.050.

Feng, Y., Chen, S., Zhang, L., 2013. System dynamics modeling for urban energy consumption and CO2 emissions: A case study of Beijing, China. Ecol. Model. 252, 44–52. http://dx.doi.org/10.1016/j.ecolmodel.2012.09.008, Ecological Modelling for Global Change and Coupled Human and Natural Systems.

Ford, 2020. Ford - model details. URL https://www.ford.co.za/cars/new-figo-2018/models/1-5-trend-mt-hatch/ [Accessed: 2021-11-17].

Fourie, P.J., 2010. Agent-based transport simulation versus equilibrium assignment for private vehicle traffic in gauteng. In: 29th Annual Southern African Transport Conference Proceedings. pp. 11–22.

Frey, H.C., Unal, A., Rouphail, N.M., Colyar, J.D., 2003. On-road measurement of vehicle tailpipe emissions using a portable instrument. J. Air Waste Manage. Assoc. 53 (8), 992–1002. http://dx.doi.org/10.1080/10473289.2003.10466245.

Gable, T., Martins-Turner, K., Nagel, K., 2022. Enhanced emission calculation for freight transport. Procedia Comput. Sci. 201, 601–607. http://dx.doi.org/10.1016/j.procs.2022.03.078, The 13th International Conference on Ambient Systems, Networks and Technologies (ANT) / The 5th International Conference on Emerging Data and Industry 4.0 (EDI40).

Gao, W., Balmer, M., Miller, E.J., 2010. Comparison of MATSim and EMME/2 on greater toronto and Hamilton area network, Canada. Transp. Res. Rec. 2197 (1), 118–128. http://dx.doi.org/10.3141/2197-14.

Gerber, J.-M., Joubert, J.W., 2022. Impact of road grade on the risk profile of driver behavior. Transp. Res. Rec. http://dx.doi.org/10.1177/03611981221089939, (forthcoming).

Gräbe, R.J., Joubert, J.W., 2021. Behavioural sensitivity towards emission concepts. Procedia Comput. Sci. 184, 734–738. http://dx.doi.org/10.1016/j.procs.2021.03.091.

Gurram, S., Stuart, A.L., Pinjari, A.R., 2019. Agent-based modeling to estimate exposures to urban air pollution from transportation: Exposure disparities and impacts of high-resolution data. Comput. Environ. Urban Syst. 75, 22–34. http://dx.doi.org/10.1016/j.compenvurbsys.2019.01.002.

Hugo, J.-M., 2021. Appending GPS Traces with Road Grade Data to Estimate Driver Behaviour Risk (Master's thesis). University of Pretoria.

Hülsmann, F., Gerike, R., Kickhöfer, B., Nagel, K., Luz, R., 2011. Towards a multi-agent based modeling approach for air pollutants in urban regions. In: Kolloquium Luftqualität an Straß En 2011: Tagungsbeiträge Vom 30. Und 31. März 2011, Bergisch Gladbach. GSV Verlag GmbH, ISBN: 978-3-941790-77-3, pp. 144–166, URL https://doi.org/10.14279/depositonce-9312.

Isuzu, 2021. Heavy commercial truck. Available at: https://isuzu.co.za/heavy-truck [Accessed: 2021-07-21].

Ježek, I., Blond, N., Skupinski, G., Močnik, G., 2018. The traffic emission-dispersion model for a Central-European city agrees with measured black carbon apportioned to traffic. Atmos. Environ. 184, 177–190. http://dx.doi.org/10.1016/j.atmosenv.2018.04.028.

Joubert, J.W., 2017. Multi-agent model of route choice when vehicles are sensitive to road grade. In: The 6th International Workshop on Agent-Based Mobility, Traffic and Transportation Models, Methodologies and Applications (ABMTrans 2017). In: Procedia Computer Science, vol. 109C, pp. 869–874. http://dx.doi.org/10.1016/j.procs.2017.05.402.

Joubert, J.W., 2022. Real driving emissions data: University of Pretoria. In: Mendeley Data, V4. http://dx.doi.org/10.17632/Y9PJTT5NGC.4.

Joubert, J.W., Gräbe, R.J., 2021. A South African scenario for emissions modelling. Procedia Comput. Sci. 184, 739–744. http://dx.doi.org/10.1016/j.procs.2021.03.092.

Joubert, J.W., Gräbe, R.J., 2022. Real driving emissions: Isuzu FTR850 AMT. Data Brief 41, 107975. http://dx.doi.org/10.1016/j.dib.2022.107975.

Kaddoura, I., Ewert, R., Martins-Turner, K., 2021. Exhaust and non-exhaust emissions from today's and future road transport: A simulation-based quantification for Berlin. Available online at https://svn.vsp.tu-berlin.de/repos/public-svn/publications/vspwp/2021/.

Kahle, D., Wickham, H., 2013. Ggmap: Spatial visualization with ggplot2. R J. 5 (1), 144–161. http://dx.doi.org/10.32614/RJ-2013-014.

Kickhöfer, B., 2016. Emission modeling. In: The Multi-Agent Transport Simulation MATSim. Ubiquity Press, pp. 247–252. http://dx.doi.org/10.5334/baw.36.

Kickhöfer, B., Agarwal, A., Nagel, K., 2018. Mind the price gap: How optimal emission pricing relates to the EU CO2 reduction targets. Int. J. Sustain. Transp. 13 (5), 378–391. http://dx.doi.org/10.1080/15568318.2018.1472321.

