Emissions in Gauteng

Ruan Johannes Gräbe

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Abstract

Title:	Emissions in Gauteng
Author:	Ruan J. Gräbe
Student number:	16004486
Supervisor:	Prof Johan W. Joubert
Department:	Industrial and Systems Engineering

Emission reduction interventions assist decision-makers in setting targets for environmental regulations and policies. These are necessary to address the growing concern of air pollution. In the UK alone, £800m have been invested in an air quality programme to meet their net-zero emissions target by 2050 (World Economic Forum, 2020a). We recognise that informed decision-making is vital for capital investment into transport interventions, especially in a developing country like South Africa.

We focus on emissions generation in the Gauteng province to understand how the actual traffic emissions vary from our estimations with the tools at our disposal. The tool we utilise is the Multi Agent Transport Simulation (MATSim) emissions model based on the Handbook Emission Factors for Road Transport (HBEFA). MATSim is a powerful modelling framework that can produce transport simulations of an entire city with a high level of detail (Fourie, 2009; Van Velden, 2012; Zhuge et al., 2014; Ziemke et al., 2019).

The problem we face is that the European-based emissions model does not account for the driving conditions and vehicle types affecting real-world driving emissions on South African road networks. We address the diversity of our local driver population by creating a synthetic population representing the Gauteng vehicle population. MATSim's Agent-Based Model (ABM) enables us to model emission profiles for each vehicle represented as an agent. In the synthetic population, we include passenger cars and heavy vehicle types. We estimate the aggregate CO_2, CO and NO_x emitted on a provincial level and the individual emissions per vehicle type.

We use PEMS equipment to conduct Real Driving Emissions (RDE) tests with which we validate our MATSim emissions model for Gauteng. We conduct these tests for both vehicle types represented in our synthetic population: a passenger car and a heavy vehicle. By comparing the PEMS data to MATSim's estimations on a predetermined test route in Pretoria, we find that the emissions model accounts for $\pm 80\%$ of the CO_2 emissions from these vehicle types. Furthermore, the observed CO emissions are 2.3–2.9 times *higher* than the simulation. MATSim also *underestimates* NO_x emissions for the heavy vehicle type and *overestimates* these pollutant emissions for the light vehicle.

Our investigation of the emissions on the test route reveals that different road types and driving conditions factor into the variance we observe in our local emissions model. MATSim struggles more to estimate the emissions on steep suburban roads than on urban or freeway sections. Regarding driver behaviour, aggressive drivers might cause more carbon and NO_x emissions than conservative drivers. Weather conditions also influence this behaviour, and we heed the notable difference between our warm South African and wet European weather.

We accomplish our research goals of building a representative Gauteng emissions model in MATSim, investigating how this model performs "out-of-the-box" and quantifying the *gap* between our local simulation and the reality of traffic emissions in South Africa.

Keywords: MATSim, RDE, PEMS, emissions model, traffic emissions, agent-based simulation

Contents

List of Figures

List of Tables

Acronyms

ABM	Agent-Based Model
ABS	Agent-Based Simulation
EFM	Exhaust Flow Meter
GPS	Global Positioning System
HBEFA	Handbook Emission Factors for Road Transport
HGV	Heavy Goods Vehicle
ICM	In-vehicle Control Module
LEZ	Low Emission Zone
MATSim	Multi Agent Transport Simulation
NEDC	New European Driving Cycle
NRF	National Research Foundation
OEM	Original Equipment Manufacturer
PEMS	Portable Emissions Measurement System
RDE	Real Driving Emissions
RRV	Road-Rail Vehicle
SANRAL	South African National Road Agency Limited
UP	University of Pretoria
WLTP	Worldwide harmonised Light vehicle Test Procedure

Chapter 1

Introduction

Air pollution is a growing concern for authorities, administrations, and governments worldwide. This environmental issue has the whole world up in arms and eager to make changes and spark innovation, promising a better, greener future.

Criteria pollutants (emissions hazardous to human health) are widely investigated to develop emission reduction interventions. These assist decision-makers in setting targets for environmental regulations and policies like the US Clean Air Act (EPA, 2021b) and the UK's target to reach net zero emissions by 2050 (World Economic Forum, 2020a).

As part of the UK's emission reduction target, the Mayor launched the central London Ultra Low Emission Zone in April 2019 (World Economic Forum, 2020b). The emission reduction intervention was paid for from £800m invested into London's air quality programme since 2016. This figure emphasises the term: *a growing concern.*

1.1 Simulation for informed decision-making

When policymakers investigate projects involving six figures and above, predicting a high success rate with certainty becomes crucial. In their Central-European case study, Ježek et al. (2018) use a verified traffic emissions-dispersion model to evaluate different emission reduction scenarios. They show that removing 10% of the highest polluting vehicles reduces the total black carbon and NO_x emissions from traffic by 39% and 33%, respectively.

In his speech on the transport department's budget vote of 2021/22, South African transport minister Fikile Mbalula announced the 15.6% increase of the public transport network grant for 2023/24 amounting to R6.8 billion (Department of Transport, 2022). Diligent planning for the appropriate applications of these infrastructure and operating grants are paramount to a third-world country with an underperforming economy (based on the forecasted 2% slip in GDP for 2022 (Tech, 2022)).

In South Africa we use simulations for transportation planning and in scenarios like Ježek et al. (2018) to investigate the effect of interventions before implementation. We show how simulated vehicle emissions compare to emissions under actual driving conditions in a South African context. Consequently, we portray the variance in our local simulations, indicating the need for accurate, representative traffic emission models in South Africa.

1.1.1 Research focus

Simulation models provide a means to capture the generation of air pollutants, their atmospheric dispersion and their impact on ambient air quality and the environment. These simulation models are traffic or (road) transport models, emission models, Gaussian or chemistry transport models, and air quality models. The simulation framework utilised for this research, Multi Agent Transport Simulation (MATSim), enables traffic and emissions modelling. Therefore, the research focus is on the generation of traffic pollutants captured by MATSim's modelling framework.

Traffic and emission models require emission factors as input parameters to calculate emissions from particular exhaust chemicals. Country-specific databases contain vehicle emission factors for different vehicle categories. Like the European-based HBEFA (2019), these databases incorporate factors for various driving conditions, hot and cold running and evaporative emissions (Forehead and Huynh, 2018).

Our research has a twofold purpose. Firstly, to investigate and understand the uncertainty and the variance in South Africa's vehicle emissions. How does our vehicle fleet compare to its European counterpart, where the emission factors we use in our simulations originate? Without knowledge of the actual performance of the South African vehicle fleet, we desperately try to improve the state of transport emissions with no measure of success. To this end, we aim to quantify the gap between state of the art emission models and what we experience as "ground truth" in a local context.

Secondly, to provide policymakers with insights that guide decision-making for setting informed and realistic targets that address (among others) some valid concerns in South Africa:

- Even though the country supports reducing greenhouse gasses emitted by the transport sector, South Africa's national Green Transport Strategy has presented no quantitative targets (Department of Transport, 2018).
- Since 2019, the inclusion of carbon tax in the fuel levy promotes the *polluter pays* principle. Getting this pricing wrong would send an incorrect message to vehicle owners, causing unintended consequences and hurting the South African economy and its citizens.
- Encouraging a modal shift to hybrid or electric vehicles is only attainable for the financial elite and not feasible in developing countries. It may potentially worsen the state of economic inequality.
- If freight vehicles are disproportionately taxed, it forces price increases across entire supply chains, adversely affecting the consumer buying off the shelf.

We want to contribute to the transport sector in South Africa to avoid ill-informed policy decisions and unintended consequences on a national level. To set informed and realistic targets, we need to validate our simulation models by acknowledging our local conditions. Therefore, we require a baseline to establish what we will use to validate against – what is our current reality?

1.1.2 Estimating "ground truth"

Modelling and simulation are, in essence, a subjective representation of reality. To guide decision-making and provide valuable insights from simulation, we require a means to validate our models. The best available measure we can use is the ground truth, but how do we estimate this for emission models? What is the "gold standard" against which we measure our representation of emissions generation?

To validate air quality models, a combination of traffic loop sensors and emission calculations can estimate the ground truth for multiple sources of air pollution in their vicinity (Ma et al., 2012). For transport emission models, laboratory tests are the industry standard. However, the Volkswagen "Dieselgate" scandal (Chossière et al., 2017) proved how unreliable these tests could be. Portable Emissions Measurement System (PEMS) tests provide a more accurate validation method for Real Driving Emissions (RDE) (Frey et al., 2003; Hao et al., 2017; Liu et al., 2010; Ropkins et al., 2007). Used alongside RDE test procedures in Europe, these technologies serve to complement lab tests like the latest Worldwide harmonised Light vehicle Test Procedure (WLTP) (ACEA, 2021).

We have at our disposal methods of validating simulation models, but what if these methods are inaccurate? Dey et al. (2019) calculate the variation in damage costs of emissions and gives an example of the consequence of over- or underestimating emission inventories on its relevant applications in Ireland. The cost of "getting it slightly wrong" was €40 million.

With taxpayers' money on the line, a developing country like South Africa, with the world's highest inequality in income distribution, can not afford to "get it slightly wrong" (Statista, 2021). The rising cost of living and volatile political climate in South Africa leaves us, the citizens, desperate for the government to make informed and calculated decisions regarding matters that affect our pockets at month-end.

1.2 Agent-based modelling in South Africa

In a developing country with high economic inequality, extreme socioeconomic and population diversity, the ability to account for diversity in our simulations becomes essential, especially when we want to ask questions like *"who gets the benefit from transport infrastructure and interventions?"* and, equally important, *"who pays for those benefits?"* To accommodate the diversity and inequality present in the South African population, we adopt an agent-based approach for transport emissions modelling. Agent-Based Models (ABMs) prove beneficial to evaluate the impact of (transport) interventions as they are adequately expressive to capture the unique attributes of individuals and the environment (Ziemke et al., 2019).

The MATSim, succeeding TRANSIMS (Barrett et al., 2001), is a powerful activity-based modelling framework that can produce transport simulations of an entire city with a high level of detail (Fourie, 2009; Van Velden, 2012; Zhuge et al., 2014; Ziemke et al., 2019). As we later show, the aggregate effect of individual vehicle emissions can be studied on a regional scale.

The problem faced in South Africa is that the emission models rely on emission factors from the Handbook Emission Factors for Road Transport (HBEFA) – the widely accepted state of knowledge for RDE in Europe (Matthias et al., 2020). These emission factors are calculated from RDE under specific European conditions.

When we conduct PEMS field tests in the Gauteng province of South Africa, we drive at an elevation between 1300–1750m above sea level, compared to Germany, Switzerland, Austria and Sweden, most located well below 1000m (Switzerland being the exception at 1350m). These are the countries where the applicable emission models are mainly used (ERMES, 2021).

In terms of physical factors, a passenger car in the European Union (EU) ages, on average, 11.5 years (ACEA, 2019) compared to 9.5 years in South Africa (Venter, 2017). The average South African passenger car is 5% lighter and has an engine-rated power of 7% more than its European counterpart. The combined effect on emissions generation would imply that the South African fleet produces around 1–2% more emissions than the European fleet. Posada (2018) indicates that this is not the case, as the published

CO_2 emissions (in g/km) from the South African fleet is, on average, 22% more than the European fleet.

Potential reasons for the misalignment of fleet emissions could be vehicle technology (the European market avails more fuel-efficient technologies for the average new vehicle than the South African market), elevation, road conditions or driving behaviour. This begs the question:

> *can we rely on our (European-based) emission models to produce useful results when compared to our (South African) PEMS validation tests?*

Well, no. Given the multiple factors influencing our vehicle fleet profiles, we (wrongly) play the simulation game on two completely different fields. Therefore, we expect variance in our local emission models.

Consequently, from our research focus, we can formulate specific research goals to address this variance:

1. Build a traffic emissions model for Gauteng in MATSim's Agent-Based Simulation (ABS) framework.

2. Investigate how good this European-based model performs "out-of-the-box" in a local context.

3. Quantify the *gap* between the Gauteng emissions model and ground truth in South Africa to use this model effectively.

1.3 Research design

We develop an ABS model in MATSim, reflecting the reality of a vehicle population with diverse emission profiles. These profiles reflect the latest specifications as contained in HBEFA version 4.1. We couple the ABS model with the daily activities of the Gauteng province's driver population and, using sampled vehicle statistics, produce a representative estimation of the pollutants generated on a regional scale.

Subsequently, we narrow our focus to the individual vehicle class. We investigate the variance in the emissions from heavy and light vehicles generated by our ABS compared to RDE from PEMS trip data. This RDE data serves to validate our agent-based emissions model of Gauteng.

1.4 Document structure

HBEFA includes emission factors for multiple vehicle categories of all regulated and significant non-regulated pollutants (ERMES, 2021). These emission factors are included in an extension of the MATSim framework – a code contribution that enables emissions modelling in the agent-based framework (Hülsmann et al., 2011). We discuss the various approaches for emissions modelling and, to this end, our choice of MATSim's agent-based framework in chapter 2.

Chapter 3 sets the stage for agent-based emissions modelling in South Africa. Here we discuss our research methodology and the steps towards a representative MATSim emissions model for the Gauteng province, addressing our first research goal.

The data we obtain from our PEMS field tests quantify RDE in South Africa. We present our findings in chapter 4 and discuss the variance in our ABM compared to the PEMS test data. This fulfills our second and third research goals.

We evaluate our research goals in chapter 5 and discuss the topics that present potential future work for South African emissions modelling in MATSim.

Chapter 2

Literature review

The many vehicles and traffic situations involved on a road network make real-world emission measurements impractical (Smit et al., 2010). Measurement is also impossible when we consider hypothetical scenarios for transport interventions. Traffic emission models can offer a practical alternative to real-world measurements (Grote et al., 2016).

