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Integrated agent-based transport simulation and air pollution modelling in urban areas

– the example of Munich

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Abstract

Against the background of high air pollution levels in urban areas, which are often related to high traffic demand and lead to adverse effects on human health and the environment, there is a demand to develop transport policies to reduce air pollution in a sustainable way. This thesis focuses on the modelling of air pollutant concentration and, thereby, addresses three fields of research: transport modelling, air pollutant emission and atmospheric dispersion modelling. In each of these fields nowadays, specific methods and tools are increasingly developed to provide new valuable insights. However, owing to their complexity these approaches often cannot be integrated in order to analyse the impact of different transport policies on air pollution. Even though less detailed methods and tools are also available and suitable for decision making processes, they do not provide all the information necessary to understand the cause-and-effect chain.

This thesis addresses this gap by presenting a new approach, an integrated air pollution model, which simulates the complete cause-and-effect chain from changes in transport behaviour and vehicle technology to the impact on air quality.

The developed approach links agent-based transport modelling with vehicle specific emission factors based on traffic situations. As a result, it is possible to include driving dynamics, in terms of traffic situations, and vehicle attributes to calculate air pollutant emissions through the use of HBEFA emission factors. In this thesis, an emission calculation tool is first developed and integrated within the environment of the multi-agent transport simulation, MATSim. It could be shown that simulated link travel times follow measured travel times and simulated emissions correlate with sophisticated emission simulations using measured driving cycles. Additionally, this methodology is projected on the real-world scenario of the Munich metropolitan area in Germany, through a large-scale simulation with MATSim. The emission level is linked to the agent causing it, as well as to where the emission level was caused forming the basis for following the cause-and-effect-chain. By mapping emissions back to their source, i.e. the road section, a disaggregated spatial analysis of air pollutant emissions is possible.

Finally, the complete integrated approach from traffic activity to air pollution modelling is developed, validated and applied to the inner city area of Munich. A street canyon approach with respect to atmospheric dispersion modelling is applied and integrated with MATSim and the emission calculation tool. The integrated approach is able to simulate air pollutant concentrations for every street canyon and on an even more disaggregated level for several points distributed within the street canyon. Furthermore, locations with high air pollutant concentration levels, so-called hotspots, and the impact on this level due to changes in travel behaviour and vehicle technology can be determined.

With the developed approach, transport policies can be evaluated. In the case of rising car user costs, for example, through the introduction of higher fuel taxes, traffic

demand and the emission level decrease to different extents. This can be shown on an aggregated and spatially disaggregated level. Car user price elasticity of commuters differ from the one of inner-urban travel demand. The introduction of a speed limit in the inner city of Munich shows an overall decrease in car trips, a slight increase in car distance travelled by commuters and reduced air pollutant concentrations within a selected street canyon.

The integrated air pollution modelling approach allows for the evaluation of a variety of further transport policies providing aggregated impacts of changes in transport behaviour and vehicle technology on traffic demand and the emission level as well as, with respect to a spatially disaggregated level, on air pollutant emissions and concentrations. As a result, it provides a basis for future research work in the modelling of agent-based transport and environmental effects as well as the application of this approach to other cities.

Zusammenfassung

Urbane Räume weisen bei dichtem Verkehrsaufkommen häufig hohe Luftschadstoffkonzentrationen auf, die sich negativ auf die menschliche Gesundheit und die Umwelt auswirken können. Um die Luftqualität in Städten nachhaltig zu verbessern, sind effektive verkehrspolitische Maßnahmen erforderlich.

Die vorliegende Arbeit befasst sich mit der Modellierung von Luftschadstoffkonzentrationen und den damit verbundenen Verursacher-Wirkungs-Zusammenhängen. Drei verschiedene Forschungsbereiche sind darin eingebunden: die Modellierung der Verkehrsnachfrage, die Modellierung der resultierenden Luftschadstoffemissionen und die atmosphärische Ausbreitungsmodellierung von Luftschadstoffen. In jedem dieser Forschungsbereiche wurden durch die Entwicklung immer speziellerer und komplexerer Methoden neue aufschlussreiche Erkenntnisse gewonnen. Aufgrund der hohen Komplexität dieser Ansätze ist eine Zusammenführung schwierig, jedoch notwendig, um die Auswirkungen verschiedener lokaler und großräumiger verkehrspolitischer Maßnahmen auf die Luftqualität analysieren zu können. Zwar existieren einige integrierte Modelle in dieser Richtung, diese sind jedoch nicht hinreichend detailliert und können meist nicht die vollständigen Wirkungszusammenhänge und somit auch nicht die Verursacher der Luftschadstoffkonzentrationen abbilden.

Ziel der Arbeit ist es, genau diese Forschungslücke zu schließen. Eine neue integrierte Modellierung zur Berechnung der Luftschadstoffkonzentrationen wurde entwickelt. Dieses Modell ermöglicht es, die Verursacher-Wirkungs-Zusammenhänge von Veränderungen im Verkehrsverhalten und bei Fahrzeugtechnologien bis hin zu den Auswirkungen auf die Luftqualität in urbanen Räumen zu modellieren.

Die entwickelte Methodik kombiniert eine agentenbasierte Verkehrsmodellierung mit fahrzeugspezifischen Emissionsfaktoren, die zusätzlich verschiedenen Verkehrssituationen zur Beschreibung der Fahrdynamik zugeordnet werden können. Unter Berücksichtigung der Verkehrssituationen und Fahrzeugattribute werden Luftschadstoffemissionen durch Anwendung von HBEFA-Emissionsfaktoren und der multi-agentenbasierten Verkehrssimulation (MATSim) modelliert. Dabei wird gezeigt, dass die modellierten Reisezeiten weitestgehend den beobachteten Reisezeiten sowie die modellierten Luftschadstoffemissionen dem Verlauf der Emissionen eines detaillierten Emissionsmodells, das gemessene Fahrzyklus-Daten verwendet, entsprechen.

Ein wesentliches Element dieser Arbeit stellt die Projektion der Methodik zur Berechnung der Emissionen auf den Großraum München und die Entwicklung eines geeigneten MATSim-Szenarios für diesen Anwendungsfall dar. Hierbei werden die Emissionen jeweils dem Verursacher und dem Ort, an dem sie ausgestoßen werden, zugewiesen; diese Verknüpfung bildet die Grundlage zur Analyse der Wirkungszusammenhänge. Das Vorgehen ermöglicht eine verursachergerechte und

räumlich hoch aufgelöste Analyse des Emissionsniveaus. Im nächsten Schritt wird dieser Modellierungsansatz um die Modellierung der Luftschadstoffkonzentrationen für den Innenstadtbereich in München ergänzt und damit die Verursacher-Wirkungs-Zusammenhänge von der Verkehrsentstehung bis hin zur Modellierung der Luftqualität abgebildet. Die atmosphärische Ausbreitungsmodellierung basiert auf der Modellierung von Luftschadstoffkonzentrationen in Straßenschluchten. Der entwickelte Ansatz ist in der Lage, Luftschadstoffkonzentrationen für jede Straßenschlucht im Innenstadtbereich Münchens und darüber hinaus für verschiedene Punkte innerhalb von Straßenschluchten zu simulieren. Damit können Orte mit besonders schlechter Luftqualität, sogenannte Hotspots, identifiziert und Veränderungen im Verkehrsverhalten und bei den Fahrzeugtechnologien in ihren Auswirkungen auf die Luftschadstoffkonzentrationen bestimmt werden.

Mit dem integrierten Modellierungsansatz können verkehrspolitische Maßnahmen mit hohem Detaillierungsgrad evaluiert werden. Die Auswirkung von Politikinstrumenten wird im Rahmen der Arbeit anhand steigender variabler Kosten des Autofahrens analysiert. Als Ergebnis zeigt sich für München, dass durch eine solche Maßnahme die Verkehrsnachfrage und die Emissionen unterschiedlich stark sinken. Dieser Zusammenhang wird durch eine Untersuchung auf aggregierter wie auf räumlich disaggregierter Ebene belegt. Deutlich wird auch, dass die ermittelten Preiselastizitäten zwischen der Verkehrsnachfrage von Pendlern und der von Verkehrsteilnehmern im innerstädtischen Raum unterschiedlich hoch bezüglich der Reduktion des Emissionsniveaus sind. Als weitere verkehrspolitische Maßnahme wird die Einführung eines Tempolimits im Innenstadtbereich von München analysiert. Ergebnis ist, dass die Pkw-Verkehrsnachfrage deutlich sinkt, wobei die Wegelängen von Pendlern geringfügig zunehmen. Gleichzeitig werden die Luftschadstoffkonzentrationen innerhalb der untersuchten Straßenschlucht reduziert.

Die integrierte Modellierung der agentenbasierten Verkehrssimulation und der Luftschadstoffkonzentrationen ermöglicht die Evaluierung einer Vielzahl von weiteren verkehrspolitischen Maßnahmen. So können Veränderungen im Verkehrsverhalten und bei den Fahrzeugtechnologien in ihren Auswirkungen auf die gesamte Verkehrsnachfrage und das Emissionsniveau und darüber hinaus auf räumlich differenzierte Luftschadstoffemissionen und –konzentrationen analysiert werden. Das Modell bietet damit einen guten Ausgangspunkt für zukünftige Forschungsarbeiten im Bereich der agentenbasierten Verkehrsmodellierung und der Modellierung von Umwelteffekten sowie für problemangepasste Anwendungen in weiteren Städten.