Li, J., Rombaut, E., Vanhaverbeke, L., 2021. A systematic review of agent-based models for autonomous vehicles in urban mobility and logistics: Possibilities for integrated simulation models. Comput. Environ. Urban Syst. 89, 101686. http://dx.doi.org/10.1016/j.compenvurbsys.2021.101686.

Linton, C., Grant-Muller, S., Gale, W.F., 2015. Approaches and techniques for modelling CO2 emissions from road transport. Transp. Rev. 35 (4), 533–553. http://dx.doi.org/10.1080/01441647.2015.1030004.

López-Martínez, J.M., Jiménez, F., Páez-Ayuso, F.J., Flores-Holgado, M.N., Arenas, A.N., Arenas-Ramirez, B., Aparicio-Izquierdo, F., 2017. Modelling the fuel consumption and pollutant emissions of the urban bus fleet of the city of madrid. Transp. Res. D 52, 112–127. http://dx.doi.org/10.1016/j.trd.2017.02.016.

Loulou, R., Labriet, M., 2007. ETSAP-TIAM: the TIMES integrated assessment model Part I: Model structure. Comput. Manag. Sci. 5 (1–2), 7–40. http://dx.doi.org/10.1007/s10287-007-0046-z.

Lozhkina, O.V., Lozhkin, V.N., 2015. Estimation of road transport related air pollution in Saint Petersburg using European and Russian calculation models. Transp. Res. D 36, 178–189. http://dx.doi.org/10.1016/j.trd.2015.02.013.

Macal, C.M., 2016. Everything you need to know about agent-based modelling and simulation. J. Simul. 10 (2), 144–156. http://dx.doi.org/10.1057/jos.2016.7.

McNally, M.G., 2007. The four-step model. In: Handbook of Transport Modelling. Emerald Group Publishing Limited.

Nocera, S., Basso, M., Cavallaro, F., 2017. Micro and Macro modelling approaches for the evaluation of the carbon impacts of transportation. Transp. Res. Proc. 24, 146–154. http://dx.doi.org/10.1016/j.trpro.2017.05.080.

Nocera, S., Ruiz-Alarcón-Quintero, C., Cavallaro, F., 2018. Assessing carbon emissions from road transport through traffic flow estimators. Transp. Res. C 95, 125–148. http://dx.doi.org/10.1016/j.trc.2018.07.020.

O'Driscoll, R., ApSimon, H.M., Oxley, T., Molden, N., Stettler, M.E.J., Thiyagarajah, A., 2016. A portable emissions measurement system (PEMS) study of NOx and primary NO2 emissions from Euro 6 diesel passenger cars and comparison with COPERT emission factors. Atmos. Environ. 145, 81–91. http://dx.doi.org/10.1016/j.atmosenv.2016.09.021.

Pukhova, A., Moreno, A.T., Llorca, C., Huang, W.-C., Moeckel, R., 2021. Agent-based simulation of long-distance travel: Strategies to reduce CO2 emissions from passenger aviation. Urban Plan. 6 (2), 271–284. http://dx.doi.org/10.17645/up.v6i2.4021.

R Core Team, 2020. R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria, URL https://www.R-project.org/.

RAC, 2020. Euro 1 to Euro 6 guide – find out your vehicle's emissions standard. Available at: https://www.rac.co.uk/drive/advice/emissions/euro-emissions-standards/, Accessed: 2021-11-17.

Rasouli, S., Timmermans, H., 2013. Activity-based models of travel demand: promises, progress and prospects. Int. J. Urban Sci. 18 (1), 31–60. http://dx.doi.org/10.1080/12265934.2013.835118.

Robinson, A., Venter, C., 2019. Validating traffic models using large-scale Automatic Number Plate Recognition (ANPR) data. J. South Afr. Inst. Civ. Eng. 61 (3), 45–57. http://dx.doi.org/10.17159/2309-8775/2019/v61n3a5.

Rushton, C., Galatioto, F., Wright, J., Nielsen, E., Tsotskas, C., 2018. City-wide emissions modelling using fleet probe vehicles. IET Intell. Transp. Syst. 12 (9), 1181–1188. http://dx.doi.org/10.1049/iet-its.2018.5217.

Wickham, H., 2016. Ggplot2: Elegant Graphics for Data Analysis. Springer-Verlag New York, URL https://ggplot2.tidyverse.org.

World Economic Forum, 2020a. London's air quality has dramatically improved since 2016. Here's how the UK capital did it. Available at: https://www.weforum.org/videos/ [Accessed: 2021-04-08].

World Economic Forum, 2020b. The Mayor's ultra low emission zone for London. Available at: https://www.weforum.org/videos/ [Accessed: 2021-04-08].

Wyatt, D.W., Li, H., Tate, J.E., 2014. The impact of road grade on carbon dioxide (CO2) emission of a passenger vehicle in real-world driving. Transp. Res. D 32, 160–170. http://dx.doi.org/10.1016/j.trd.2014.07.015.

Zheng, F., Li, J., van Zuylen, H., Lu, C., 2017. Influence of driver characteristics on emissions and fuel consumption. Transp. Res. Proc. 27, 624–631. http://dx.doi.org/10.1016/j.trpro.2017.12.142.