The need for simulating traffic emissions stems from the environmental and health impacts of air pollution. Among other use cases for risk assessment (El-Fadel, 2002; Qiu and Li, 2015; Wismans et al., 2011), emissions modelling is particularly useful for evaluating emission reduction scenarios like introducing a Low Emission Zone (LEZ).

This intervention aims to reduce vehicle emissions, improving the local air quality in a given geographical area. Air quality and dispersion models can indicate the associated health risk and spread of traffic pollution. However, these models require as crucial input spatially and temporally resolved emissions from the relevant sources (Matthias et al., 2020).

Therefore, as enabling factors for future air quality estimation, we focus in the subsequent sections on the *generation* of emissions simulated by *traffic and emission models*. We also discuss our modelling framework of choice and means of validation from Real Driving Emissions (RDE) tests with a Portable Emissions Measurement System (PEMS).

2.1 Elements of road traffic emissions

There are different sources of emissions, grouped in four categories: point (factories and power plants – stationary), biogenic (livestock), area, and mobile (dynamic) (EPA, 2021a). We classify *traffic emissions* as a mobile source of air pollution. Traffic emission models capture the *generation* of criteria pollutants that provide emission estimates at high spatial and temporal resolution (Forehead and Huynh, 2018). Additional sources of traffic emissions like evaporative and non-exhaust vehicle-wear emissions are also included in updated emission inventories required by emission models (EEA, 2021).

Transport modelling and calculation of the related fuel consumption and emissions form the basis of quantifying emissions from mobility (Nocera et al., 2018). Nocera et al. (2017) discuss the main characteristics and link between the two-step process of simulating emissions: combining the traffic and emissions model. In the following section, we discuss the different types of traffic and emission models and highlight the reason for our choice in the South African context, where we apply our case study.

2.1.1 Traffic models

Traffic assignment is the first step in transport modelling, enabling the study of various externalities. Traffic models capture this step that allows researchers and practitioners to analyse the effects of congestion, traffic safety, global warming, air pollution and noise pollution (Wismans et al., 2011). We distinguish between static and dynamic traffic models.

The four-step model

The traditional four-step model (like VISUM, (Fellendorf et al., 2000)) is a static model that relies on the spatial distribution of a population. It calculates average traffic volumes in different areas of a network. Contrary to (microscopic) Agent-Based Models (ABMs), modelling an individual on a network, the unit of measure in four-step models is the number of trips emanating from particular zones (Rasouli and Timmermans, 2013). The four-step model comprises *(i) trip generation, (ii) trip distribution, (iii) modal split* and *(iv) traffic assignment*. These models offer a macroscopic traffic description, but the static description is useful on large spatial scales (Shorshani et al., 2015).

Policy questions often only require aggregate estimates on a system level to understand the impact of changes and interventions (Linton et al., 2015). This explains why we see, especially in our local context, the four-step model overused in the industry where practitioners are slow to adopt state-of-the-art practices and instead opt for the "tried and tested" methods that (still) fail on multiple fronts.

Rasouli and Timmermans (2013) discuss the initial promises of activity-based models – an alternative to the traditional four-step model. They summarise the progress made over two decades and identify unsolved issues requiring further research. A few shortfalls were identified in the four-step model that fueled the development and use of activity-based (microscopic) 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.

Rasouli and Timmermans (2013)'s review provides compelling evidence that suggests dynamic traffic models better address the issues inherent to the traditional four-step model. We discuss the underlying principles of these models on different spatial scales.

Dynamic models

Macroscopic dynamic modelling approaches like system dynamics, techno-economic models and integrated assessment models allow planning on larger spatial and temporal scales than microscopic approaches. These models use an aggregate representation of vehicles and assume continuous traffic flow based on *homogenous vehicle behaviour*, thus limiting their ability to predict congestion (Shorshani et al., 2015).

Macroscopic models require three main parameters for implementation: the fundamental traffic flow diagram, OD matrices and traffic control devices. The simulation model produces as output time-dependent traffic densities for each segment on the road network and traffic flows on these segments (Shorshani et al., 2015).

- *System dynamics modelling (SDM)*, positioned between small-scale microsimulations and large-scale techno-economic models, rely on causal loop diagrams (CLDs) to explore qualitative relationships between different system aspects. They also include quantitative techniques and analysis, making them highly versatile tools (Pfaffenbichler et al., 2010). An advantage of this approach lies in its ability to capture multiple stakeholder dynamics and policy outcomes from complex systems (Linton et al., 2015).

- *Techno-economic models* use the occurrence of socio-economic changes in a top-down approach to capture large-scale dynamics of the transport system. These models estimate travel demand by drawing on socio-economic characteristics and forecast changes (Linton et al., 2015).

- *Integrated assessment models (IAMs)* model the interactions between the economy and environment on a macro scale. It includes a sub-module for transport as a component of economic activity. Similar to techno-economic models in terms of scale and scope, IAMs further explore economic-related changes in the environment (Linton et al., 2015).

Microscopic models take into account the time-space behaviour of individual vehicles, influenced by interactions with the road network and their proximity to other vehicles. These models calculate each vehicle's location, speed, and acceleration on the network at every time step during the simulation. Microsimulation also allows the analysis of small changes in the network in terms of their impact on road traffic. This provides a valuable series of techniques for road transport emissions modelling (Linton et al., 2015).

- *Traffic network models (microsimulations)* are built on the principles of the four-step model and car-following and lane-changing rules that determine individual vehicle interactions (Linton et al., 2015).

- *Behavioural models* draw on behavioural economics and social psychology disciplines to provide greater detail on individual travel choices and decision-making. Also referred to as *activity-based models*, they view travel as the result of individual activities and decisions. These activities that necessitate mobility are explored to understand transport levels and picture individual decision-making (Linton et al., 2015).

- *Agent-based modelling* has been used in activity-based and microsimulation approaches (Balmer et al., 2006; Bekhor et al., 2011). The benefit of using ABMs within the transport sector is that we can model a series of *heterogenous* agents, allowing a "bottom-up" approach and detailed insights into system interactions. We can depict complex systems where agents interact with one another and their environment to produce "emergent behaviour" (Bernhardt, 2007).

The traffic emission model uses as input the fleet activity (trips) generated by these *traffic models*. Together with vehicle emission factors, the *emission model* generates emissions data for the network.

2.1.2 Emission models

Smit et al. (2010) validated different types of emission models. Here we present them in increasing complexity, cost and time resources. (a) – (c) constitutes *average speed-based* models, and (d) – (e) *instantaneous* emission models:

(a) *Average speed* models (e.g. COPERT (Ntziachristos et al., 2009), MOBILE (EPA, 1994)), widely used for emission estimation and air quality modelling studies (Shorshani et al., 2015). These models implicitly account for some congestion influence because the driving cycles used to realise the emission model has dynamic speed-time profiless (Grote et al., 2016);

(b) *Traffic-situation* models (e.g. HBEFA (2019), ARTEMIS (Boulter and McCrae, 2007), COPERT Street Level (Emisia, 2021)), where discriptions of particular traffic situations like *stop-and-go* or *freeflow driving* determine emission factors. These models explicitly account for congestion influence through the user-defined qualitative description of traffic conditions: each traffic situation (characterised by road type) in the emission model is referenced to an average emission factor for different vehicle categories (Grote et al., 2016);

(c) *Traffic-variable* models (e.g. TEE (Negrenti, 1996), Matzoros model (Matzoros, 1990)), which require traffic flow variables like average speed, traffic density, queue length and traffic signal settings. These can be sourced from both microscopic and macroscopic traffic models;

(d) *Cycle-variable* models (e.g. VERSIT+ (Smit et al., 2007)) require detailed information on vehicle movement (speed, acceleration, and road grade), which can only be obtained from a microscopic traffic model or, for example, Global Positioning System (GPS) equipment. This limits their application to microscopic traffic emission models (Smit et al., 2010); and

(e) *Modal* models (e.g. PHEM (Zallinger et al., 2008), CMEM (Scora and Barth, 2006)), requiring similar input to cycle-variable models. They produce emission factors via engine or vehicle operating models at the highest resolution.

Instantaneous emission models are useful for small-scale applications because of the intensive input data requirements and high computational burden. These models use any given vehicle trajectory to estimate second-by-second vehicle emissions and fuel consumption. Hence, the emission factor unit of measure is given *per second*, contrary to *per vehicle kilometre* in the average speed-based models.

Smit et al. (2010) found that complex models do not necessarily lead to more accurate estimations. This explains the primary use of average speed and traffic-situation models across Europe and in the US (ERMES, 2021). Our research utilises the latter of these models but our local application requires a dedicated approach for the South African context.

2.2 MATSim and HBEFA

Quite often, a single approach cannot fully capture the dynamics of a complex system, especially when we are interested in gaining insights from and understanding traffic emissions. Therefore, we prefer a modelling approach that captures the critical elements of the transport system essential for our purpose of traffic emissions modelling.

Linton et al. (2015) describe Multi Agent Transport Simulation (MATSim) as an agent-based modelling approach that, through agents in the traffic network, captures the transport system dynamics with a behavioural-oriented approach. In his thesis, Kickhöfer (2014)'s agent-based approach advocates MATSim for several reasons:

(a) Firstly, its high degree of modularity and focus on the agent facilitates an individualised behavioural model.

(b) It provides a mesoscopic traffic flow model: on a scale large enough to consider emergent behaviour and small enough to study a single agent. Calculating externalities like congestion and vehicle-specific emissions requires this type of model.

(c) It can handle large networks with several million agents and enables investigation at one second time steps. This allows us to observe traffic scenarios at different times in a day, e.g. peak and off-peak.

(d) Finally, MATSim offers performance functions that capture travel preferences by assigning weights to agent attributes. With this, we can examine the impact of externalities like LEZ interventions on individual travel decisions.

These support our inclination toward MATSim for agent-based emissions modelling. Shorshani et al. (2015) mention that emission models based on microscopic transport models, like MATSim, perform better than those based on macroscopic models due to better vehicle dynamics estimation, high temporal resolution and the ability to account for congestion.

2.2.1 The value of agent-based simulations

Agent-Based Simulation (ABS)'s can provide valuable insights and decision support to situations that possibly require a counter-intuitive approach (Kickhöfer et al., 2018). This enforces the concept that ABSs are ideal for studying the unintended consequences of interventions applied on a large scale. The invaluable characteristic of ABSs lie in the fact that they show emergent behaviour of complex systems – unplanned for, unrealised, and sometimes counter-intuitive behaviour (Bernhardt, 2007). Uncertainties arise when we try to model the real world with (relative) accuracy while accounting for this complex behaviour between interacting agents. It is when our intuition fails to accurately portray this uncertainty that we realise the value of ABS.

Macal (2016) defines four agent properties for agent-based modelling and simulation: *individuality, autonomy, interactivity* and *adaptability.* The value of ABS lies in its capability to capture all four of these properties in a single model.

By *individuality*, we refer to the diversity of each agent's attributes that presents it as a distinct individual. These attributes may include a daily plan with home and work locations and vehicle type with a particular emissions profile in traffic simulations. *Autonomy* implies that each agent can act independently and make its own decisions based on its individual characteristics. Emphasis on agent individuality and autonomy regularly coincide where interaction is not required, like traffic or taxation models – large in scale and computationally intensive. Social simulations model the *interactivity* between agents to study the emergence of patterns, social structures and institutions. This property implies that behaviour is independently or interdependently with other agents and the environment. Adaptive models capture changing behaviour among agents. The *adaptability* of agents can represent a learning process by which previous encounters are remembered and used to guide future decision-making.

Why MATSim?

MATSim allows us to examine the emergent behaviour of agents as a result of their individuality, autonomy, interactivity and adaptability. These properties are essential to a transport simulation with a focus on individual emission profiles: when modelling a synthetic population with various emission profiles, the modeller depends on the ability to simulate a distinct individual (by its vehicle type) that can act independently by interacting with other agents on the given road network. If required, these agents should also react and adapt to external influences of the simulated environment imposed by the modeller.

MATSim incorporates all of these essential agent properties in its ABM. It models a population of individuals (agents), each representing a person with unique attributes, as they execute their daily plans on a transport network. A *plan* is a sequence of activities and trips richly described in terms of timing (start time and duration), location (detailed facilities or coordinates instead of zones) and mode. The agent's experience is scored using a generalised cost function that accounts for the (positive) utility of participating in value-adding activities and the (negative) utility of travelling and incurring cost to overcome the distance between activities. The experience is based on and influenced by multiple agents trying to execute their individual plans on the limited infrastructure, causing congestion. Autonomous decision-making is embedded in the MATSim machinery as interchangeable and complementary modules like changing the timing of an activity, altering a route, or changing mode, depending on the supporting data available and the intent of the model investigation. As agents adapt their daily plans and execute the revised plans iteratively, they build up a memory of plans, favouring those that promise a higher expected utility. This co-evolutionary machinery of MATSim allows for a relaxed state to be achieved over a sufficient number of iterations when no agent can consistently improve its state of maximising its utility.

2.2.2 Similar work

Work and research done by Kickhöfer and peers set the global stage for emissions modelling in MATSim. The essence of his work centres around the relationship between emissions, traffic congestion and emission tolls, applied as transport intervention in most of his studies. In Hülsmann et al. (2011), they develop the approach to link the agent-based transport model MATSim with emissions factors and traffic situations in Handbook Emission Factors for Road Transport (HBEFA). This approach links the traffic flow model in MATSim with the database of HBEFA. It calculates time-dependent cold and warm emissions specific to each vehicle type. Its reusability and transferability to other scenarios are among its main features. The `emissions` contribution comprises two main steps:

1. Deduction of kinematic characteristics from MATSim simulations: when an agent enters a link (road segment) on the road network, MATSim saves a timestamp and compares it to the time at which this agent exits the link, resulting in the free-flow travel time.