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List of abbreviations

µg	microgram
µm	micrometre
h	hour
km	kilometre
kW	kilowatt
m^3	cubic metre
s	second
vkm	vehicle kilometre
CO	carbon monoxide
HC	hydrocarbons
NH_3	ammonia
NO	nitrogen monoxide
NO_2	nitrogen dioxide
NO_x	nitrogen oxides
O_3	ozone
Pb	lead
PM	particulate matter
PN	particle numbers
SO_2	sulphur dioxide
ADMS	Atmospheric Dispersion Modeling System
AERMOD	AMS/EPA Regulatory Model
AUSTAL2000	Computer programme according to the Appendix 3 of the German regulation *TA Luft*
BImSchV	Ordinance for the implementation of the Federal Immission Control Act
CALPUFF	California Puff Model
CFD	Computational fluid dynamics
COPERT	Computer Program to calculate Emissions from Road Transport
CPBM	Canyon Plume Box Model
EU	European Union
FAC2	fraction of predictions within a factor of two of observations

FB	fractional bias
GPS	Global positioning system
GRAL	Graz-Lagrangian Model
GRAMM	Graz Mesoscale Model
HBEFA	Handbook on Emission Factors for Road Transport
IARC	International Agency for Research on Cancer
LASAT	Lagrange-Simulation of Aerosol-Transport
LfU	Bavarian Environment Agency
MATSim	Multi-agent transport simulation
MICRO-CALGRID	Microscale Californian Photochemical Grid Model
MiD	Mobility in Germany
MISKAM	Microscale Flow and Dispersion Model
MOVES	Motor Vehicle Emission Simulator
MVV	Munich public transport system
NAD	normalised absolute difference
NMSE	normalised mean-squared error
NUTS	Nomenclature of Statistical Territorial Units
OSPM	Operational Street Pollution Model
PBM	Photochemical Box Model
PHEM	Passenger car and Heavy duty Emission Model
pt	public transport
RUM	Random Utility Model
TSP	total suspended particulates
VERSIT+	State-of-the art emission model
VOC	volatile organic compounds
WHO	World Health Organization

1 Introduction

1.1 Background

Urban air quality is on the political agenda whether it comes to holding the limit values in the European Union (EU) or when measuring concentration levels in Asian cities, which are far beyond any thresholds announced by the World Health Organization (WHO) and highly damaging to human health. In October 2013, the International Agency for Research on Cancer (IARC) – the specialised cancer agency of the WHO – classified outdoor air pollution as carcinogenic to humans. Reviewing the latest scientific literature, they found that there is sufficient evidence that air pollution is a leading environmental cause of death due to lung cancer. Even though air pollution is a serious problem in newly industrialised countries this finding applies to all regions worldwide (IARC, 2013; IARC, 2014). Particulary in urban areas humans are often exposed to high levels of air pollution.

According to the IARC (2013), “the predominant sources of outdoor air pollution are transportation, stationary power generation, industry, agriculture and residential heating and cooking”. Motorised traffic contributes to 25–40 % of the ambient levels of air pollution (Straif et al., 2013). In some areas the share can be even higher. Air pollutants are airborne substances that can originate from natural and from anthropogenic sources. High air pollutant concentrations lead to adverse effects on the environment and human health (Bickel and Friedrich, 2005).

The most relevant air pollutants in German cities, which are mainly related to road traffic, are nowadays particulate matter (PM) and nitrogen oxides (NO_x), especially nitrogen dioxide (NO_2), and as a secondary pollutant ozone (O_3). The European Union (EU) has initiated limit values for air pollutants, which must be complied with at air pollution measurement stations in European cities (EC, 2008). Over the past years NO_2 concentrations have shown no reduction in German cities. In 2013, the EU limit value of annual average NO_2 concentrations was exceeded at 56 % of all traffic related measurement stations. PM concentrations have been reduced in several cities over the last years, which can be mainly explained by technological improvements of exhaust gas treatment and the implementation of transport policies such as environmental zones and bans on freight traffic passing through cities. However, with respect to daily average PM concentrations, EU limit values were still exceeded at 3 % of the measurement stations in 2013. Ozone concentrations depend largely on the meteorological conditions. O_3 concentrations have reduced over the last years and exceeded the limit value only by 8 % for the averaging period 2011 - 2013 (Graff et al., 2013).

Against this background, several cities are required to reduce air pollution to comply with EU limit values. Any reductions beyond these limit values are also desirable. According to the WHO (2000, 178), “there is no evidence for a clearly defined concentration–response relationship for nitrogen dioxide exposure.” In its “Global Update 2005”, the WHO renewed its guidelines from 2000 and reviewed new scientific findings on short-term and long-term exposure to NO_2. NO_2 levels are regarded as an appropriate marker of exposure to traffic-related emissions. The main challenge in setting up reasonable guidelines is the cocktail of combustion related pollutants NO_2 is part of. If NO_2 is used as a marker for this mixture, a lower annual limit value is suggested by the WHO. Beyond complex combustion-generated pollution mixtures, some scientific studies reviewed by the WHO also support a lower NO_2 limit value than 40 $\mu g/m^3$, but the existing evidence is not sufficient for revising the limit values (WHO, 2006).[1]

Transport policies should address innovations in emission control technologies and more important, in order to develop sustainable solutions, travel behaviour. Examples of transport policies include regulations such as environmental green zone, emission standards and speed limits, pricing measures directed at travel behaviour also including internalisation strategies of external effects of traffic, measures regarding a sustainable urban and regional planning, information and communication strategies to raise public awareness for environmentally friendly transport modes as well as supportive measures of multimodal transport behaviour and low emission technologies. The effectiveness and efficiency of these transport policies can be evaluated by using quantitative or qualitative methods or a combination of both. An ex-ante evaluation of transport policies is often required to assist decision makers in designing suitable measures. Ex-post evaluations of transport policies are usually conducted to allow for policy corrections in case of undesirable developments.

Possible methodological approaches to assess air quality include the use of measured concentration data, air pollution modelling or a combination of both. Measurement stations are often sparsely distributed over an urban area, making it difficult to determine the air quality for the entire city or specific locations. Air pollution modelling allows researchers to address different scopes of air pollution. A variety of air pollution models have been developed to study air quality at different levels of detail, ranging from global and regional to microscopic approaches. Measurement data is also used for calibration purposes of air pollution modelling or as input data, for example, in the case of measured background concentration (Fenger and Tjell, 2009).

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[1] The section on the assessment of the concentration-exposure response relationship refers to Hülsmann et al. (2013).

Air pollution modelling approaches are complex and require various input data. The most important input data are air pollutant emissions caused by traffic. In the field of traffic-related emission modelling, different approaches have been developed to link travel behaviour to emission calculations. There are, on the one hand, macroscopic transport models, which are designed for large-scale scenarios often using emission factors, which show little variations in driving dynamics and vehicle technology. Microscopic traffic flow simulations, on the other hand, are suitable for the analysis of a small study area if the simulation time should remain reasonable. Emission calculations that can be linked to these transport models are often based on detailed emission models (Barlow and Boulter, 2009).

1.2 Aim and approach of the thesis

Urban areas are associated with high traffic density. Here, road traffic is a major source for air pollution in cities. The cause-and-effect chain, from traffic activity to the concentration of air pollutants and population exposure, is complex. Modelling this cause-and-effect chain and the impacts transport policies have on air pollutant concentrations requires complex methodologies, suitable modelling techniques and reliable input data. This is one of the main reasons, why traffic, emission and air pollutant concentration modelling are often separately approached. However, working with separate models and tools makes it difficult and sometimes impossible to integrate them because input and output data formats differ between the approaches and complex interfaces are needed. An integrated approach is needed to address current air quality regulations as well as to identify the right transport policies to reduce air pollutant concentrations and to achieve EU limit values. Local analyses of the impact of transport policies such as a speed limit along a single street section are possible by microscopic traffic and emission models, which provide detailed input data for microscopic air pollution modelling. However, the effects on the entire city cannot be assessed in this way. Macroscopic traffic and emission modelling would generate this large-scale information, but this approach only considers, to a limited extent, variations in driving dynamics and vehicle technology. The identification of the vehicle, i.e. person, causing the pollution is necessary to link the resulting adverse environmental effects to the polluter as well as to consider changes in individual decision making as a product of transport policies. By doing this, for example, it is possible to internalise external environmental effects and address the polluter, who causes adverse effects on a third party such as people exposed to the pollution.

Against this background an approach is here developed that (i) integrates all parts of air pollution modelling, (ii) combines both large-scale scenarios and detailed emission calculations and air quality modelling and (iii) is able to analyse transport policies. Challenging tasks are to modify and adjust existing methodologies, amend them with new methods, create seamless interfaces, prepare the data on a spatially disaggregated level, transform the data to be used for modelling and validate the interim and final results. The developed methodology is implemented for the city of Munich with respect to base and policy scenarios and, therefore, serves as a starting point for application in other cities.

The objective of the thesis is to analyse the impact of transport policies on air pollutant emissions and concentrations with a seamless and integrated approach modelling the complete cause-and-effect chain from changes in transport behaviour and vehicle technology to air quality. An integrated air pollution model is developed addressing the following main research questions:

- How can the influencing factors of air pollutant emissions be considered within the multi-agent transport simulation (MATSim), focusing on driving dynamics on a link (street section) basis and vehicle attributes?
- How can the link-based emission calculation tool be projected on a citywide modelling approach?
- How can the output and level of detail of the transport model and emission calculation tool be linked to the modelling of air pollution?
- How can single street canyon modelling be projected on a citywide modelling approach?

The focus of each chapter and how it is related to the objective of the thesis is described in the following section.