2. Generation of emissions factors identified per (varying) vehicle type, road category and speed limit. MATSim assigns these factors to each agent and link it traverses.

We use the vehicle-specific emission factors from HBEFA 4.1 to define the unique attributes assigned to each agent. Only using the vehicle types with their emission factors relevant to *our* South African context, we apply the emissions contribution to our small scale experiment(s).

The results from our study serve to provide a starting point for answering questions similar to the one from Kickhöfer et al. (2011). They affirm that the inclusion of individual income in utility calculations do allow a better understanding of public acceptance issues.

They conclude this by estimating income-dependent utility functions for each individual to depict human mobility behaviour and testing the implementation in the MATSim framework. By using (updated) emission factors in HBEFA 4.1 to enhance the current emissions contribution, we gain a better understanding of the relationship between traffic congestion and emissions in our South African context when applying some travel intervention.

We seek a similar response in agent behaviour as presented by Agarwal and Kickhöfer (2015). They evaluate the outcome of pricing emissions and congestion, respectively. The former shows agents preferring shorter distances whereas the latter steers them towards shorter travel times which could mean longer distances. A travel intervention applied to a population of agents could produce unintended and unplanned consequences. We aim to produce simulated behaviour for which we can plan, applying interventions where *we* control the consequence.

Kickhöfer et al. (2018) also use the emissions contribution to study air pollutant emissions in the transport sector (likewise in Kickhöfer et al. (2013)). They test optimal emission pricing strategies that would result in reaching set policy targets regarding greenhouse gas emissions. The population to which these pricing strategies apply largely influence the efficacy of such travel interventions. If they failed to represent the agent population accurately, the authors' study would be flawed in any localised context. To this end, we seek a representative population of agents in the Gauteng province to which we apply the emissions contribution.

2.2.3 Uncertainty in emissions models

Shorshani et al. (2015) describe the uncertainties in the internal model parameters that cause erroneous emission estimates. The most typical among these are: *traffic data* (flows and speeds), *vehicle fleet composition* (e.g heavy, passenger car, bus), and *emission factors*.

The first among these depends on how we build our simulated road network. The HBEFA links to the traffic flow model of MATSim to realise an emissions modelling tool in an agent-based framework. MATSim can assign descriptions to each road segment (link) in the given network, which correlate with the traffic situations in HBEFA's database. In doing so, the uncertainty of *traffic data* is cleared.

In chapter 3, we address the second uncertainty. We perform data fusion to build a synthetic vehicle population that captures the diversity and accurately depicts the South African *vehicle fleet composition*.

The traffic situations in HBEFA are tailored explicitly to European driving conditions. However, Sun et al. (2014) found HBEFA to be suitable for the Chinese fleet and roads. Our model validation in chapter 4 indicates if the *emission factors* from HBEFA are sound for estimating emissions in South Africa.

2.3 PEMS in emissions modelling

Multiple studies demonstrate PEMS instrumentation 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 on a second-by-second (1Hz) basis (Frey et al., 2003; Hao et al., 2017; Liu et al., 2010; Ropkins et al., 2007).

Engine output can be computed at each sampling instance using the test vehicle specifications. This enables the prediction of instantaneous fuel consumption and exhaust emissions (Wyatt et al., 2014).

PEMS measurements provide actual emissions in the absence of a standard test cycle, making it an unrepeatable and time-intensive experiment. However, it includes 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).

The benefit of PEMS tests is that the researcher can study a distribution of emissions measured across multiple trips, which is more comprehensive than point values from static measurements. Simulation models can produce similar distributions from ensemble runs, making PEMS tests the ideal validation method.

Use cases for PEMS

The combination of local PEMS measurements for *validation* and emission models contributes to producing a validated emissions model in a localised context. However, PEMS also play an equally important role in *generating* the results for emission models.

In-laboratory campaigns most often provide emission factors required in emission models. López-Martínez et al. (2017) remark that PEMS produce measurements from tunnel studies, remote sensing and on-road or onboard experiments that improve the estimation of these emission factors.

PEMS tests also provide essential RDE data to verify the adherence to legislative caps for pollutants like NO_x. The conditions for these RDE tests include:

- up and downhill driving;
- driving on urban roads, rural roads and motorways (low, medium and high speeds);
- additional vehicle payloads;
- year-round temperatures; and
- varying elevation.

Europe is the first region globally to introduce on-road RDE testing under these conditions. These tests complement the Worldwide harmonised Light vehicle Test Procedure (WLTP) test, introduced in 2017. It replaced the New European Driving Cycle (NEDC) test designed in the 1980s, which relied on outdated technology and driving cycles (Car Emissions Testing Facts, 2016). This emphasises the (increasing) value and usefulness of PEMS tests in the environmentally-conscious era in which we find ourselves.

2.4 Summary

Air pollution's environmental and health impacts drive policymakers towards simulation for informed decision-making when considering hypothetical scenarios for transport interventions. We discuss traffic modelling approaches of travel demand on micro and macro scales. These transport models perform traffic assignment, estimating the fleet activity (trips) required by emission models. We conclude with Rasouli and Timmermans (2013) that dynamic models perform better than the traditional four-step model for traffic assignment. As a result, we prefer the valuable series of techniques for traffic emissions modelling offered by micro- and mescopic models.

The MATSim framework captures transport system dynamics with a behavioural-oriented approach (Linton et al., 2015). The emissions integration in MATSim (Hülsmann et al., 2011) realises a traffic-situation model with a low level of complexity and lower cost and time resources than instantaneous emission models (Grote et al., 2016). MATSim's agent-based approach can depict agents with essential properties like individuality, autonomy, interactivity and adaptability, making it the favoured simulation tool for traffic emissions modelling (Kickhöfer, 2014).

PEMS instrumentation proves helpful for RDE tests in various case studies (Frey et al., 2003; Hao et al., 2017; Liu et al., 2010; Ropkins et al., 2007). They also provide a means of validating local emission models. This solidifies our inclination to utilise PEMS to uncover the variability in our local measurements. In doing so, we address our first research goal of investigating and understanding the uncertainty and variance in South Africa's transport emissions. Consequently, we can compare these measurements to our ABS model's estimations. To this end, we get one step closer to validated emission models in South Africa. This enables us to provide policymakers with insights that guide decision-making for setting informed and realistic targets, achieving our final research goal.

Chapter 3

MATSim for emissions modelling

Agent-based modelling has gained more attention increasingly in the field of transport simulations due to its significant advantage over the well-known four-step sequential model (Shiftan and Suhrbier, 2002). The agent-based model provides richer insights into individual behaviour and decision-making as opposed to the aggregate approach followed by the four-step model.

In this chapter, we establish a baseline scenario in the Multi Agent Transport Simulation (MATSim) framework that can be used to evaluate emissions generation on a regional scale. The scenario covers the multi-metropolitan economic centre of the country, the province of Gauteng, which is made up of the City of Johannesburg, Tshwane (Pretoria) and Ekurhuleni, along with two district municipalities: Sedibeng and West Rand. We focus on the Gauteng province as it accounts for less than 2% of the country's land surface but 25% of the population and more than a third of the country's gross domestic product (GDP).

Ideally, we want to use this MATSim model in future policy work. The baseline scenario developed in this chapter creates a "safe space" to investigate various *what-if* scenarios to inform policy decisions.

3.1 Emissions modelling in Gauteng

MATSim models an entire driver population in a large-scale Agent-Based Simulation (ABS). Its open-source framework allows users to add various extensions (code contributions) for scenario-specific interventions.

The database of the Handbook Emission Factors for Road Transport (HBEFA) links to the traffic flow model of MATSim to realise an emissions modelling tool in an agent-based framework. Emission factors from HBEFA provide each agent (driver) with vehicle-specific, time-dependent characteristics based on its vehicle type.

This HBEFA integration produces the `emissions` contribution, developed and tested by Hülsmann et al. (2011), further improved by Kickhöfer et al. (2013) and presented in Kickhöfer (2016). This extension has been used to perform spatial analysis of air pollutant emissions (Kickhöfer et al., 2013), calculate local air pollution exposure costs (Kickhöfer and Kern, 2013) and compare optimal pricing and backcasting approaches and costs required to reach the EU's 2020 emission reduction targets (Kickhöfer et al., 2018).

Gräbe and Joubert (2021) utilise the emissions contribution in a small-scale MATSim model. They demonstrate behavioural sensitivity with a population of agents, each having unique emission profiles. Joubert and Gräbe (2021a) build on this work to simulate emissions for passenger cars on the Gauteng road network. However, this Gauteng model does not include heavy vehicles types in its agent population. The functionality tested by Gräbe and Joubert (2021) and the large-scale model of Joubert and Gräbe (2021a) lays the foundation for the development of the case study for the Gauteng road network in section 3.3. We expand Joubert and Gräbe (2021a)'s model to include Heavy Goods Vehicles (HGVs) in the Gauteng vehicle population.

3.2 Research methodology

The research design, materialising our first research goal, has three components: For the *(1) simulation input*, we provide the network and generate initial demand – the synthetic agent population. Agents receive a daily plan with activities to execute during the simulation period. These activities comprise an agent's commute from home to work and back home again. Along with daily plans, we assign a vehicle class to each agent. Additionally to the work of Joubert and Gräbe (2021a), agents can also be assigned an HGV vehicle class (as opposed to only passenger car vehicle types). The *(2) mobility simulation* places the initial demand on the network and allows agents to execute their daily plans for a simulation period of 24 hours. The *(3) simulation output* quantifies the emissions generated on each link in the road network. We aggregate these results to compute the emissions generated on a system level from the provincial road network. Then, we consider the emissions per vehicle class, reporting the pollutants generated from a passenger car and heavy vehicle type.

3.3 Gauteng allocation

An earlier version of this section was published in Joubert and Gräbe (2021a).

Traditional transport models rely primarily on origin-destination (OD) matrices to describe the patterns in trip distribution. These OD matrices typically cover only a short time window like the morning peak traffic. As a result, the majority of trips accounted for during this window are the routine home-to-work commute. The benefit of activity-based travel demand is that it typically covers an entire day with richer activity sets. However, to realise these activity-based models, richer input data is required from detailed trip diaries, frequently inaccessible (Ilhai et al., 2019; Zhuge et al., 2014).

Consequently, several research contributions show how a trip-based model's OD matrices can be converted into an activity-based set of travel chains for discrete individuals. Fourie (2009) and Zhuge et al. (2014) convert *EMME/2* data into a MATSim population of agents. They both confirm that the agent-based equivalent yields more accurate travel time predictions and richer overall result sets.

This study adopts a similar approach to Fourie (2009) and Zhuge et al. (2014) to generate synthetic travel demand for Gauteng, South Africa. Joubert and Gräbe (2021a) describe this process using the Saturn-based transport model of the South African National Road Agency Limited (SANRAL) for 2016, validated by Robinson and Venter (2019).

The initial demand translates into a MATSim population of agents with daily trips, called plans. Given these initial plans, 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 loads every agent into the mobility simulation (Gao et al., 2010). The applicable travel modes are private cars (commuters), light vehicles (business), light-heavy goods vehicles or heavy goods vehicles.

Table 3.1 distinguishes between two vehicle classes representing these four agent types included in the MATSim population:

Table 3.1: Vehicle classes representing different agent types

Passenger car	Heavy
Private car (commuter)	Light-heavy goods vehicle
Light vehicle (business)	Heavy goods vehicle

3.3.1 Vehicle population

The next step is to assign a dedicated vehicle to each agent in this population. A vehicle should have a specific type that accounts for its emissions concept. It should distinguish on the vehicle class (passenger car or heavy goods vehicle), fuel type (petrol or diesel, in South Africa) and the Euro concept, for example, Euro 4.

Nevertheless, such a detailed breakdown of the vehicle type is not available in public data. For example, the electronic National administration Traffic Information System (eNaTIS) provides a live vehicle population (eNaTIS, 2020). eNaTIS only indicates the number of registered vehicles in each province and only distinguishes between the classes shown in Table 3.2. No fuel-related or emissions data is available for any of the vehicle types. Consequently, this study employs a strategy to infer the emissions concepts using second-hand vehicle sales data as a proxy for the distribution of vehicle types in the country. Why *this* strategy? Unfortunately, we can not obtain detailed vehicle profiles from eNaTIS. Therefore, second-hand car sales are our best effort because it is the *only* proxy to estimate vehicle age at this stage.

Table 3.2: Live eNaTIS vehicle population for the province of Gauteng (July 2020).

Vehicle class	Province Gauteng	Percentage of total
Motor cars and station wagons	3 128 479	**70.34**
Minibuses	130 207	2.93
Buses, bus trains, midibuses	20 460	0.46
Motorcycles, quadrucycles, tricycles	139 445	3.13
LDV's, panel vans, other light load vehicles, GVM $\leq$ 3500kg	853 293	19.18
Trucks (heavy load vehicles), GVM $>$ 3500kg	140 033	3.15
Other	36 029	0.81

Even though we ignore light delivery vehicles (LDVs), comprising about 20% of the vehicle population, this strategy still caters for at least 70% with the passenger vehicle class (shown in bold in Table 3.2). A possible implication of only modelling 70% of Gauteng's vehicle population might be an inaccurate representation of the daily traffic volumes, especially on busy national and metropolitan freeways.

We sample from over 65 000 listed passenger vehicles from AutoTrader (2020) to obtain the proportion of fuel types[1]. For each sampled vehicle we infer its emissions concept from secondary sources like True Rating (2020) or the Australian Drive (2020) (see Table 3.3).

[1]We disregard all but the main fuel types (petrol and diesel) in our South African context.

Table 3.3: Vehicle sampling results for 20 years. Each row contains the Euro emissions concept % of the vehicles sampled in that year (Joubert and Gräbe, 2021a).

Year	**Sample population**	**Petrol Euro concept**					**Diesel euro concept**				
		2	**3**	**4**	**5**	**6**	**2**	**3**	**4**	**5**	**6**
2000	0.09	5.3	77.0	—	—	—	2.7	15.0	—	—	—
2001	0.14	5.3	77.0	—	—	—	2.7	15.0	—	—	—
2002	0.13	5.3	77.0	—	—	—	2.7	15.0	—	—	—
2003	0.21	5.3	77.0	—	—	—	2.7	15.0	—	—	—
2004	0.32	5.3	77.0	—	—	—	2.7	15.0	—	—	—
2005	0.50	—	37.1	46.8	—	—	—	8.1	8.1	—	—
2006	0.67	na	na	na	na	na	na	na	na	na	na
2007	1.03	na	na	na	na	na	na	na	na	na	na
2008	1.14	—	8.5	63.1	—	—	—	13.1	15.3	—	—
2009	1.27	—	6.5	62.0	5.0	—	—	4.5	20.5	1.5	—
2010	2.20	—	3.6	57.1	11.4	—	—	4.3	18.6	5.0	—
2011	3.11	0.7	—	23.0	46.0	—	—	0.7	2.2	27.3	—
2012	4.29	3.0	3.0	18.0	56.0	—	—	4.0	4.0	12.0	—
2013	5.39	—	—	9.7	53.6	1.9	—	—	7.1	27.7	—
2014	7.00	—	—	19.5	36.3	10.6	—	—	5.3	25.7	2.7
2015	8.50	—	0.7	9.2	29.0	30.9	—	2.0	2.0	18.4	7.2
2016	9.70	—	1.8	10.0	23.8	19.6	—	1.1	4.4	26.5	11.1
2017	9.30	—	—	8.7	31.4	30.8	—	—	5.4	15.1	8.7
2018	10.10	5.0	4.0	15.0	13.0	44.0	—	1.0	3.0	6.0	9.0
2019	16.41	na	na	na	na	na	na	na	na	na	na
2020	18.50	—	—	3.0	24.1	37.6		—	6.8	15.2	12.0
Median		0.86	2.32	13.45	28.15	23.97	0.03	1.28	5.56	16.82	7.11

Note: "na" values indicate years from which sampling is yet to be done.

With the detailed emissions concepts known for each year, we follow a Monte Carlo sampling approach to estimate the overall likelihood of a specific emissions concept. A single run will first sample the vehicle's production year, using the probabilities from the *Sample population* column in Table 3.3. Because we sample for ten emission concepts and from more than 80% of the sample population, the value we lose from incomplete sampled years is negligible.

Next, we sample the Euro emissions concept conditional on the production year. We repeat this 10 000 times. One can now, for this run, tally the total number of each of the ten emission concepts.

We repeat this process for an ensemble of 1 000 runs and report the median values of the (symmetric) distributions for each emissions concept at the bottom of Table 3.3.

3.3.2 MATSim

With the probabilities for each emissions concept estimated, we recommence assigning a vehicle type to each agent. We do this in the MATSim scenario by sampling a concept using a cumulative probability distribution of the median probabilities. At this point, no additional person attributes are taken into account to discern, for example, that a more affluent individual is more likely to have a newer and environmentally friendlier (higher Euro concept) vehicle. This is left for future work as it will require additional proxy variables like the appraised value of each vehicle.

Moreover, we do not specify the fuel type (petrol or diesel) and emissions concept for heavy vehicle classes in the current scenario. This is because there is no reliable way (yet) to estimate the vehicle sizes and emission concepts for these vehicles. As a result, MATSim compensates when these parameters are not specified. For every heavy vehicle added to the Gauteng population, MATSim assigns an "average" emissions concept for lack of the current ability to specify different emission profiles. This is sufficient for aggregate analyses but lacks detail when validating these vehicle types on an individual (agent-based) level. However, we can now do better for the passenger car vehicle type, specifying emission profiles representative of the Gauteng vehicle population.

HBEFA data

A typical vehicle type in MATSim's synthetic population can be `PC D Euro 4`, indicating a *passenger car* that runs on *diesel* with a *Euro 4* emissions concept. This attribute necessitates the connection to the exported emission factors from HBEFA's database.

HBEFA 4.1 allows users to export emission factors for various vehicle categories, ①, under multiple traffic scenarios, ②, and ambient conditions, ③. Figure 3.1 shows the selection of passenger car and HGV vehicle categories for pollutants like CO_2 (also selected are CO, NO, NO_2 and NO_x), ④. Further shown are the inclusion of hot and cold-start emission factors, ⑤, ⑥, specified ambient conditions and aggregation level of output, ⑦.

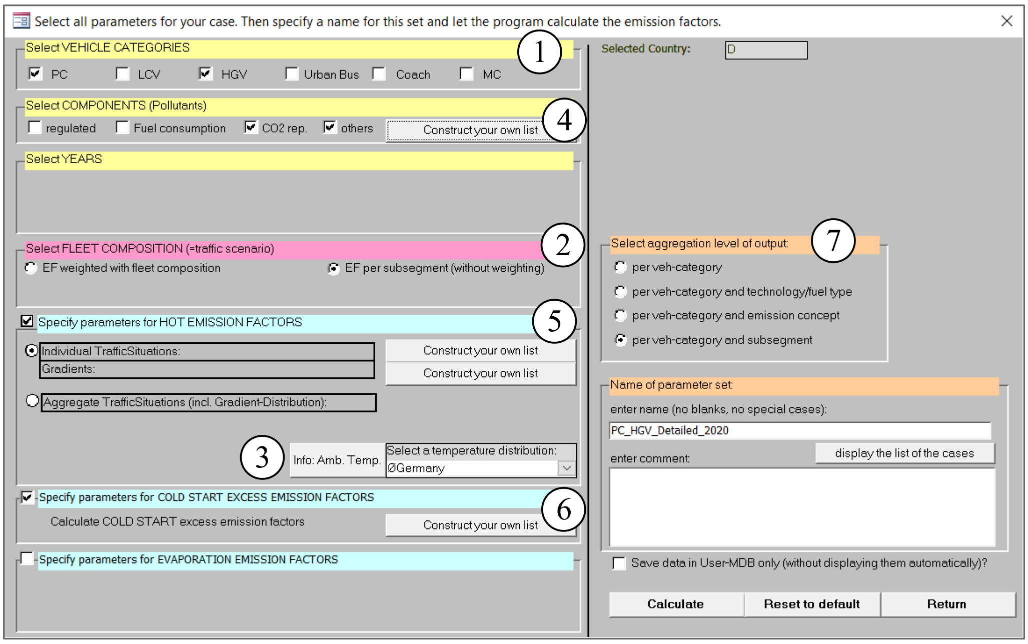
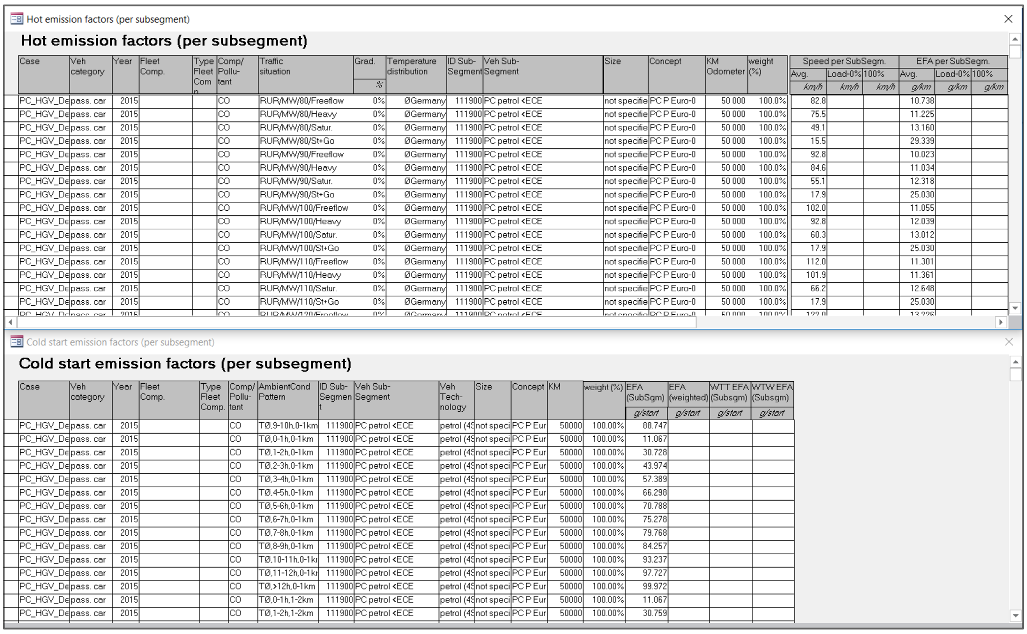


Figure 3.1: HBEFA database configuration for exporting emission factors.

HBEFA 4.1 extracts the emission factors according to the configuration from Figure 3.1, shown in Figure 3.2



Hot emission factors (per subsegment)

Case	Veh category	Year	Fleet Comp.	Type Fleet Comp.	Comp/ Pollutant	Traffic situation	Grad. %	Temperature distribution	ID Sub-Segment	Veh Sub-Segment	Size	Concept	KM Odometer	weight (%)	Speed per SubSegm. Avg. km/h	Load-0% km/h	100% km/h	EFA per SubSegm. Avg. g/km	Load-0% g/km	100% g/km
PC_HGV_De	pass. car	2015			CO	RUR/MW/80/Freeflow	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	82.8			10.738		
PC_HGV_De	pass. car	2015			CO	RUR/MW/80/Heavy	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	75.5			11.225		
PC_HGV_De	pass. car	2015			CO	RUR/MW/80/Satur.	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	49.1			13.160		
PC_HGV_De	pass. car	2015			CO	RUR/MW/80/St+Go	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	15.5			29.339		
PC_HGV_De	pass. car	2015			CO	RUR/MW/90/Freeflow	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	92.8			10.023		
PC_HGV_De	pass. car	2015			CO	RUR/MW/90/Heavy	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	84.6			11.034		
PC_HGV_De	pass. car	2015			CO	RUR/MW/90/Satur.	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	55.1			12.318		
PC_HGV_De	pass. car	2015			CO	RUR/MW/90/St+Go	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	17.9			25.030		
PC_HGV_De	pass. car	2015			CO	RUR/MW/100/Freeflow	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	102.0			11.055		
PC_HGV_De	pass. car	2015			CO	RUR/MW/100/Heavy	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	92.8			12.039		
PC_HGV_De	pass. car	2015			CO	RUR/MW/100/Satur.	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	60.3			13.012		
PC_HGV_De	pass. car	2015			CO	RUR/MW/100/St+Go	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	17.9			25.030		
PC_HGV_De	pass. car	2015			CO	RUR/MW/110/Freeflow	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	112.0			11.301		
PC_HGV_De	pass. car	2015			CO	RUR/MW/110/Heavy	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	101.9			11.361		
PC_HGV_De	pass. car	2015			CO	RUR/MW/110/Satur.	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	66.2			12.648		
PC_HGV_De	pass. car	2015			CO	RUR/MW/110/St+Go	0%	ØGermany	111900	PC petrol <ECE	not specifie	PC P Euro-0	50 000	100.0%	17.9			25.030		

Cold start emission factors (per subsegment)

Case	Veh category	Year	Fleet Comp.	Type Fleet Comp.	Comp/ Pollutant	AmbientCond Pattern	ID Sub-Segment	Veh Sub-Segment	Veh Technology	Size	Concept	KM	weight (%)	EFA (SubSgm) g/start	EFA (weighted) g/start	WTT EFA (Subsgm) g/start	WTW EFA (Subsgm) g/start
PC_HGV_De	pass. car	2015			CO	TØ,9-10h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	88.747			
PC_HGV_De	pass. car	2015			CO	TØ,0-1h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	11.067			
PC_HGV_De	pass. car	2015			CO	TØ,1-2h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	30.728			
PC_HGV_De	pass. car	2015			CO	TØ,2-3h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	43.974			
PC_HGV_De	pass. car	2015			CO	TØ,3-4h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	57.389			
PC_HGV_De	pass. car	2015			CO	TØ,4-5h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	66.298			
PC_HGV_De	pass. car	2015			CO	TØ,5-6h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	70.788			
PC_HGV_De	pass. car	2015			CO	TØ,6-7h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	75.278			
PC_HGV_De	pass. car	2015			CO	TØ,7-8h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	79.768			
PC_HGV_De	pass. car	2015			CO	TØ,8-9h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	84.257			
PC_HGV_De	pass. car	2015			CO	TØ,10-11h,0-1kı	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	93.237			
PC_HGV_De	pass. car	2015			CO	TØ,11-12h,0-1kı	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	97.727			
PC_HGV_De	pass. car	2015			CO	TØ,>12h,0-1km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	99.972			
PC_HGV_De	pass. car	2015			CO	TØ,0-1h,1-2km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	11.067			
PC_HGV_De	pass. car	2015			CO	TØ,1-2h,1-2km	111900	PC petrol <ECE	petrol (4S	not speci	PC P Eur	50000	100.00%	30.759			

Figure 3.2: Extracted hot and cold-start emission factors from the HBEFA database.

When MATSim calculates link emissions – pollutants emitted by an agent on a particular section of the road network – these factors come into play.

In this Gauteng scenario, the HBEFA data includes emission factors for passenger cars and heavy vehicle types. Before the mobility simulation, MATSim reads the HBEFA data in `csv`-format and creates lookup tables for hot and cold-start emission factors. It queries these tables to calculate link emissions when all agents have completed their daily plans. Consequently, estimated emissions can be reported on a network level, per agent or vehicle type by using the emission factors extracted from HBEFA 4.1.