1.3 Structure

The thesis consists of six parts. Chapter 2 gives an overview of traffic-related air pollution describing sources and health impacts of air pollutants (see Section 2.1) and the political framework on emissions and air quality (see Section 2.2). This is followed by a description of air pollutant concentrations in Munich and plans on how to reduce them (see Section 2.3). Additionally, an overview of transport, emission and air quality models is provided (see Section 2.4). The subsequent three chapters address the integrated air pollution modelling approach regarding traffic modelling, the calculation of air pollutant emissions and the modelling of air pollutant concentrations in the city of Munich. In Chapter 3, the linkage between traffic and emission modelling is presented. This is followed in chapter 4 with an analysis of the effect of a traffic policy, i.e. rising car user costs, on NO_x emissions, in order to show the large-scale applicability of the approach. Chapter 5 describes the complete integrated approach of air pollution modelling and how it is able to analyse transport policies on an aggregate and local level. Chapter 6 summarises the results of chapters 3 to 5 and contains a concluding discussion on future research needs and an outlook.

Figure 1.1 shows the structure of the integrated air pollution modelling approach. Throughout this thesis the focus will be on NO_x emissions and concentrations.

However, the approach developed can be easily extended to other air pollutants, for example PM, sulphur dioxide (SO_2) and carbon monoxide (CO).

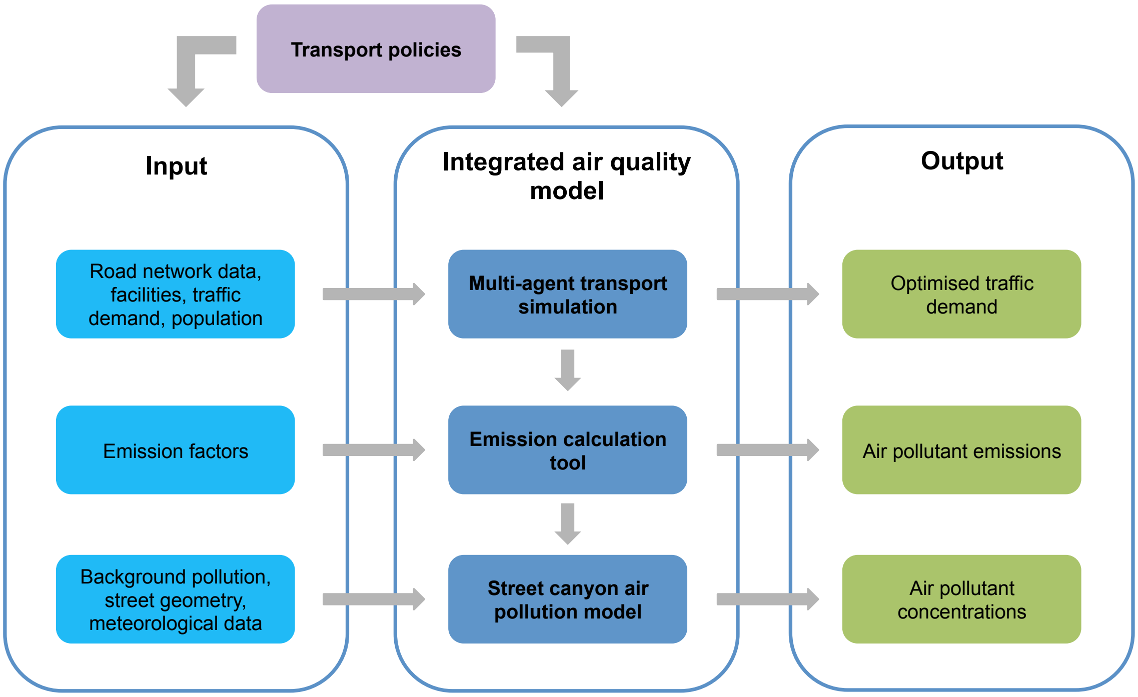

Figure 1.1: Structure of the integrated air pollution modelling approach

The integrated approach from modelling traffic activity and emissions to the simulation of air pollution, which is shown in Figure 1.1, is developed, implemented and validated in already published papers (chapters 3 to 5). A brief description of these papers is provided here:

Chapter 3 is based on *Hülsmann, F., Gerike, R., Kickhöfer, B., Nagel, K., Luz, R. (2011). Towards a multi-agent based modelling approach for air pollutants in urban regions, in Luftqualität an Straßen, Bundesanstalt für Straßenwesen, FGSV Verlag GmbH, Bergisch Gladbach, 2011, 144–166.*

In this chapter, the developed approach links the agent-based transport model MATSim with the emission factors and traffic situations of the Handbook on Emission Factors for Road Transport (HBEFA). The goal is to approximate link travel times as well as the resulting emissions of air pollutants while still being applicable to large-scale scenarios. This work aims to lay out the foundations for this innovative approach. By using MATSim it is possible to include driving dynamics in terms of stop-and-go and free-flow traffic situations as well as vehicle attributes to calculate emissions by using HBEFA emission factors. A test case is developed where link travel times are simulated and the resulting emissions are calculated for MATSim test vehicles. It could be shown that they follow approximately measured travel times, especially when the system converts to a Nash-equilibrium. A relationship between MATSim simulated emissions and emission simulations by the Passenger car and Heavy duty Emission

Model (PHEM) using measured driving cycles is shown. Further, the chapter discusses how to extend this approach to a large-scale scenario including what prerequisites are needed. The implementation of these conceptual ideas can be found in Chapter 4. Finally, the chapter analyses what additional information the model provides in order to achieve a more sustainable transport and urban planning.

Chapter 4 is based on *Kickhöfer, B., Hülsmann, F., Gerike, R., Nagel, K. (2013). Rising car user costs: comparing aggregated and geo-spatial impacts on travel demand and air pollutant emissions, in T. Vanoutrive, A. Verhetsel (eds.), Smart Transport Networks: Market Structure, Sustainability and Decision Making. NECTAR Series on Transportation and Communications Networks Research, Edward Elgar.*

This chapter investigates the calculation of air pollutant emissions for the entire urban area of Munich and studies the effects of a scenario with rising car user costs. When estimating future transportation costs for car users, there is some agreement that these costs are likely to increase over the upcoming decades. The reasons could be multifaceted: rising prices for crude oil, huge investments in alternative energy supply and in demand-side infrastructure as well as road pricing schemes or taxes in order to internalise negative external effects of road traffic. Rising costs are likely to change aggregated air pollutant emissions and result in spatially differentiated emission levels. Especially in urban areas where the road traffic demand is high, a reduction of air pollutant emissions could mitigate negative impacts on human health and the environment. The question is whether congestion relief resulting from rising car user costs can significantly reduce air pollutant emissions. For this purpose, a real-world scenario of the Munich metropolitan area in Germany is set up and simulated with MATSim. The software is capable of simulating complete daily plans of several million individuals and allows emission calculations on a detailed level, e.g. for a single street or a single vehicle over time of day. Varying emission levels due to different vehicle characteristics, road categories, speed levels and traffic situations are, hence, considered. By mapping emissions back to their source, i.e. the road section, a spatial analysis of air pollutant emissions is possible, which can identify congested areas and the change in emissions due to congestion relief. In this chapter, car user price elasticity of different user groups including commuters and inner-urban travel demand are found to be in a reasonable range. As a result, congestion relief can be shown for some formerly congested roads but also higher emissions are found along major arterials due to higher vehicle speeds above the emission minimising speed level.

Chapter 5 is based on *Hülsmann, F., Gerike, R., Ketzel, M. (2014). Modelling traffic and air pollution in an integrated approach – the case of Munich. Urban Climate, DOI information: 10.1016/j.uclim.2014.01.001.*

As road traffic is a major source for urban air pollution there is a need to link traffic models with the modelling of air pollution in order to analyse the impacts of transport policies on the environment and human health. In this chapter, an approach is developed that links MATSim with the calculation of air pollution using the Operational

Street Pollution Model (OSPM), which is a street canyon model. An overview of air pollution models and the linkage between traffic and air pollution models are given. A complete integrated approach to air pollution modelling is developed, validated and applied to the inner city area of Munich. Simulated hourly mean NO_x concentrations are compared with concentration measurements showing a similar pollution level and diurnal pattern at a site along a street canyon in Munich, Germany. NO_2 emissions and concentrations are simulated for an area bounded by the major ring road of Munich, Germany. As a result, the air pollution level along each street canyon, with several receptor points along the facades, is simulated. Locations with a high concentration level can be identified and the effects of changing traffic demand through the introduction of a speed limit are shown.

2 Traffic-related air pollution

This chapter presents fundamental information on traffic-related air pollution and discusses its relevance for this thesis. It begins with basic information on air pollutants (see Section 2.1), the political context (see Section 2.2, 2.3) and the development of air pollutant concentrations in Munich (see Section 2.3). Following this, with respect to the integrated air pollution modelling approach, this chapter provides a literature review of models and tools and a subsequent discussion on the applied modelling approaches (see Section 2.4).

2.1 Air pollutants, sources and external effects

The dominant source of air pollution in transportation in the EU is road traffic, followed by domestic and international shipping. Road traffic-related air pollutants are NO_x, PM (PM_{10} and $PM_{2.5}$), CO, hydrocarbons (HC) and sulphur oxides. With respect to NO_x, the transport sector contributes 58 % to total NO_x emissions, with road transport exhaust specifically showing a share of 33 % (EEA, 2012). Air pollutants originate from combustion processes of petrol and diesel engines, evaporation as well as from abrasion and resuspension. Under ideal conditions burning hydrocarbon fuel would react to carbon dioxide and water. Combustion processes are usually not perfect because combustion is not necessarily complete and the reactants are impure. They contain other substances such as nitrogen, sulphur and other compounds and thus perfect mixing cannot be achieved. Consequently, during combustion processes nitrogen and atmospheric oxygen react to NO_x under high temperatures. Heavy metals and sulphur oxides result as bi-products due to impure fuel. Imperfectly combusted fuel reacts to HC, CO and PM (Tiwary and Colls, 2010).

2.1.1 Particulate matter

Sources

In addition to carbon, particulate matter consists of unburnt fuel, ash, unburnt oil and sulphate and water. Particles of 1 µm or less in diameter are most damaging to human health. Policies and regulations have focused on the mass concentration of particulates, but nowadays the number of ultrafine particulates is also addressed because they may dominate the particle population. Petrol engines show lower PM emissions than diesel since diesel fuel consists of agglomerated solid carbon and ash as well as volatile organic and sulphur compounds (Tiwary and Colls, 2010). Apart from combustion, road dust, tyre and brake abrasion are further sources of PM (Ketzel et al., 2007).

Health impacts

Health impacts of PM range from irritations of mucosa to respiratory and cardiovascular diseases. Small particles with an aerodynamic diameter of 2.5 µm or less are more dangerous to human health than larger particles such as PM_{10}. $PM_{2.5}$ can penetrate into the lower respiratory tract (Tiwary and Colls, 2010).

Vehicle emission control technologies

PM emissions are decreased by particulate filters, which have been incorporated into the vehicle fleets since 2007, as initiated by governmental subsidies as well as penalties in the case of non-refitting (UBA, 2009). Furthermore, the introduction of the environmental green zone in German cities has supported the installation of particulate filters. Environmental green zones are specifically declared areas, most often in inner cities, where vehicles are only allowed to enter if they meet specific emission level requirements.

2.1.2 Nitrogen oxides and ozone

Sources

The emission level of NO_x varies based on the air-fuel ratio during the combustion process. The stoichiometric ratio is the chemically optimum air–fuel ratio. At this ratio though, NO emissions are high due to the high combustion temperatures. A lower air-fuel ratio results in comparably lower NO emissions due to less energy use and thus cooler engine conditions (Tiwary and Colls, 2010). A leaner combustion also reduces NO emissions. NO_2 is directly emitted and as secondary pollutant formed when NO reacts with ozone (O_3). Petrol engines mainly emit NO and to a very small extent NO_2, whereas for diesel engines and petrol engines based on direct injection the share of NO_2 in NO_x can be between 10 % and 60 %. A large share of NO_2 is mainly caused by the processes within oxidation catalysts. NO is oxidised to NO_2 in the oxidation catalyst (Klemp et al., 2012).

Under natural conditions, tropospheric ozone is formed by the photolysis of NO_2 (see equation 1) and the combination of oxygen atoms with oxygen molecules (see equation 2). The resulting NO reacts with O_3 to form NO_2 (see equation 3).

$$NO_2 + hv \rightarrow NO + O \tag{1}$$

$$O + O_2 + M \rightarrow O_3 + M \tag{2}$$

$$NO + O_3 \rightarrow NO_2 + O_2 \ , \tag{3}$$

where hv are photons and M is a third body molecule (e.g. N_2, O_2). By these reactions ozone background concentrations in the atmosphere are reduced. Additional ozone is formed if NO reacts with a radical to form NO_2 (see equation 4).

$$RO_2 + NO \rightarrow RO + NO_2 \; , \tag{4}$$

where RO_2 is an organic peroxy radical and NO an alkoxy radical. The formation of ozone depends on the mixing, the availability of radicals, the weather conditions and the concentration of NO_x in the atmosphere. The concentration of NO_2 as secondary pollutant depends on the availability of NO and O_3, with increasing NO_2 concentrations in the case of high NO exhaust emissions and a high level of O_3 background concentration (Fenger and Tjell, 2009).

Health impacts

NO_x emissions are part of the formation of acid rain and contribute to ozone layer depletion. In addition to adverse environmental effects, NO_2 irritates the respiratory system including bronchial reactivity and asthma, and can exacerbate chronic respiratory diseases. Long-term exposure to NO_2 can result in impaired lung functions and resistance to respiratory diseases (WHO, 2006). NO_2 has also been associated with the incidence of breast cancer and prostate cancer (Crouse et al., 2010; Parent et al., 2013).

Ozone irritates eyes and is considered harmful for the respiratory system. Asthmatic attacks are provoked and pre-existing respiratory diseases can be exacerbated due to it. Environmental impacts include the impaired ability of plants to produce and store food. This effect can already occur at low concentrations (Tiwary and Colls, 2010).

Vehicle emission control technologies

Filtering systems have been installed in most vehicles to reduce air pollution. Among these are three-way catalytic converters that have been in use since the early 90s to reduce CO, HC and NO_x. Exhaust gas recirculation, additionally, reduce NO_x emissions by recirculating small proportions of the exhaust gas back to the air inlet. Diesel engines and lean-burn petrol engines, which are an attractive alternative to conventional petrol engines due to their fuel efficiency, often come along with excessive oxygen. As a consequence, NO_2 emissions cannot be efficiently reduced as described in a previous section. In order to reduce NO_x emissions along with PM emissions further catalysts exist. Among these are the NO_x storage/reduction and selective catalytic reduction using ammonia to reduce NO_x emissions (Liu and Gao, 2011). O_3 concentrations can be reduced by decreasing the precursor hydrocarbons and NO_x emissions from the vehicle exhaust.

2.2 Policy framework

Air pollution is an important topic on the political agenda in the European Union as many cities do not meet the limit values set in the EU Directive on ambient air quality and cleaner air for Europe (EC, 2008). The EU Directive on Ambient Air Quality in 2008 is transposed into German law via the Federal Immission Control Act. The 39th Ordinance implementing the Federal Immission Control Act (BImSchV) has been modified accordingly on a one-to-one basis (The Federal Government, 2010). Table 2.1 gives an overview of the air quality standards in the EU.

Table 2.1: Air quality standards (EC, 2008)

Air pollutant	**Concentration**	**Averaging period**	**Permitted exceedances each year**	**Legal nature**
PM 2.5	25 $\mu g/m^3$	1 year	n/a	Target value entered into force 01/01/2010 Limit value enters into force 01/01/2015
PM 10	40 $\mu g/m^3$	1 year	n/a	Limit value entered into force 01/01/2005
	50 $\mu g/m^3$	24 hours	35/year	
NO_2	200 $\mu g/m^3$	1 hour	18	Limit value entered into force 01/01/2010
	40 $\mu g/m^3$	1 year	n/a	
SO_2	350 $\mu g/m^3$	1 hour	24	Limit value entered into force 01/01/2005
	125 $\mu g/m^3$	24 hours	3	
Ozone	120 $\mu g/m^3$	Maximum daily 8 hour mean	25 days averaged over 3 years	Target value entered into force 01/01/2010
CO	10 mg/m^3	Maximum daily 8 hour mean	n/a	Limit value entered into force 01/01/2005

In Germany, the 16 federal states are responsible for the enforcement of air quality standards. For most cities the compliance with EU limit values cannot be achieved because air pollutant concentrations are still too high. Therefore, under certain circumstances it is possible to postpone the deadline (BMU, 2010). If it is foreseeable or very likely that EU limit values on ambient air quality are exceeded, air quality plans for each municipality must be drawn to present the various measures reducing air pollution in order to meet the limit values. If such plans are not ambitious enough to comply with the limit values, the EU can reject the postponement of the deadline. In case of non-compliance with the EU limit values, the municipalities may face penalties (District Government of Upper Bavaria, 2013).

In addition to air quality standards, EU emission standards for passenger cars, light commercial and heavy duty vehicles exist. They regulate the emissions of NO_x, HC, CO, PM and the introduction of Euro 6 particle numbers (PN). With the introduction of the emission standard Euro 1 in 1992-93 by Directive 91/441/EEC (EEC, 1991), three-way catalytic converters in petrol vehicles have spread widely to most European countries. The emission limits for CO, HC+NO_x and PM emissions for diesel passenger cars were tightened until 2000 (Euro 3) when a separate emission limit was introduced for NO_x emissions. This was further tightened for diesel passenger cars with 250 mg/km in 2005 (Euro 4), 180 mg/km in 2009 (Euro 5) and 80 mg/km in 2014 (Euro 6). For petrol passenger cars, a NO_x emission limit of 80 mg/km has already existed since 2005 and has reached 60 mg/km (Lindqvist, 2012; EC, 2007).

With respect to Euro 6 NO_x limit values, in a vehicle emission test programme of the Dutch Ministry of Infrastructure and the Environment real-world NO_x emissions of mainly large Euro 6 diesel passenger cars were measured. It was found that measured Euro 6 NO_x emissions are higher than Euro 6 type approval emission levels. The measured real-world emission levels on motorways have been roughly stable from Euro 1 to Euro 6, whereas for traffic in urban areas a reduction is found. NO_x emission control technologies such as exhaust gas recirculation, lean NO_x trap and selective catalytic reduction have a significant impact on real-world NO_x emissions. These emission control technologies can lead to differences in the emission level between onboard measurements and type approval tests because during real-world driving conditions every technology is not necessarily switched on. There is still a need to test more Euro 6 vehicles, especially compact and small passenger cars (Ligterink et al., 2013).

Similar results were found by the Institute of Internal Combustion Engines and Thermodynamics (IVT) at TU Graz. They also tested EURO 5 passenger cars to be updated in HBEFA 3.2. NO_x emission levels of EURO 5 diesel passenger cars increased compared to EURO 4. It is found that higher speeds and engine loads lead to higher NO_x emissions. NO_x and consequently NO_2 emissions have actually not been reduced since EURO 1. With the introduction of EURO 6c in 2017/18, which includes a test procedure and limit values for real driving emissions, reductions in NO_x emissions are expected (IVT, 2013).

The emission standard for PM was also steadily reduced and reached 5 mg/km for diesel passenger cars in 2009. Regarding Euro 6, a number limit for particle numbers (PN) has been introduced by Regulation (EC) No 715/2007 (EC, 2007). A reason for this decision was that vehicle emission control technologies for PM emissions, i.e. particulate filters, have shown that a high number of ultra-fine particles can pass the filters (Lindqvist, 2012).

In order to comply with standards, emissions have to be measured using standardised test cycles. These test cycles have been developed as a requirement for automobile manufacturers in order to determine the emission level for passenger car registrations. There is gap between the emissions measured on standardised test cycles and real-world emissions though, which is due to heating and air conditioning systems as well as other auxiliary equipment (Mock et al., 2012).