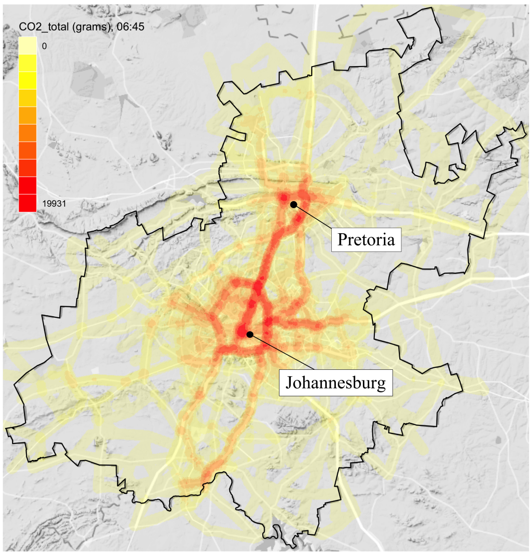
3.3.3 Results

The road network, emission factor data and the initial travel demand of light and heavy vehicles are loaded into the MATSim scenario and executed. Without optimising the computational setup, the simulation runs for approximately 208 seconds per iteration for the 62 990 agents, a 10% sample of Gauteng. We use an HP Elitebook 850 with 4GB of RAM allocated to the process. Within the MATSim configuration, four threads are made available for mobility simulation (taking up most of the computational time) and events processing.

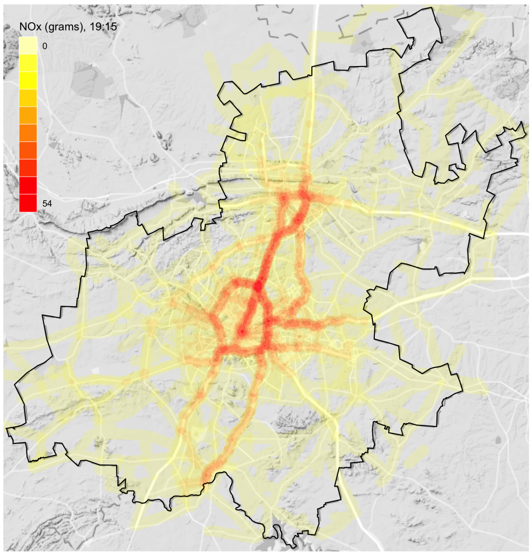
For the size of the network and the number of agents, MATSim generates 26 million events during the mobility simulation. When the mobility simulation shuts down, the warm and cold event types are extracted and aggregated per vehicle. A valuable characteristic of a high-resolution, agent-based setup is that one can aggregate to any required level.

We can introduce both spatial and temporal dimensions to the results because of each emissions event. We know the detailed link on the network (spatial) and when the vehicle left the link (temporal). We show the emissions generation on a regional level by aggregating the total CO_2 and NO_x at specific times in the simulation. Figures 3.3a and 3.3b respectively show these pollutants on the Gauteng road network. High pollutant concentrations (in red) are evident on the major national and metropolitan freeways centred around and between the two city centres: Pretoria (North) and Johannesburg (South).

The traffic volumes that cause these emissions are as expected: Pretoria and Johannesburg are among the top five highest populated cities in South Africa (by the number of inhabitants), attracting the most economic activity, and therefore road traffic, in the Gauteng province.



(a) Total CO_2 produced



(b) Total NO_2 produced

Figure 3.3: Pollutants generated on the Gauteng road network.

Based on our 10% sample, we estimate that the Gauteng vehicle population emits ±4 500 tonnes of CO_2, 19.2 tonnes of CO (carbon monoxide) and 9.1 tonnes of NO_x over a 24-hour period.

Local sources estimate that, without including freight transport (heavy vehicle types), passenger vehicles in Gauteng emit 15 000–20 000 tonnes of CO_2 per day (Moeletsi and Tongwane, 2020; WWF, 2016).

Per-vehicle emissions show how we arrive at these aggregate estimates on a regional level. The agent-based simulation models two agent types: a light and heavy vehicle class. These agent types produce the following distributions (Figure 3.4) that capture *individual* CO_2 emissions for the entire vehicle population.

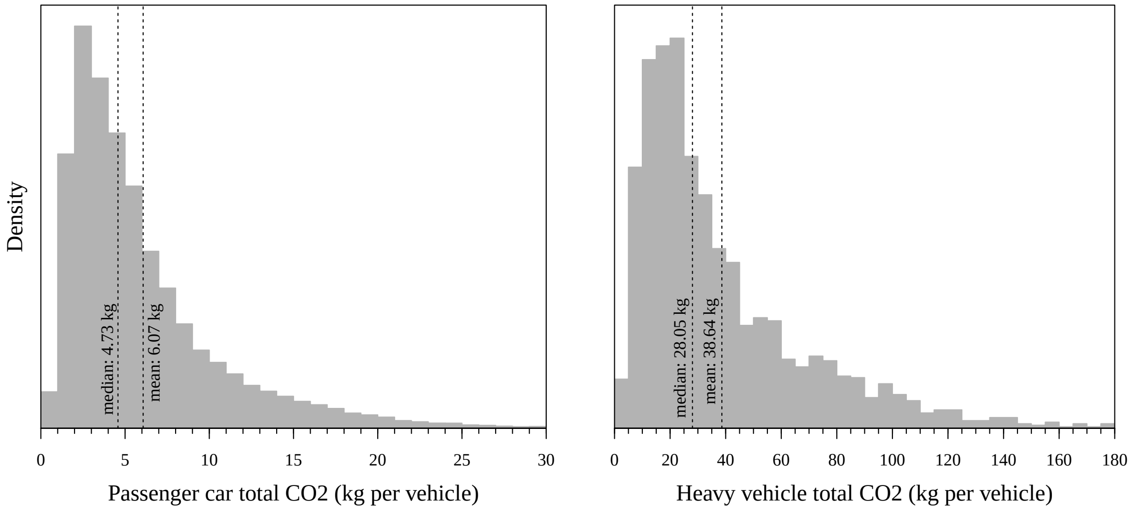


Figure 3.4: Distribution of the total CO_2 produced from (daily) home-work-home trips.

Similar distributions for CO and NO_x emissions provide the same daily estimates for the passenger car and heavy vehicle class. Table 3.4 combines the average emission estimates for these agent types executing their daily plans.

Table 3.4: Average daily pollutant emissions per vehicle class.

Vehicle class	Pollutant (g)		
	CO_2	CO	NO_x
Passenger car	6 070	29.9	12.6
Heavy Goods Vehicle	38 640	47.3	67.2

We recognise that the initial demand for our Gauteng model, based on SANRAL's four-step model, only considers morning and afternoon peaks. This four-step model only captures peak traffic, accounting for the highest daily traffic volumes. Offpeak emissions are not included in the regional emission estimates, yet: parents fetching their children from school, people going shopping during the day and couriers making trips to deliver online orders. The emissions from these daily activities are unaccounted for in the regional emissions model. This might paint an inaccurate picture of what truly happens daily on Gauteng's road network. However, when comparing simulation to reality, to have a discrepancy of a factor of *three*, based on local source estimates, seems unusual. Could the omission of these offpeak emissions cause such a significant discrepancy? This raises concern when put in perspective: government entities make multi-billion Rand decisions on figures that may be largely overestimated – they could be wholly over-taxing or over-charging based on data that is not the ground truth.

3.3.4 Validation

New cars come labelled in their windscreens with a chart that indicates the vehicle's emissions and fuel consumption. Figure 3.5 illustrates this data on the windscreen of a common passenger car at a South African car dealership in Hatfield, Pretoria. In reality, we never experience these mileages and emission standards. This is because original equipment manufacturers (OEMs) obtain these values from factory testing under stringent condi-

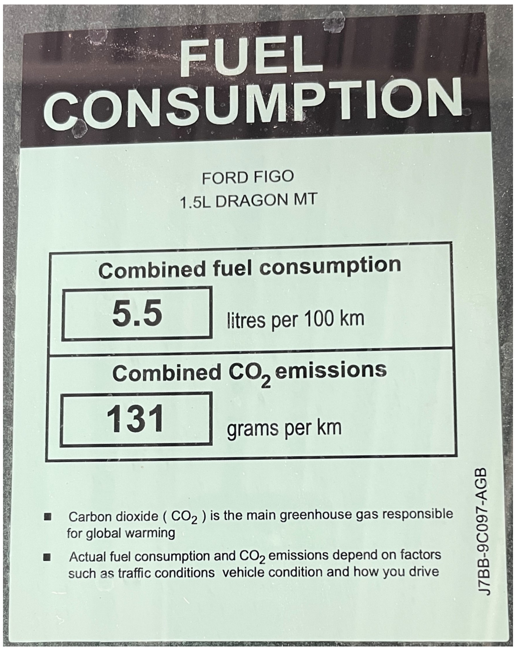


Figure 3.5: Fuel consumption and carbon emissions data for a new vehicle from a South African car dealership.

tions. As commuters, we experience *real* driving conditions. Our driving behaviour does not match the conditions set in these rigorous factory tests. Therefore, we can not rely on OEM data to validate an emissions model applied to a real-world scenario. Fortunately, there exists equipment that allows us to measure Real Driving Emissions (RDE) in our local context.

Europe introduced on-road RDE testing under specific conditions that utilises Portable Emissions Measurement System (PEMS) instrumentation. These units record the movement, geographical position and exhaust emissions of a vehicle driven over a real-world test route. In chapter 4 we apply PEMS instrumentation to study the variance present in our Agent-Based Model (ABM) compared to emissions from real driving conditions. If we can compensate for this variance in future models, we move one step closer to validated emission models in South Africa.

Chapter 4

Real driving emissions

The infamous Volkswagen "Dieselgate" scandal (Chossière et al., 2017), amongst others, sparked an international movement to improve vehicle certification by incorporating Real Driving Emissions (RDE) testing. This development opened up a new field of research in the transport sector. Consequently, the Centre for Transport Development at the University of Pretoria (UP), in the Faculty of Engineering, Built Environment and Information Technology (EBIT), acquired a Portable Emissions Measurement System (PEMS) in 2020[1].

The PEMS unit allows one to accurately measure a variety of vehicle exhaust emissions under real-world driving conditions. The unit and the Centre's capability is the first of its kind in Africa (Joubert and Gräbe, 2021c). The team at the Centre is building up a database of emissions and vehicle diagnostics on various road types and vehicle loads in Gauteng (Joubert, 2021). The current cohort of test vehicles includes the University fleet of light vehicles and the NRF Road-Rail Vehicle (RRV), a heavy goods vehicle.

This chapter addresses the second and third research goals: investigating how good our emissions model performs "out-of-the-box" and quantifying the *gap* between our simulation and *real* (local) driving emissions.

4.1 PEMS

In reality, South Africans never experience the mileages and emission standards boldly advertised on a chart in the windscreens of their new cars. This is because Original Equipment Manufacturers (OEMs) obtain these values from factory testing under stringent conditions. These South African commuters experience *real* driving conditions. Their driving behaviour does not match the conditions set in these rigorous factory tests. Therefore, OEM data is an unreliable source to validate an emissions model applied to a real-world scenario. Fortunately, PEMS allow the measurement of RDE in a local context.

PEMS instrumentation is utilised to study the variance present in Multi Agent Transport Simulation (MATSim)'s agent-based emissions model of Gauteng compared to emissions from real driving conditions. PEMS driving tests are conducted with a passenger car and heavy vehicle to estimate the "ground truth" of emissions generation for these vehicle classes in a South African context. By measuring RDE for the same vehicle classes represented in MATSim's emission model, the author justly compares apples with apples.

[1]We acknowledge the funding contributions for this initiative from UP, the National Research Foundation (NRF) (through the National Equipment Programme), and the Department of Science and Innovation (through the RDI Waste Roadmap managed by the CSIR)

4.1.1 Field test setup

The PEMS unit is mounted on two vehicles from the UP's fleet. The unit measures instantaneous emissions for various pollutants at a rate of 1Hz. Summating these measurements produce the total emissions generated per trip. Multiple trips are conducted with each test vehicle to account for the variability associated with driver behaviour. Each trip conducted follows the same predetermined route that starts and ends at the main Hatfield campus of the University of Pretoria in Gauteng (Figure 4.1). The 61.7km long C-shaped route

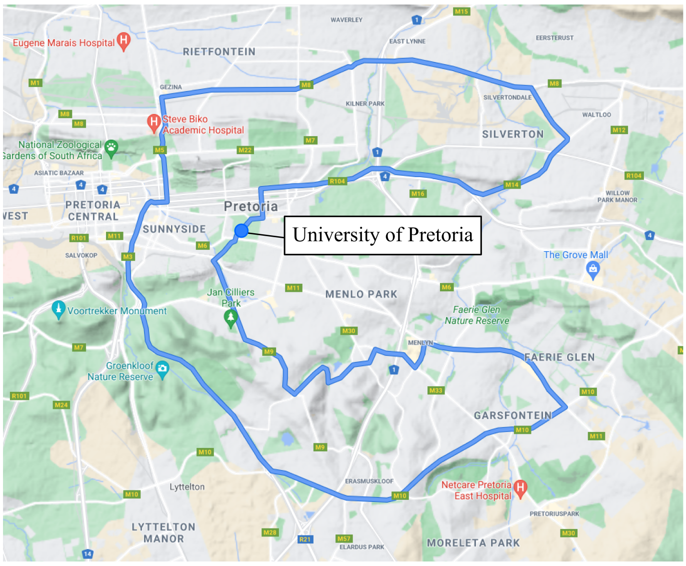


Figure 4.1: The C-route starting and ending at the University of Pretoria.

includes different road types: residential, local, secondary, primary and freeway sections. The test vehicle types are described as follows.