Regarding heavy duty vehicles, emission standards have been tightened since 1992 with another significant difference between EURO V as introduced in 2008 and Euro VI introduced in 2013 by Regulation (EC) No 595/2009. Euro VI comprises much stricter NO_x and PM emission levels and the introduction of a number limit for particle numbers (Lindqvist, 2012; EC, 2009).

2.3 The situation in Munich

Munich is the third biggest city in Germany and is densely populated with 1,364,920 inhabitants (Federal Statistical Office, 2011). It has a monocentric structure with two major ring roads surrounding the city centre and the inner city area. The public transport network is organised radially, with public transport lines leading into and out of the city centre. In the city of Munich, 37 % of the citizens use the car, 21 % take public transport, 14 % take the bicycle and 28 % walk, as of 2008. For the entire area of the MVV (Munich public transport system), which includes the city of Munich and the suburban area, 47 % use the car, 15 % public transport, 13 % take the bicycle and 25 % walk as of 2008 (City of Munich, 2010).

In the following section, the situation of Munich related to air pollution is discussed. Air quality in cities is influenced by several different factors. Among these are the traffic situation, the meteorological conditions, the transport and diffusion of the air, and the street geometry.

Meteorological conditions

In Munich southwest winds prevail with a share of about 36 % of the hourly measured wind directions blowing from the southwest, as measured between 1998 and 2009. During this time, higher wind speeds blow from the west and lower wind speeds originate in the south and southwest. In addition, eastern and north-eastern winds occur with a relatively high share of about 22 %. Thermal inversion is also a phenomenon, which is typical for Munich. It develops during the night and can last until the next day. As a result, it prevents mixing of vertical air masses and can, therefore, deteriorate air quality because air pollutant concentration remains below the inversion layer (DWD, 2010).

Air pollution measurements

Air pollutant concentrations at measurement stations can be influenced by three main sources: local road traffic, urban background and regional background concentrations. Different measurement stations exist to identify the overall concentrations and the contribution caused by road traffic in the urban area. Traffic measurement stations are located along the major middle ring road at Landshuter Allee in Munich surrounding the inner city area, along the inner ring road at Stachus surrounding the city centre and at Prinzregentenstrasse, which is an east-west directed road located in the inner city area. They measure total concentrations including emissions from local traffic in the street and traffic from surrounding roads as well as concentrations prevailing in the region. Regional background measurement stations aim to capture the concentrations which exist in the region and which are caused by industry, emissions from domestic heating and biomass, secondary contributions and long-range transport of air pollutants. For example, in the municipality Andechs, a measurement station exists where the share of local road traffic is negligible. Finally, urban background measurement stations are installed to measure the concentrations which do not include local traffic emissions in the city. They look at traffic emissions from other roads, industrial and biogene emissions as well as emissions from domestic heating, secondary contributions and other sources such as construction sites. Urban background stations are located at Lothstrasse and Johanneskirchen.[2]

Development of air pollutant concentrations

PM_{10} concentrations show a decreasing trend from 2005 to 2012 for daily and annual average values at the measurement stations Landshuter Allee, Stachus and Lothstrasse. In 2005, at Landshuter Allee daily average values were exceeded on 107 days and at Stachus on 51 days. The EU limit value for the annual average concentrations was still exceeded in 2006. A significant drop of PM_{10} concentrations occurred in 2007 at Landshuter Allee and stayed at a similar level showing some fluctuations until 2011. Since 2012 EU limit values are complied with at both traffic measurement stations, with the consideration that regional background concentrations are comparably low since then (District Government of Upper Bavaria, 2013; LfU, 2013).

Over the last few years a different development of NO_x concentrations has been found. At traffic measurement stations NO_2 concentrations have been stagnating or even increasing since 2005. This means that average annual limit values are still exceeded. At Landshuter Allee annual average NO_2 concentrations have fluctuated around 80 µg/m^3 since 2005. There has been a decrease in NO concentration levels and

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[2] For more details see http://www.lfu.bayern.de/luft/immissionsmessungen/index.htm (accessed 27/04/2014).

ozone concentrations have been stagnating over the last few years at all measurement stations (District Government of Upper Bavaria, 2013; LfU, 2013).

Air quality plan

In 2004, the air quality plan was enacted in Munich and since then four updates have followed. Due to the exceedance of limit values regarding PM and NO_2 concentrations, the air quality plan was amended in 2007 with the establishment of a ban on heavy duty vehicles passing through the city. This was followed by the second update of the air quality plan with the introduction of the environmental green zone inside the Mittlerer Ring in 2008. Two years later the environmental green zone was further regulated by the second level in 2010, followed by the third level in 2012. The different levels imply that vehicles should exhibit a certain EU emission standard described in Section 2.2 to be allowed to drive into the environmental green zone. These measures were mainly directed at the reduction of PM concentrations. Other air quality measures were introduced by the air quality plan in 2010 addressing all relevant air pollutants. Among these were road traffic-related measures to create free flow conditions, the support of public transport and cycling as well as mobility and parking space management (District Government of Upper Bavaria, 2013).

Since air quality standards are still exceeded in Munich, a draft of the fifth update was drawn in cooperation with the district government of Upper Bavaria, the Bavarian Environment Agency (LfU) and the city of Munich at the end of 2013. It contains various transport measures, such as a 50 km/h speed limit along Landshuter Allee, feasibility studies to improve air quality and reduce noise exposure, environment oriented traffic management, support and further development of non-motorised traffic, public transport and alternative vehicle concepts such as carsharing and the use of alternative vehicle technologies (District Government of Upper Bavaria, 2013).

2.4 Modelling approaches

Variety is large when considering transport, emission and air pollution models. In the following three sections an overview of modelling approaches with respect to their characteristics, scale, limitations and applicability is given. The applied transport, emission and air pollution models and their relevance for the policy-sensitive integrated approach developed in this thesis are discussed.

2.4.1 Transport models

A range of transport models exist. Among these are the following transport models, which are used in many case studies and research projects:

- Trip-based models
- Activity-based transport models

- Agent-based transport models
- Traffic flow models

The traditional **4-stage trip model** exhibits a general framework for transport system analysis. It follows a sequence of demand procedures including trip generation, trip distribution, mode choice and route choice. Feedback mechanisms between route choice, trip distribution and mode choice are included in the modelling procedure (Hensher and Button, 2000). The 4-step modelling approach yields a unique solution of route assignment and it can be used at a macro scale for urban, region and countrywide areas. It is often accessed via a user interface, which simplifies usage and analysis of the transport data. However, some limitations exist: daily dynamics cannot be modelled and the decisions taken are agent-independent, which makes a person resolved analysis impossible (Meyer and Miller, 2001).

Activity-based transport models consider the decision making process of individual travellers. They model activity plans of all travellers. Chains of activities are derived from travel diaries and the scheduling of activities is reflected in time and space. Interpersonal distribution effects are also addressed. The quality of activity-based transport modelling depends highly on reliable input data. Activity-based transport models are suitable to model travel behaviour in urban areas (Hensher and Button, 2000; Bhat and Koppelman, 1999).

Agent-based transport simulations model traffic demand on an individual level following a stochastic, queue based traffic simulation (Cetin, 2005). With respect to the multi-agent transport simulation, MATSim, a synthetic population, which shows the demographic structure of the modelled area, is generated by using census or survey data. Initial individual traffic demand described by daily plans is executed in the physical environment. Each agent of the synthetic population chooses between different daily plans with iteratively varying activity chains to optimise individual traffic demand with respect to departure times, transport mean and routes. MATSim allows for daily time-dependent analysis keeping the agent‘s identity throughout the modelling process. It is possible for additional modules to be added to the simulation and post-processing on a person and space-resolved level. Furthermore, MATSim scenarios can be developed for modelling transport in urban areas. Nevertheless, agent-based transport models have some deficiencies because they depend on reliable input data and on a large database. Furthermore, the use of the models and user specific modifications require detailed knowledge and the computational requirements are high (Balmer, 2007; Balmer et al., 2009).

Microscopic **traffic flow models** depict each vehicle as part of the traffic flow. The interactions between the vehicles as well as their individual attributes are simulated. They follow specific rules, such as speed and lane choice, using calculation algorithms and are simulated time-discretely. Three elementary driving behaviour models exist: the car-following model, lane-changing model and route choice model. The computational requirements that come along with such detailed modelling are high.

This is why traffic flow models are often only applied to few street sections in order to precisely simulate travel behaviour (FGSV, 2006).

Figure 2.1 shows the classification of MATSim as compared to a traffic flow simulation and trip-based model with respect to the spatial and person specific resolution as well as its suitability for large-scale scenarios. The higher the resolution the more demanding the computational requirements such as simulation time, which increases with resolution.