Heavy goods vehicle

The test vehicle we use for the heavy vehicle class is the RRV – a heavy goods research vehicle based on an Isuzu FTR850 AMT (Figure 4.2). The 7.8-litre, six-cylinder turbocharged, intercooled, common-rail diesel engine has a Euro 3 emissions rating (Isuzu, 2021). The RRV takes approximately 110 minutes to complete one trip along the C-route in typical urban traffic conditions.

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 minutes to complete one trip along the C-route in typical urban traffic conditions.

4.1.2 Equipment

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. This is useful to specify the start and end time of successful field tests or to mark a point when an unexpected event occurs during the test, like being forced to take a slight detour. The ICM also connects to and records the vehicle's Onboard Diagnostics (OBDII) port while driving.

Exhaust gasses pass through the 4-inch (±100mm) 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.

The SEMTECH DS+ unit is loaded and secured onto the RRV's deck, close to the exhaust or on the backseat of the Ford Figo. The layout of the setup on the vehicles are shown in Figures 4.2 and 4.3. The exhausts, ①, are connected to the EFM flow tube, ②, using a flexible stainless steel tube with a conic reducer. In the RRV's setup, the EFM connects directly to the gaseous analyser, ③. The Ford Figo requires a heated line, ⑦, to connect the EFM with the gaseous analyser inside of the vehicle. We position the GPS unit's antenna, ④, and weather probe, ⑤, close to the centre of the RRV's deck and similarly on the Ford Figo's roof. The ICM connects via an extended cable and is located inside the RRV's driver cab or on the passenger seat inside the Ford Figo, ⑥, to connect to the vehicles' OBDII ports.

Figure 4.2: UP's Road Rail vehicle (RRV) fitted with the SEMTECH® DS+ PEMS unit.

Figure 4.3: The SEMTECH® DS+ PEMS unit fitted to a light vehicle from UP – a passenger car of the same vehicle class as the Ford Figo (UP, 2020).

For a detailed description of the data and the experimental design, materials and methods employed for the PEMS field test, the reader is encouraged to read the data article by Joubert and Gräbe (2021b).

After installation and once calibration is completed, the unit is switched over from shore power to its dedicated power source: a 13V Lithium Iron Phosphate (LiFePO4) battery with a 108Ah 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 ICM unit, and the driver starts the vehicle.

4.1.3 Trip data

The SEMTECH® DS+ PEMS unit comes with software for postprocessing the recorded trip data. This data includes the pollutant concentrations of CO, CO_2, NO and NO_2, ambient conditions, and vehicle diagnostics collected from different sensors mounted to the vehicle during the field tests. The postprocessor enables the user to specify settings that determine the format of the output data file. Among many others, but relevant to this study, are:

- transport delays for emissions, temperature measurements, vehicle and GPS information;
- fuel properties; and
- user-preferred output parameters, like date and time format, imperial/metric units and the data interval (set to 1Hz).

All of which influence the result of various calculated data fields, i.e. the humidity corrected NO_x measurement. The author refrains from using any "corrected" data fields due to the vast amount of configuration settings that may (unknowingly) taint our picture of *real* driving emissions.

Data analysis is performed on the post-processed data file in the open-source software environment, R (R Core Team, 2020). From this file, the time, latitude, longitude, RPM, vehicle speed, elevation and instantaneous mass emissions are extracred for each 1Hz measurement. The cleaned datasets containing these measurements for the RRV and Ford Figo are published in **?**. Consequently, the emissions generated by the Ford Figo and the RRV are compared to their simulated counterparts in MATSim. This serves to validate the local MATSim emissions model, addressing the second research goal. In addition, it serves the third (and final) research goal of quantifying the variance in South Africa's vehicle emissions – what we *estimate* and what we *measure*.

4.1.4 MATSim setup

Joubert and Gräbe (2021a) utilise MATSim's `emissions` contribution (Hülsmann et al., 2011) to develop an emissions model for the Gauteng road network that simulates heavy vehicles and Euro 1–6 (petrol/diesel) passenger cars. The heavy vehicles types are not distinguished by a particular Euro emissions concept or fuel type. The author builds on Joubert and Gräbe (2021a)'s work to model heavy vehicle types with a dedicated Euro emission concept. This improvement allows the simulation of the RRV and Ford Figo test vehicles as heavy and passenger car vehicle types, respectively. The RRV's simulated counterpart is modelled as an agent with a Heavy Goods Vehicle (HGV) type (diesel) and a Euro 3 emissions concept. The Ford Figo is modelled as an agent with a passenger car (petrol) vehicle type and a Euro 5 emissions concept.

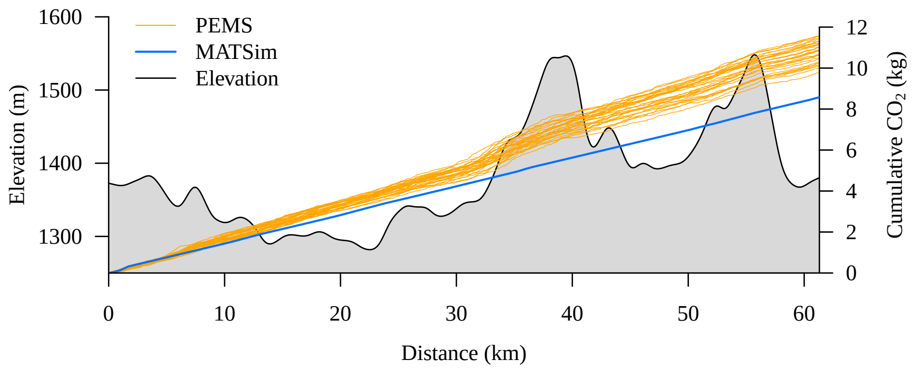
MATSim's agent-based framework models each agent as an individual with unique daily activities, called a *plan*. The only activity in the simulated test vehicles' plan is to complete a single trip on the 61.7km C-route that starts and ends at the University of Pretoria. This route is created programmatically in MATSim's Gauteng road network.

The simulated test vehicle agents are injected into a 10% sample of the Gauteng vehicle population. The sample population executes their daily home-work-home activities alongside the newly modelled test vehicles. The number of vehicles on the road network causes congestion which mimics the urban traffic conditions encountered in the PEMS field tests. The simulation is set up to perform 30 ensemble runs to account for the inherent variability in the simulation model.

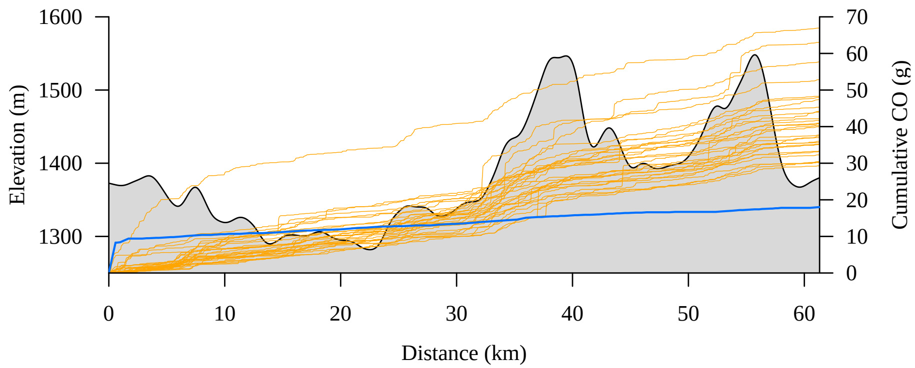
4.2 Results and discussion

Elevation data from the GPS unit fitted with the PEMS equipment provides additional insights when plotted together with the cumulative emissions. Figures 4.4 and 4.5 show the rate at which the cumulative CO_2 emissions are generated as the test vehicles and their simulated counterparts travel along the C-route.

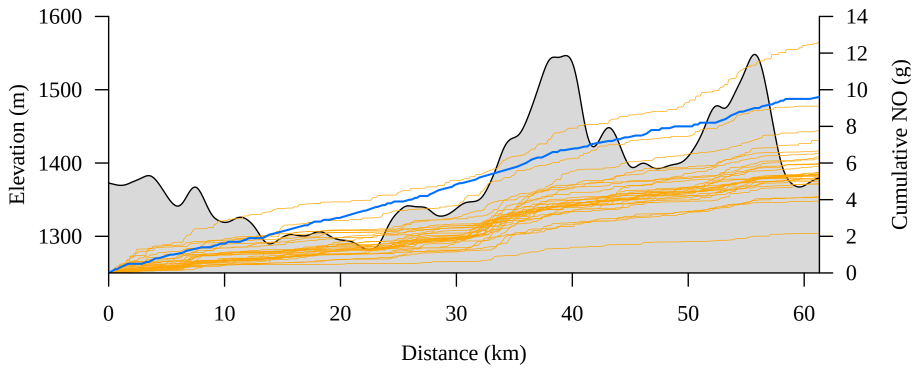
The MATSim model shows negligible variance in the emission results from 30 ensemble runs. Hence, these cumulative emissions are only plotted as a single (blue) line.



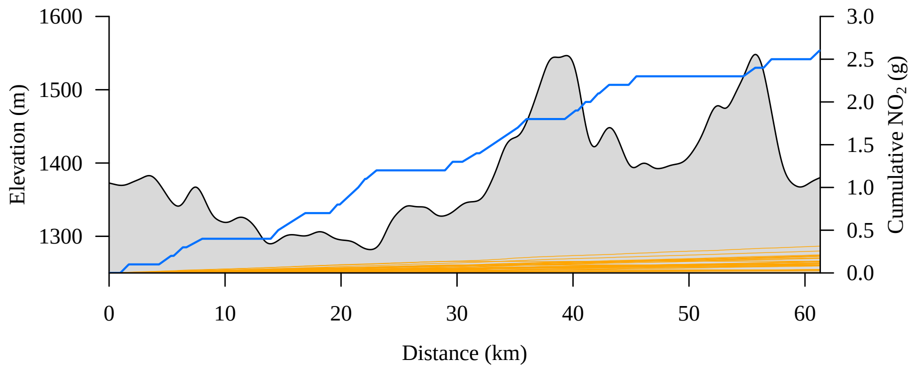
(a) CO_2



(b) CO

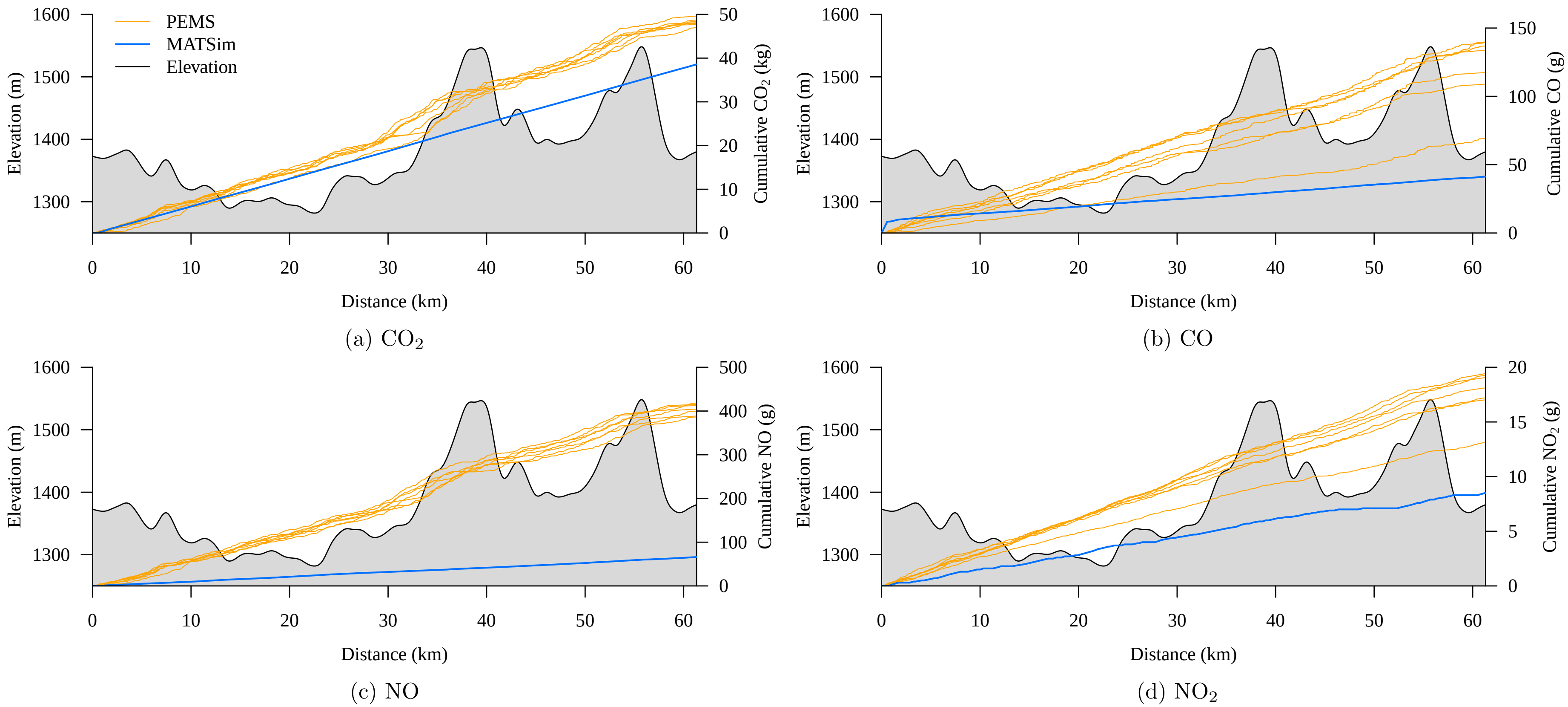


(c) NO



(d) NO_2

Figure 4.4: The C-route elevation profile with the light vehicle's cumulative emissions.