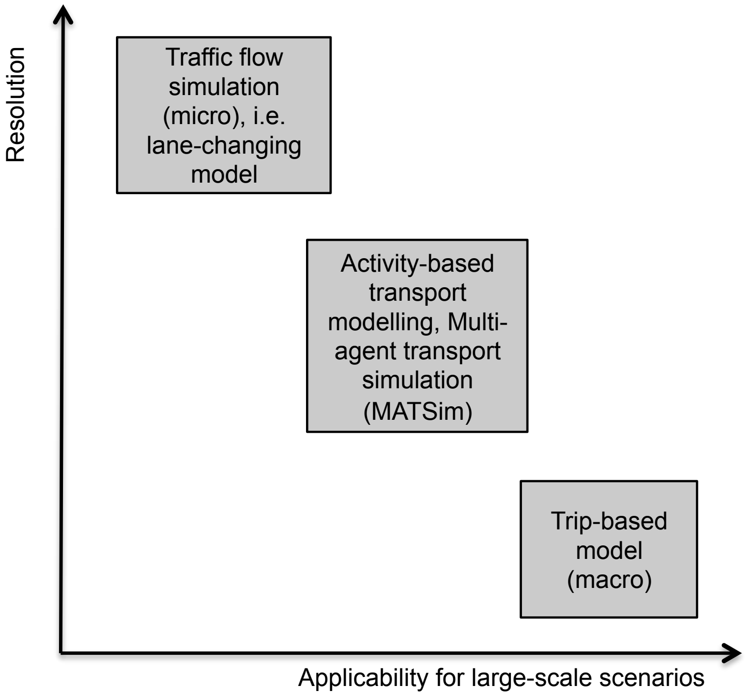

Figure 2.1: Classification of MATSim among microscopic and macroscopic transport models

2.4.2 Emission models

Emission models differ with respect to the generic model type, the level of detail and the geographic scale of application as well as the emission types (Barlow and Boulter, 2009). Three types of exhaust emissions exist: warm, cold-start and evaporative emissions. Warm emissions occur during driving, when the engine is already warmed up. Cold-start emissions develop during the warm-up phase of the engine, for example due to incomplete combustion, catalyst inefficiency or increased friction (Boulter and Latham, 2009). Evaporative emissions, which are mainly diurnal, hot soak and running losses, can develop during parking and driving due to thermal changes in the fuel system (Hausberger et al., 2005). The contribution of each emission type to the overall emission level depends on the air pollutant. The different emission models, which are described below, focus on warm emissions, which are most relevant, especially with respect to the air pollutants that are currently causing exceeded EU limit values.

Aggregated emission factors are typically applied to national and regional emission inventories and are used for environmental and strategic impact assessments. A single emission factor for a vehicle type and a general driving behaviour is used. The traffic data required is based on the area or road type. The European Environment Agency's model COPERT[3] provides a set of aggregated emission factors (Barlow and Boulter, 2009).

Average speed models, which are often used along with macroscopic transport models, relate emissions and fuel consumption to the average speed of each driving cycle for each vehicle category. Emission and fuel consumption factors are generated from chassis dynamometer measurements. Average speed models are suitable for large-scale scenarios and, for example, used by COPERT. The required input data – average trip speed –, can, for example, be obtained from trip-based models, which are common transport models applied to large-scale scenarios. Limitations exist with respect to the driving dynamics on a link because they can only be approximated by the average speed. This implies that the level of emission factors is the same for driving cycles with the same average speed, but different driving dynamics (Barlow and Boulter, 2009).

In **multiple linear regression models** a relationship between driving dynamics and emission rates is drawn. The driving dynamics are described by various model parameters and their derivatives. Speed-time profiles are used as input data and are generated by micro-simulated traffic models. The regression model is derived for the air pollutant considered and the vehicle category. The emission model, VERSIT+[4], uses such an approach and can be applied at different geographical scales with road sections at the lowest resolution. In contrast to average speed models VERSIT+ determines different emissions factors for a driving cycle and vehicle category with similar average speed but different driving dynamics (Smit et al., 2007).

Traffic situation models relate emissions and fuel consumption to vehicle categories operating in a specific type of traffic condition. A typical example is the Handbook on Emission Factors for Road Transport 3.1, which models emission factors based on a large number of predefined traffic situations (INFRAS, 2010). It follows a discrete approach based on traffic situations. Required input data to use traffic situation models are the road type, speed limit, average speed and the level of congestion. Most emission factors in HBEFA 3.1 are based on the instantaneous emission model PHEM[5]. An emission factor is assigned to each area (urban, rural, motorway), road type, speed limit and the following four traffic situations: free-flow, heavy and saturated

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[3] COPERT is a "Computer Program to calculate Emissions from Road Transport" (Samaras and Zierock, 2009).

[4] VERSIT + is a "State-of-the art emission model" (Smit et al., 2007).

[5] PHEM is a "Passenger car and Heavy duty Emission Model" (Hausberger et al., 2009).

traffic and stop-and-go. Traffic situation models are suitable for local and link-based applications, but can also be applied to regional and national inventories (INFRAS, 2010; Barlow and Boulter, 2009).

Table 2.2: Overview of the emission models based on Barlow and Boulter (2009) and Mahmod and van Arem (2008)

Generic type	**Characteristics**	**Requirements**	**Geographical scale / application**	**Example**
Aggregated emission factor models	Single emission factor for a vehicle type and general driving, simple approach	Not suitable for other situations beyond general driving	Large-scale applications	
Average speed models	Vehicle specific emission factor as a function of average trip speed.	Emission variations based on driving dynamics at the same speed are not considered	Large-scale applications, Emission inventories, local air pollution prediction models	COPERT
Traffic situation models	Emission factor related to driving cycle parameters, e.g. average speed, relative positive acceleration, share of congestion	Determination of road types and traffic situations difficult	Urban air pollution scenarios, local applications, link-based, used by many German local authorities	HBEFA
Multiple linear regression models	Multivariate regression functions to predict average emissions per vehicle over various parameters related to driving dynamics	Large and detailed traffic database required	Emission inventories	VERSIT+
Instantaneous emission models	Vehicle-specific emissions are calculated from a second-by-second basis of vehicle operation, including e.g. variations of road gradients	Driving cycle required as input data.	Link-based applications, detailed space and time resolved emission analysis	PHEM, MOVES

Instantaneous emission models are typically used at a micro-scale and are able to precisely simulate emissions. They are based on second-by-second activity data and often map the amount of emissions at a given time to the generating "engine state".

The engine power is calculated based on the driving cycle, road gradient, driving resistance and the losses in the transmission system. Typical applications are MOVES[6] of the US Environmental Protection Agency and PHEM (Abou-Senna et al. 2013; Hausberger, 2009). PHEM was mainly developed to model heavy duty vehicle emissions, but is currently also used for simulating the emissions of passenger cars and light commercial vehicles. The impact of different driving cycles, gear shift strategies, vehicle loadings, road gradients and vehicle characteristics on emissions can be simulated. Additionally, PHEM is capable of including future vehicle technologies and characteristics (Hausberger et al., 2009). In combination with transport models, a traffic flow model is required to provide the instantaneous traffic data. Instantaneous emission models are typically not used for large-scale application on a regional and national level due to their high level of detail (Mahmod and van Arem, 2008). A summary of emission models is given in Table 2.2.

2.4.3 Air pollution modelling

There is an extensive diversity of air quality models that can be applied to local and urban case studies. This section presents an overview of air pollution modelling and the diversity of different approaches followed by a more detailed description of street canyon modelling, which is applied in this thesis.

Overview of air pollution modelling

Air pollution modelling can be classified by the following criteria:

- **Model scales** range from micro (few meters) and local scales (km) via meso scales (hundreds of km) to the regional (thousands of km) and global scale. The Atmospheric Dispersion Modeling System (ADMS), Canyon Plume Box Model (CPBM) and California Puff Model (CALPUFF) are, for example, regional dispersion models, whereas the Microscale Flow and Dispersion Model (MISKAM) is a microscopic model (Fenger and Tjell, 2009; EEA, 2014).
- **Model types**: The type of air pollution models can be physical, empirical, statistical, deterministic (physical-chemical) or a combination of these. Box models are a simplified approach with respect to transport mechanisms of air pollutants, but can show complex chemical reaction schemes. Air masses are emitted into a box, in which they are physically and chemically modified assuming well-mixed and homogenous conditions. Examples are the CPBM and the Photochemical Box Model (PBM). The Gaussian plume model uses the Gaussian distribution of the plume in both directions, vertically and horizontally, and usually considers the diffusion and advection of air pollutants. The wind field is assumed to be homogenous. Limitations exist with respect to low wind

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[6] MOVES is a “Motor Vehicle Emission Simulator” (EPA, 2012).

conditions, which cannot be adequately modelled, and recirculation effects of pollutants in street canyons, which are not included. Gaussian puff models are able to include continuous emissions from the source to model temporal and spatial variations in the wind field. Gaussian plume and puff approaches are widely applied in models such as CALPUFF, the Operational Street Pollution Model (OSPM), AMS/EPA Regulatory Model (AERMOD) and the ADMS Urban. The Lagrangian model uses a box which contains the initial concentration of pollutants and trajectories particulates are moving along. The approach includes mean fluid velocity, turbulence and molecular diffusion. It is used by the Graz-Lagrangian Model (GRAL) and by the Lagrange-Simulation of Aerosol-Transport (LASAT). In contrast to the Lagrangian model, the Eulerian model simulates the fluid in a control volume, with the fluid moving through the volume. Diffusion, advection, transport and the removal of pollutant emissions are considered. Computational fluid dynamics (CFD) is a complex approach solving the Navier-Stokes equation and the continuity equation. MISKAM and the Microscale Californian Photochemical Grid Model (MICRO-CALGRID) are typical applications of the CFD (Fenger and Tjell, 2009; Gurjar et al., 2010; EEA, 2014).

- **Source types**: Point sources are typically small openings such as a stack from which air pollutants are discharged. Line sources often represent a long narrow source such as street sections, which are used by the OSPM. A large surface area is an area source. This can be a landfill source or liquid surface. The model CALPUFF, for example, can use both line and area sources. Volume sources are bulky sources as fugitive emissions from a building (Fenger and Tjell, 2012; Gurjar et al., 2010).
- **Atmospheric stability** can follow Pasquill stability classes or the Boundary Layer Scaling (Holmes and Morawska, 2006).
- **Atmospheric and traffic-related turbulence**: Vehicle induced turbulence and turbulence of ambient air represent two types of turbulence with the former applied by the OSPM and the latter by MISKAM (Holmes and Morawska, 2006).
- **Meteorology**: Some models such as the OSPM and CPBM apply measured meteorological data, for example, with respect to wind speed and wind direction. Other models use wind field modelling (Neunhäuserer et al., 2011).
- **Wind field models**: Wind field models can be diagnostic or prognostic. Diagnostic wind field models solve the mass conservation equation. Examples are CALMET and the dispersion calculation according to the Appendix 3 of the German regulation *TA Luft* – Technical Instruction on Air Quality Control (AUSTAL2000). Prognostic wind field models can solve the conservation equation for the mass, momentum and internal energy, e.g. within an Eulerian grid field. In comparison to diagnostic wind field models, obstacles such as buildings can be better simulated. Computer capacity and the running time of

such models are high. Such wind field models are used by MISKAM and the Graz Mesoscale Model (GRAMM) (Zenger, 1998; EEA, 2014).

- **Air pollutants:** Dispersion modelling is carried out for two types of air pollutants: gases and particles, which are both addressed by most models. The modelled pollutants can be SO_2, CO, NO_x, NO, NO_2, volatile organic compounds (VOC), O_3, benzene, ammonia (NH3), lead (Pb), $PM_{2.5}$ and PM_{10}, total suspended particulates (TSP) and buoyant (EEA, 2014).

Street canyon modelling

Street canyon modelling is applied to a specific location or an area. The aim is to identify the additional air pollutant concentration induced by the traffic in street canyons. In order to simulate air pollution in street canyons, dispersion models are used. Only the emission source in the simulated area is considered by these models because it depicts the source of the additional concentration. Background regional and urban concentrations are often obtained from measurement stations, which typically measure air pollutant concentrations on an hourly basis. They can also be simulated by using regional scale models.

Among street canyon modelling, screening models are found, which simulate hotspot related air pollution citywide. They represent simplified approaches generating a result per street section. These models do not consider complex building structures and topographic variations. Examples of this type of model are IMMIS^{luft} [7] and Prokas_B[8]. There are additionally more detailed models, which can be assigned to two main groups:

- Microscopic models, which simulate the dispersion processes in detail with a high spatial resolution, but come with long simulation times. Complex building structures and topographic variations are often considered. These are, for example, the dispersion model LASAT, which is a 3-dimensional Lagrangian particle model based on the guideline VDI 3945 Blatt 3. The 3-dimensional microscopic flow and dispersion model MISKAM calculates wind flow distribution and air pollutant concentration on a microscale in built-up areas.
- Semi-parametric approaches are another type of street canyon modelling. Two examples are the CPBM and the OSPM. The OSPM – Operational Street Pollution Model is developed especially for street canyons. It combines a plume for the direct impact of pollutants and a box model for the additional impact of pollutants trapped within the wind vortex (Berkowicz et al., 1997). In contrast to microscopic models, this approach is not able to consider complex building

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[7] IMMIS^{luft} models traffic induced air pollution in street canyons, see http://www.ivu-umwelt.de/front_content.php?idcat=94 (accessed 27/04/2014).

[8] Prokas_B calculates traffic induced air pollution, see http://www.lohmeyer.de/en/content/software-sales-distribution/product-overview/prokas#PROKAS_B (accessed 27/04/2014).

structures and intersections, and simplifies the dispersion processes by empirically determined constants.

In order to identify the model appropriate for a specific case study, accuracy and availability of the required input data need to be fundamental preconditions (Vardoulakis et al., 2003; Neunhäuserer et al., 2011).

2.4.4 Applied models of the integrated air pollution modelling approach

The simulation of the complete cause-and-effect chain from traffic activity to air quality requires the combination of different models and databases. With respect to transport modelling the applied transport model, MATSim, is able to simulate travel behaviour including variations in driving dynamics. It is further possible to map the caused traffic demand to the traveller and, thus, integrate vehicle attributes regarding car users. The applied emission model, HBEFA 3.1, which is based on traffic situations, is able to link the MATSim output with specific vehicle and traffic situation emission factors. HBEFA is an approved emission database, which is clearly shown by the fact that it is used in many research studies and by several municipalities to calculate the environmental effects of road traffic. The integrated use of MATSim and HBEFA is not only suitable for single street sections, but also to simulate the effect changes in vehicle technology or in travel behaviour have on emissions for large-scale scenarios. As a result, the level of emissions throughout the road network as well as the polluter can be identified. These issues, especially the linkage between MATSim and the emission calculation tool, which is based on HBEFA, as well as the projection on a large-scale scenario are addressed in chapters 3 and 4.

Up to this point the cause-and-effect chain is not complete since the emission level cannot be directly linked to the air pollution level. This is due to further influencing factors such as meteorology, street geometry and background concentration. Therefore, air pollutant concentrations are modelled in this thesis to capture the air pollution level the population is actually exposed to. The applied street canyon approach, the OSPM, is able to use not only the emissions but also traffic information directly obtained from MATSim. It calculates air pollutant concentrations from receptor points along street canyons and allows for a differentiation of concentration levels between subsections and sides of street canyons. As a result, the detailed output produced by MATSim and the emission calculation tool can be used by the OSPM to be transformed to detailed space-resolved air pollutant concentrations (Chapter 5). Microscopic models such as MISKAM would provide a higher spatial resolution than the OSPM, but they are not suitable for large-scale scenarios within a reasonable simulation timeframe.

This approach, which provides an analysis on an individual and disaggregated spatial level, forms the basis for policy analyses. It allows for the analysis of pricing measures with a higher resolution than typical macroscopic transport models. Agents can be charged, for example, with an individual toll for the emissions they cause per link. The external costs then become part of the individual decision making function of each agent in the MATSim simulation. Transport policies aimed at internalising the external effects of traffic can then be analysed. In addition, with respect to local measures such as speed limits, a spatially differentiated analysis is possible. Chapter 5 assesses, for example, the implications of a speed limit on air pollutant concentration within a street canyon. Apart from the analysis of the effect of a transport policy at the locality, this approach allows for studying the effect of a transport policy on the surrounding area and beyond, as well as identifying the population causing air pollution and where this population lives. This is, for example, important if a transport policy is directed at a specific subpopulation such as commuters to assess which part of the population actually changes its travel behaviour. Chapter 4 addresses the integration of car user costs into the individual decision making function and the impact on traffic and emissions caused by subpopulations as well as the spatial impact.

3 Towards a multi-agent based modelling approach for air pollutants in urban regions

3.1 Introduction

Environmental effects that are related to road traffic depend on various factors. The air pollutant concentration is particularly affected by the type of air pollutant, the emission level and the atmospheric conditions. In order to reduce the impacts on humans and the environment in a sustainable way, the polluter has to be identified. Furthermore, the air pollutants with high concentrations in urban areas should be focused on. These are nitrogen dioxide and particulate matter. In this context it is an important task to model and evaluate the impacts of transport policies to improve air quality.

For a detailed assessment of the environmental effects a transport model is needed that produces enough information about the travel behaviour, but is able to model an entire urban area to assess transport policies. The multi-agent transport simulation MATSim is able to simulate large-scale scenarios. It is particularly suitable for modelling the air pollution on a detailed level as complete daily plans are modelled and the traveller's identity is kept throughout the simulation process. The goal of this chapter is to link the kinematic characteristics per traveller and road section obtained from the transport model MATSim with emission factors that fit to the travel behaviour and the road category. The questions are how the parameters used in the MATSim simulation need to be set up, modified or adapted, what kinematic value serves best to calculate the emissions, what and how the emission factors should be applied.

The chapter starts with a presentation of the transportation model in Section 3.2, followed by an exposure of the emission calculation tool in Section 3.3. This basically gives an overview of the two parts to be linked. In Section 3.4, a test case is developed. It aims at showing that link travel times can be approximated in a meaningful way for each traveller on this road section. The resulting emissions of air pollutants are analysed in Section 3.5. Section 3.6 discusses what extensions of the emission calculation tool are possible and how to adapt the modelling and calculation process to a large-scale real-world scenario of the Munich metropolitan area. The chapter ends with a conclusion.

3.2 Simulation approach

This section (i) gives a brief overview of the general simulation approach the software tool MATSim uses and (ii) describes in more detail the representation of traffic flow. The understanding of the general simulation approach presented in Section 3.2.1 is relevant for the outlook towards a real-world application, given in Section 3.6.2, in order to fully capture the possibilities that MATSim opens up for transport planners and decision makers. Section 3.2.2 is relevant for the simulation runs and emission calculations presented in this chapter. For further information please refer to Raney and Nagel (2006) and Balmer et al. (2005) or to Charypar et al. (2007), respectively.

3.2.1 MATSim at a glance

In MATSim, each traveller of the real system is modelled as an individual agent. The approach consists of an iterative loop that has the following important steps:

1. **Plans generation**: All agents independently generate daily plans that encode among other things his or her desired activities during a typical day as well as the transportation mode. There is always one plan for each mode.
2. **Traffic flow simulation**: All selected plans are simultaneously executed in the simulation of the physical system.
3. **Scoring**: All executed plans are scored by an utility function which is, in this chapter, personalised for every individual by individual income.
4. **Learning**: Some of the agents obtain new plans for the next iteration by modifying copies of existing plans. This is done by several modules that correspond to the choice dimensions available: time choice, route choice and mode choice. Agents choose between their plans with respect to a Random Utility Model (RUM).

The repetition of the iteration cycle coupled with the agent database enables the agents to improve their plans over many iterations. This is why it is also called learning mechanism which is described in more detail by Balmer et al. (2005). The iteration cycle continues until the system has reached a relaxed state. At this point, there is no quantitative measure of when the system is “relaxed”; we just allow the cycle to continue until the outcome is stable.

3.2.2 Traffic flow simulation

For the simulation runs in this chapter that will focus on a single test road, only the first two steps of the overview above are relevant. For the test road, even the first step is done in a very basic way since there is no need of constructing activity locations and transportation modes based on real-world data. The mental layer within MATSim that describes the planning of activities and the behavioural learning of agents does not add additional information for the test road scenario since there are no alternatives to choose from. Therefore, only the physical layer that is responsible for traffic flow simulation is now of special interest.