(a) CO_2 (b) CO

(c) NO (d) NO_2

Figure 4.5: The C-route elevation profile with the heavy vehicle's cumulative emissions.

Table 4.1 contains the average 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.

Table 4.1: 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.

Vehicle	Pollutant (g)				
	CO	CO_2	NO	NO_2	NO_x
Light vehicle					
UP Ford Figo	41.2	10 824	5.77	0.112	5.88
MATSim	18.0	8 578	9.60	2.60	12.2
*OEM data**	$\leq$ 61.9	8 171	–	–	$\leq$ 3.71
Heavy vehicle					
UP RRV	120.8	48 191	403.4	17.6	421.0
MATSim	41.3	38 569	66.2	8.50	74.7
*OEM data**	$\leq$ 58.81	18 570	–	–	$\leq$ 48.28

* 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 740kg (Joubert and Gräbe, 2021b), is classified as an *N2*-category vehicle, having a total mass of between 3.5 and 12 tonnes.

Except for the light vehicle's NO_x emissions, the simulation underestimates all other pollutant emissions generated on the C-route. The emissions model accounts for ±80% of the greenhouse gas, CO_2, measured by the PEMS test on the 61.7km long C-route. The observed (true) CO emissions are 2.3–2.9 times *higher* than the simulation. This raises concern when considering how much these local estimations of an odourless, colourless and poisonous gas (CO) might be off on a regional scale. The simulation accounts for merely a fifth of the NO_x emissions of the HGV but estimates more than double the actual amount for the light vehicle.

Often with simulation we compensate for the worst: results are never taken for granted because we always expect the reality to be *worse*. This is because a simulation is only a *representation* of reality, but never *really* reality. This is evident in most of these emission graphs where we see the simulation not fully capturing the true amount of pollutant emissions.

With light vehicles comprising 70% of the Gauteng vehicle population (Table 3.2), we project that MATSim's emissions model would overestimate NO_x's on a regional scale. Even though this might be seen as the "safer" estimate (rather than *underestimation*), this overestimation causes uncertainty for planners considering the adverse effect of NO_x on the human respiratory system and its contribution to acid deposition in the natural environment (Bhandarkar, 2013).

In the subsequent sections, we investigate cold-start emission events, road type, driver behaviour and driving conditions as factors that affect our PEMS measurements.

4.2.1 Cold-start events

Some of the cumulative emission plots show that a single PEMS trip exhibits particularly low (4.4c, 4.5b and 4.5d) or exceptionally high (4.4b) emissions compared to most other trips . We identify these outlier trips as "cold-start" events. A cold-start event occurs 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). Consequently, in our PEMS tests, only the first trip of a given day has a cold-start event.

The current MATSim emissions model of Gauteng does not account for cold-start emissions of HGVs. This causes inaccuracies in the estimated cumulative emissions during the initial portion (about five minutes) of the C-route trip. The measure of these inaccuracies remains unknown while the functionality is not added to the MATSim `emissions` contribution[2].

Figures 4.6 and 4.7 illustrate the total emissions during the first five minutes of each PEMS trip. These five minutes capture the cold-start emissions for the applicable trip. Comparing cold-start and hot-start pollutant emissions, we see, similar to Du et al. (2020), that CO and NO_x (especially NO) cold-start emissions often exceed that of a hot-start trip.

Cold-start pollutant emissions usually account for a significant proportion of the urban trip emissions in an RDE test (Du et al., 2020). Therefore, given a cold-start event on specific trips, one would expect to see these trips' cumulative emissions totalling *more* than hot-start trips. This begs why the outlier trips from 4.4c, 4.5b and 4.5d are *lower* than most other trips.

Our research focus is not on the analysis of these cold-start events. However, based on findings from Du et al. (2020), we speculate that these unexpected trip totals could also be attributed to external factors like driving behaviour – a noteworthy factor affecting the inconsistency of cold-start emissions results in RDE tests.

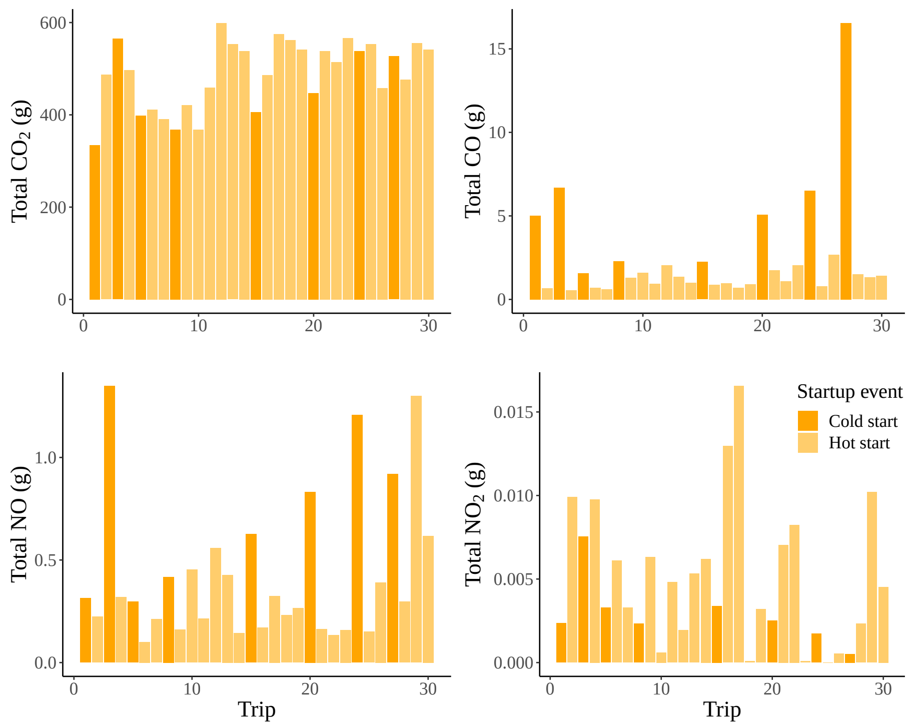


Figure 4.6: Emissions from the Ford Figo during the first five minutes of each PEMS trip.

[2]MATSim's developers incorporated this functionality in August 2021 by adding a lookup table that adds the necessary reference values for the `emissions` contribution to include before executing the mobility simulation. At the time of writing, the authors had not applied the changes to reflect the latest version of the `emissions` contribution in their MATSim model for Gauteng. Thus, remaining as future work.

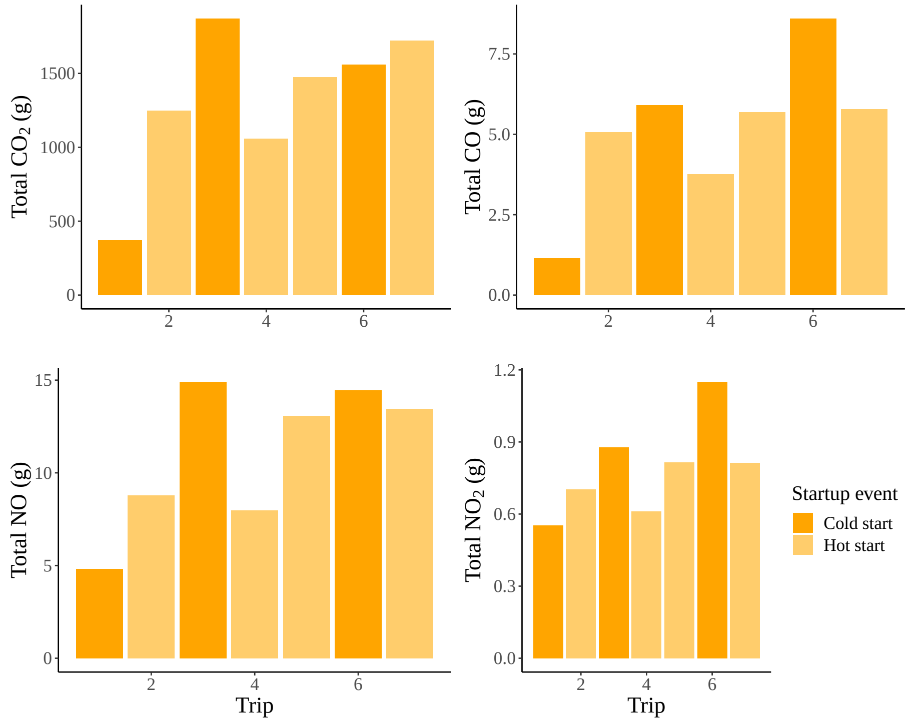
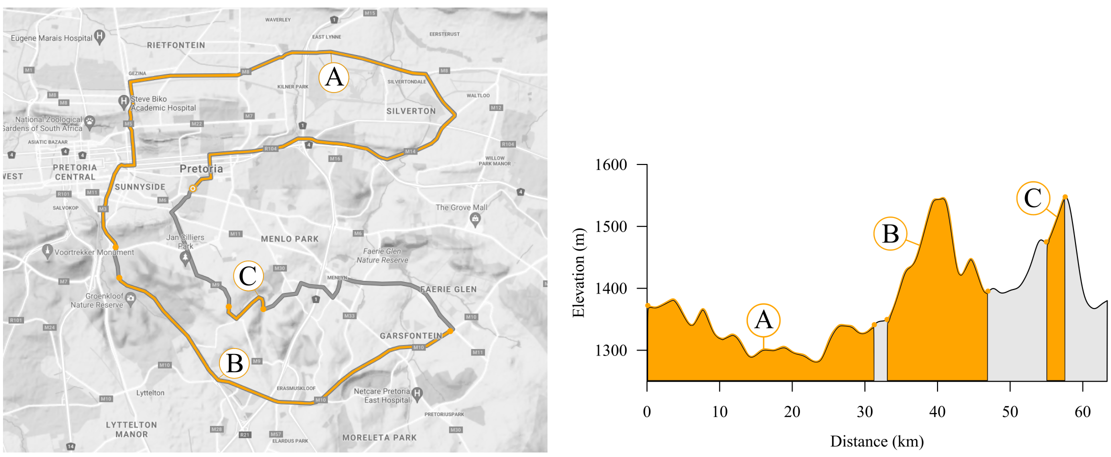


Figure 4.7: Emissions from the RRV during the first five minutes of each PEMS trip.

4.2.2 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 road sections on the C-route are used to compare the total emissions generated between different road types (Figure 4.8): *urban*, located around the city centre, *freeway*, with allowed speeds of 80–120km/h and *steep* (suburban) sections, with lower speeds in "stop & go" traffic conditions.



(a) Road sections on map

(b) Road section elevation

Figure 4.8: Different road sections used for pollutant comparison per vehicle type, where A = *Urban*, B = *Freeway* and C = *Steep (suburban)*.

The purpose of this comparison is to show, irrespective of the cumulative emissions over the entire C-route, how accurately the MATSim model simulates emissions generated on different road types.

Table 4.2 shows the calculated proportion of pollutant emissions accounted for by MATSim's emission model. This emphasises the *factor* by which the simulation overestimates (shaded cells) or underestimates the actual emissions measured on the specific road section of the C-route. When MATSim underestimates the light vehicle's CO_2 emissions on the urban road section, Table 4.2 indicates that the simulation only accounts for *0.78*, or 78% of the observed (true) emissions. Similarly, when MATSim overestimates the light vehicle's NO_x emissions on the freeway section, the estimated value is indicated as *2.16* times (216%) greater than observed from the PEMS test.

Table 4.2: The proportion of PEMS emissions accounted for by MATSim on different road sections of the C-route. Overestimations are indicated with shaded cells.

		Light vehicle		**Heavy vehicle**	
Pollutant	Road type	PEMS emissions (g)	MATSim proportion	PEMS emissions (g)	MATSim proportion
CO_2	Urban	5 500.67	*0.78*	22 789	*0.83*
	Freeway	2 175.66	*0.86*	10 393	*0.83*
	Steep	501.29	*0.53*	3 235	*0.36*
CO	Urban	18.89	*0.71*	61.97	*0.40*
	Freeway	10.72	*0.24*	16.24	*0.44*
	Steep	2.79	*0.09*	9.31	*0.12*
NO_x	Urban	2.59	*2.39*	201.44	*0.18*
	Freeway	1.48	*2.16*	91.00	*0.17*
	Steep	0.39	*0.83*	28.43	*0.09*

Note: a value close to 1.0 is a better estimate.

The most prominent distinction between emissions estimation is that of the NO_x pollutants. The simulation comes close to the observed emissions on steep sections for the light vehicle, but greatly overestimates these emissions for urban and freeway sections. In stark contrast to the light vehicle, the heavy vehicle's NO_x emissions are severely *underestimated*. This correlates with the observation that NO_x emissions often exceed the approval test in real-world driving conditions, especially for heavy (diesel) vehicles (RAC, 2020).

"Stop & go" traffic conditions also 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, especially on these short road sections, with MATSim's average speed emissions model based on Handbook Emission Factors for Road Transport (HBEFA). This is in line with Frey et al. (2003), which find emission models are limited in their ability to predict short-term variation in pollutant emissions.

The absence of road *grade* in the emissions model, in line with Wyatt et al. (2014), may further explain the differences found between estimated and real driving emissions. HBEFA's extracted emission factors incorporated into MATSim's emission model does not (currently) compensate for road grade. This might be causing the inconsistencies in emissions estimation we see in Table 4.2.

In a section on future work (chapter 5) the author mentions the influence of road grade as the (possible) underlying factor of these discrepancies. A project topic is discussed to address this issue, improving the accuracy of emissions estimation for different road types.

4.2.3 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, increasing 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.

Driving behaviour is considered a cause of variation in this study's PEMS emission data. Due to a lack of trip data for the RRV (with one driver), the authors only compare the drivers of the Ford Figo. Figure 4.9 shows the different pollutant emissions for three drivers, all having performed ten trips on the C-route (±15 driving hours each).

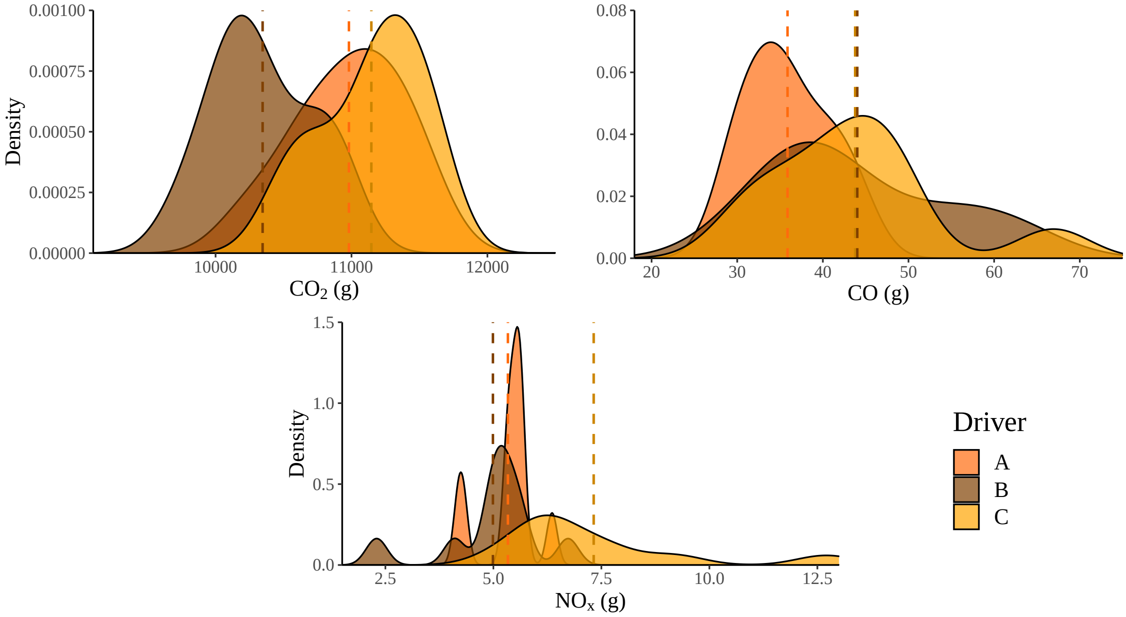


Figure 4.9: Total pollutants emitted by the Ford Figo, differentiated between drivers. Dashed lines indicate averages per driver.

Notice how driver C (yellow) seems to have a "heavy right foot" when comparing CO_2, CO and NO_x emissions with the other drivers. By solely examining driver C's emissions, he arguably fits the profile of an *aggressive* driver. Similar reasoning could be made for driver B (dark brown). Low CO_2 and NO_x emissions reflect the expectation that this would be a *cautious* driver when conducting field tests.

The results from this investigation confirm the findings of Zheng et al. (2017). Driver behaviour influences vehicle emissions and is, therefore, an essential factor for future PEMS testing.

A comprehensive analysis including the driving experience, fuel consumption, and saturation flow as factors would further support these conclusions on driving behaviour and emissions. This remains as future work.

4.2.4 Driving conditions

We have not considered different weather conditions as a factor affecting driving conditions in our simulation of emissions generation. Our European-based emissions model might be biased toward European weather conditions – much colder and wetter than South Africa. Wet road conditions change how drivers accelerate and brake, which, as we see from Zheng et al. (2017), influences our driving behaviour and consequently our emissions.

Ambient temperature influences fuel combustion, which in turn affects emissions. Bielaczyc et al. (2011) found that significant excess levels of exhaust emissions and fuel consumption is required to achieve start-up when the oil, coolant and engine block temperatures are equal or close to the ambient temperature. These cold-start emissions generally increase with low ambient (European) temperatures.

4.2.5 Summary

Consequently, we find that various factors like driving experience, driver behaviour, and driving conditions are crucial in estimating the emissions of a diverse vehicle population. We recognise that without incorporating these factors into MATSim's emission model, we would be incapable of providing reliable estimations for evaluating the generation of traffic emissions in South Africa.

This study of RDE in Gauteng, South Africa, gives insights into what we set out to accomplish in our second and third research goals. We provide these former analyses on the RDE for different road types and drivers to substantiate our assumption that variance exists in our local emission models. We address our primary research focus in this chapter of investigating and understanding the current reality of transport emissions in South Africa:

> MATSim's state of the art emissions modelling framework provides the *means* – an enabling *tool* to implement agent-based emission models for local applications. The "gap" identified between simulation and reality indicates where research focus is needed to (accurately) apply this model in a South African context.

Chapter 5

Conclusion

In this chapter, we report on how our research addressed the goals we set out to achieve. We review the simulation results from our Gauteng emissions model, the variance captured in our local simulations and elaborate on topics or projects for future work arising from this research.

5.1 Local estimations

We can not rely on our European-based emission models to produce near-perfect results compared to our South African Real Driving Emissions (RDE) tests. We attribute this remark to country-specific factors like driving elevation, vehicle age and technology, and driver behaviour influencing our vehicle fleet profiles. All of these factors contribute to the variance in our local emission models.

We set out to build an emissions model in Multi Agent Transport Simulation (MATSim)'s agent-based framework for the first research goal. We accomplished this goal in chapter 3 by creating a synthetic driver population representing the Gauteng province's vehicle population in South Africa. The traffic emissions estimated on a regional scale includes passenger cars and heavy goods vehicles in the synthetic driver population. The inclusion of these two vehicle types caters for 73.49% of the vehicles on Gauteng's road network.

We quantified and spatially aggregated the vehicle emissions to a regional level, indicating the unusual discrepancy compared to local sources. They estimate CO_2 emissions on the Gauteng road network three times that of our simulated results.

On an individual level, we depict the distribution of the per-vehicle emissions for the same period, distinguished between a passenger car and a heavy goods vehicle type. We found that on average, the simulated passenger car emits 6.07kg of CO_2, 29.9g CO and 12.6g NO_x per day. Similarly, the heavy vehicle emits 38.64kg of CO_2, 47.3g CO and 67.2g NO_x by executing its daily plan.

Based on the emissions per vehicle kilometre travelled, these figures do not even comply with Euro 4 standards for petrol and diesel vehicles. Compared to international regulations where Low Emission Zones (LEZs) necessitate fines for non-complying drivers with unacceptable EU-rated vehicles, we (in South Africa) fall short of such standards. This is to our detriment because these standards have successfully reduced harmful traffic emissions (like CO and NO_x) by up to 85% in 25 years, contributing to the betterment of human health in urban settings (RAC, 2020).

5.2 Validation

With no means of validating our estimated emissions on a regional level, we turn to Portable Emissions Measurement System (PEMS) tests to validate RDE on an individual level, based on vehicle type. In doing so (at this level of detail), we obtain a "gold standard" of real-world driving conditions in a local context. We weigh our European-based emission model against this standard to better understand the reality of transport emissions in South Africa. With this, in chapter 4, we accomplished our second and third research goals of investigating how MATSim's emission model performs "out-of-the-box", and quantifying the *gap* between our local emissions model and RDE in South Africa.

Our PEMS tests reveal that MATSim's emission model *underestimates* the CO and CO_2 emissions generated on the 61km long test route in Pretoria, Gauteng. MATSim accounts for an encouraging 80% of the CO_2 but only 34% and 44% of the CO emitted by the heavy and light test vehicle, respectively.

We see contrasting results for NO_x emissions between the two vehicle types. While MATSim hardly accounts for a fifth of the NO_x emissions measured from the heavy vehicle, it estimates more than double the actual amount for the light vehicle.

Therefore, we find that in hindsight, our aggregate emissions estimation of the Gauteng province in chapter 3 is not that accurate, as we confirm with our PEMS validation tests in chapter 4. However, we anticipated this in chapter 1, which leads us to future work.

5.3 Future work

We aim to compensate for the variance in our local simulations, leading us yet another step closer to validated emission models for South Africa. Firstly, we identify areas for improvement in our *current* methodology that might help steer us in this direction. Then, we consider the potential for future projects arising from this research.

(a) We have yet to calibrate our model of daily plans for the synthetic Gauteng population. We mentioned how Robinson and Venter (2019) validated South African National Road Agency Limited (SANRAL)'s four-step *EMME/2* model. In our research methodology, similar to (Fourie, 2009; Zhuge et al., 2014), we convert this four-step model to a MATSim equivalent without calibrating it. This means that our simulation of "realistic" traffic conditions for 24 hours might not be valid. Addressing this would produce a model that captures traffic volumes during morning and afternoon peak periods *and* daily working hours. As a result of this, we would see realistic congestion effects representative of the Gauteng province. Consequently, we could then find the (new) variance in real-world traffic emissions compared to our estimates in MATSim, as we did in chapter 4.

(b) For our simulation, we inject the test vehicles into the 10% sample population of Gauteng. This population executes their home-work-home activities, which create travel demand during the morning and afternoon peaks. We expect that by simulating the *entire* Gauteng population, the higher traffic volume during peak periods will create even more congestion on the road network affecting our test vehicles' emission data along the C-route.

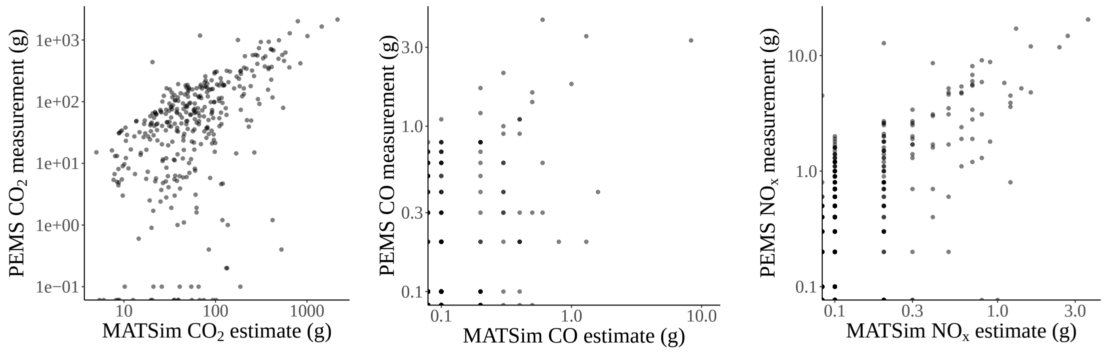
(c) The cold-start pollutant emissions are crucial for validating emission models when considering their significant contribution to RDE (Du et al., 2020). MATSim developers added the functionality to account for cold-start emissions of heavy vehicle types. At the time of writing, the author had not included this update to the MATSim emissions model of Gauteng, remaining as future work.

Now that we know the *gap* emerging from and quantified by our research goals, how do we address or fix it? Fortunately, MATSim is modular in its design. The source of emissions estimation in MATSim, Handbook Emission Factors for Road Transport (HBEFA)'s emission factors, can be adapted to bring our simulations closer to the ground truth. Alternatively, we can study the relationship between simulated emissions and ground truth, which we capture with PEMS data. This leads to the first project for possible future work:

1. We assume that the variation between our model and reality might be attributed to some external influence, like road grade. Wyatt et al. (2014) confirm 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. A parallel Masters study by Hugo (2021) on the accurate estimation of road grade in MATSim reveals that this attribute is not all that simple to estimate, contrary to the assumption that it would be straightforward to add elevation to the start and end of a network link and calculate the trigonometric slope. However, the emission factors extracted from HBEFA can be configured to compensate for road grade. Including this attribute in MATSim's emission model remains future work to address the discrepancy it might be causing for emissions estimation of different road types.

2. Our synthetic vehicle population provides detailed emission profiles for passenger cars only. We determined these profiles from our vehicle sampling strategy in section 3.3. The heavy vehicle types in our population are not allocated a specific fuel type and emissions concept. This is because we do not have a reliable way to estimate vehicle sizes and emission concepts for these vehicles yet. Performing the same sampling strategy to infer our local heavy vehicles' emission profiles will add a valuable level of detail to our synthetic population. Applying this refinement to the Gauteng emission model would provide a more accurate estimation of emissions on a regional scale, fully utilising the advantage of an agent-based simulation.

3. This research successfully identified the gap between our local emission models and what we measured as ground truth. Now, we seek a function that describes the relationship or an order ascribed to this discrepancy. Figure 5.1 presents a starting point. We plot the emission totals estimated for each link on MATSim's C-route network with the true, measured PEMS emissions on that road section. We argue that if one can quantify the relationship between local simulations and reality, we close the gap by explicitly addressing the variance in South Africa's traffic emissions.



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

Figure 5.1: Individual link emissions estimated by MATSim compared to measured values from PEMS tests for the Road-Rail Vehicle (RRV).

5.4 Summary

MATSim provides the modeller with a state of the art framework for modelling emissions on a regional scale but with individual-level detail. Researchers have advocated MATSim for its agent-based approach to emissions modelling (Kickhöfer, 2014; Shorshani et al., 2015). Our application of the agent-based framework confirms that MATSim effectively handles large-scale scenarios and enables detailed investigations on an individual level, which we utilised to address our research goals (chapter 3).

We also utilised PEMS, giving a better idea about the reality of traffic emissions in South Africa. We performed multiple PEMS tests to account for the variability associated with driver behaviour and, in doing so, obtained a “gold standard”, ground truth, which we used to identify the gap in our local emission models (chapter 4). By quantifying this gap, we report (with a better understanding) the uncertainty of traffic emissions in South Africa. Our research output presents a starting point for future studies that can produce accurate *and* representative emission models, informing policymakers to guide decision-making for setting realistic targets to benefit the country and its citizens.

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