MATSim currently implements a so-called queue-based traffic flow simulation (Charypar et al., 2007). This implies the following characteristics:

- Instead of travelling cars, the links (= roads) of a road network are simulated.
- Links are among others represented by parameters like flow capacity, storage capacity (deduced from length), maximum velocity and number of lanes. The flow capacity defines how many cars can leave the link in a time step. The storage capacity defines how many cars can be on the link at the same time.
- The cars that enter a link are stored in a first-in-first-out queue with their individual entry time.
- A car can only leave the link if it was at least in the queue for the free speed travel time of the link, all other cars that entered earlier already left the link and if the next link has enough storage capacity.

The reason for this rather abstract model is that it considerably reduces computation complexity and time. It therefore allows modelling large-scale scenarios with several million agents while considering upstream moving traffic jams and gridlock effects. However, its major drawback in the context of emission modelling is that there is very little information available about an agent's position during his or her time spent on a link. This makes it difficult to directly deduce driving patterns which do have big impacts on the emission level. This issue is addressed in Section 3.3.2.

3.3 Emission calculation tool

3.3.1 Overview of air pollutants and emission sources

The two air pollutants that exceed the limiting values prescribed by the European Union in several municipalities in Germany to a large extent are nitrogen dioxides and particulate matters. The concentration of PM is composed of engine exhaust gas emissions as well as abrasion and resuspension. Regarding health effects, the smaller the particle the worse the impact on humans. The effects range from damages of the respiratory system to carcinogenic effects. Only small amounts of NO_2 are emitted directly from fuel burning. However, the larger part originates from the reaction of nitrogen monoxide with ozone. Even though the nitrogen oxide concentration has been found to show lower levels nowadays than in recent years, the concentration of NO_2 in the urban area is still increasing. Such development can result from a mixture of effects, one being the introduction of oxidation catalyst and particle filters and another one being the increased ozone concentration in urban regions. A trade-off effect between NO_2 and PM can therefore be identified. NO_2 has a negative impact on the environment and human health mainly with respect to irritations of the respiratory system. Beyond nitrogen oxides and particulate matter, hydrocarbons and benzene are emitted by road traffic (Becker et al., 2009).

According to the emission factors presented in the Handbook of Emission Factors for Road Transport (INFRAS, 2010), different traffic situations exhibit different emission levels. Whereas a free flow, heavy and saturated traffic situation shows relatively similar emission factors, the stop-and-go traffic situation comes along with considerably higher emission factors. The observation applies to both emission types described above, NO_2 and PM. With respect to the overall emission calculation, a focus should be, thus, on defining the stop-and-go fraction when driving.

There are several sources of air pollution that can be assigned to road traffic: Warm emissions are emitted when the vehicle's engine is already warmed-up, whereas cold-start emissions occur during the warm-up phase. They differ with respect to the distance travelled, the parking time, the average speed, the ambient temperature and the vehicle characteristics (Weilenmann et al., 2009). Furthermore, emission sources are caused by evaporation and air conditioning, which are not further regarded in the modelling process. Cold-start emissions that have a considerable impact on the total emission level cannot be included in this study since the test case refers to a road section not considering start and end location of the travel. Therefore, only warm emissions are analysed. The other emissions types will be analysed in consecutive studies. The emissions per distance travelled differ significantly with respect to driving speed, acceleration and stop duration as well as vehicle characteristics such as fuel type (André and Rapone, 2009).

3.3.2 Methodology of the emission calculation tool

The emission tool is composed of two main steps: first, the deduction of kinematic characteristics from MATSim simulations and, second, the generation of emission factors. As described in Section 3.2.1, the MATSim approach exhibits activity chains for every agent over the entire day. Using this information, kinematic information per agent and link can be deduced. The emission tool can be executed as a post processing step of MATSim or directly integrated into the simulation. When an agent enters and leaves a link a timestamp is created. Thereby, it is possible to calculate the free flow travel time and the travel time in a loaded network for every agent and link. As MATSim keeps the demographic information until the system is relaxed, information about each agent's vehicle is available at any time. This information comprises the vehicle type, age, engine size and fuel type and is therefore relevant for emission modelling.

In the second step emission factors per air pollutant are identified. They can vary per vehicle type, road category and speed limit. Such emission factors are assigned to each agent and link the agent drives along. Emission factors are taken from HBEFA 3.1. The handbook provides emission factors depending on four traffic situations, free flow, heavy, saturated and stop-and-go. Such traffic situations show different kinematic characteristics depending on the road category and speed limit. The traffic situations are deduced from driving cycles, which are described by time-velocity profiles. Typical driving cycles form the basis for the emission factor calculation in HBEFA 3.1. In order to adjust such driving cycles to the traffic situations in Munich, they are compared with a variety of driving cycles that were collected by global positioning system (GPS) tracking on different road sections in Munich. In order to determine typical traffic situations for a specific road category and speed limit following the methodology developed by André (2004), a two-stage clustering approach is applied. A cluster represents a typical driving cycle. Important kinematic characteristics that determine the emission level are applied when clustering: stop duration, average driving speed, and relative positive acceleration. The parameter, relative positive acceleration, is chosen because it shows how steady the traffic flow behaves. By looking at the idling time an indication about the share of stop-and-go is given. In addition to these two parameters, the average speed has major influence on emission levels depending on the type of air pollutant. The resulting Munich specific traffic situations are compared with the ones in HBEFA 3.1 and adapted when the kinematic characteristics of the same road category and with the same speed limit differ.

In order to assign the emission factors to the traffic demand generated with MATSim, the driving behaviour of an agent on a certain link in the MATSim simulation is linked to the respective HBEFA driving cycle. Beyond the traffic situation the emission factors in HBEFA are further varied by vehicle and fuel type, emission EURO-class and engine size corresponding to the attributes vehicle and fuel type, age and cubic capacity provided by MATSim. In this chapter, only the fuel type is varied. The road categories of the Munich VISUM[9] road network (RSB, 2005) used in the traffic flow simulation differ from the categories defined in HBEFA. The road categories are differentiated by the number of lanes, speed limit and their function. These characteristics are used to link the road categories of the Munich VISUM road network with the HBEFA ones. The latter is less detailed, thus, a few road categories of the MATSim road network can be assigned to one HBEFA road category. HBEFA defines five road functions: a high-speed and high capacity road which can either be an urban motorway or a major arterial or ring road, a medium capacity road including arterial, distributor and district connectors, a local connector and a residential road. The test road in this work corresponds with a major arterial.

Having identified the HBEFA road category, two approaches are developed to assign the emission factors to each agent and link. First, the four typical average speed values of one road category that represent the typical four traffic situations, free flow, heavy, saturated and stop-and-go are compared with the average speed an agent drives on a link in the MATSim road network. The corresponding emission factor is then calculated by interpolating the HBEFA emission factors. The second approach divides each link into fractions representing stop-and-go and free flow traffic following the methodology

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[9] “Verkehr In Städten UMlegung“ developed by PTV AG (see www.ptv.de).

developed by Hatzopoulou and Miller (2009) with a few modifications. The difference between the actual travel time and the free flow travel time per link corresponds with travel time spent in stop-and-go. The average speed that represents a kinematic characteristic of the typical stop-and-go driving behaviour can be obtained from HBEFA. It is used to calculate the fraction of the link the agent spends in the stop-and-go traffic situation. The respective emission factors can be assigned to the resulting stop-and-go and free flow fraction.

3.4 Test scenario: Frankfurter Ring, Munich

In order to test the correctness and plausibility of the emission tool implementation, a test scenario for a single road is set up in this section. The road is named Frankfurter Ring and is located in the north of Munich. There is some data available, on the one hand from counting stations and on the other hand for a test vehicle that was driving on this road several times per day. Based on this real-world data, the traffic flow simulation in MATSim is set up and it is shown how to approximate the measured travel times with the simulation.

3.4.1 Input data and design

The test road is designed based on VISUM network information delivered by the municipality of Munich (RSB, 2005). Only one direction (east to west) along Frankfurter Ring is considered, between the counting station and the intersection Frankfurter Ring / Schleißheimer Straße, resulting in a total distance of 304 meter for this road. The network data also contains information about the total capacity of 36,000 vehicles per day and the maximum speed of 60 km/h. Since VISUM is handling aggregated traffic flows for e.g. 24 hours and MATSim is a time-dependent microsimulation model, the capacity was fine-tuned with information about traffic signals at the intersection Frankfurter Ring / Schleißheimer Straße (own calculations based on KVR, 2010). Based on this, the time-dependent flow capacities are defined as follows:

- midnight – 6am: 1,900 veh/h
- 6am – noon: 2,100 veh/h
- noon – 9pm: 2,240 veh/h
- 9pm – midnight: 1,905 veh/h

Counts data from counting stations that were provided by the municipality of Munich (KVR, 2006, 2009) give information about vehicle inflow patterns over time of day in two minutes time intervals as it is shown exemplarily in Figure 3.1 for July 07th, 2009. Based on this, individual agents are generated in MATSim format. An open question at this point is how to distribute these agents within the two minutes time bins. One could think – as a first approach – of distributing them randomly within these two minutes; as discussed further in Section 3.4.2, this seems to produce implausible results for the time-dependent link travel times. Therefore, following a second approach, the agents were told to depart all together at the end of their corresponding interval. It can be argued that this is more in line with reality since the upstream inflow is regulated by the upstream signalling system, which does not let them drive on the link equally distributed but as a bulk when the signal turns green. For a better inflow modelling, one would need input data from the upstream signalling system. But since it is not part of this project to model signal systems for a large-scale scenario, this possibility is not further examined.

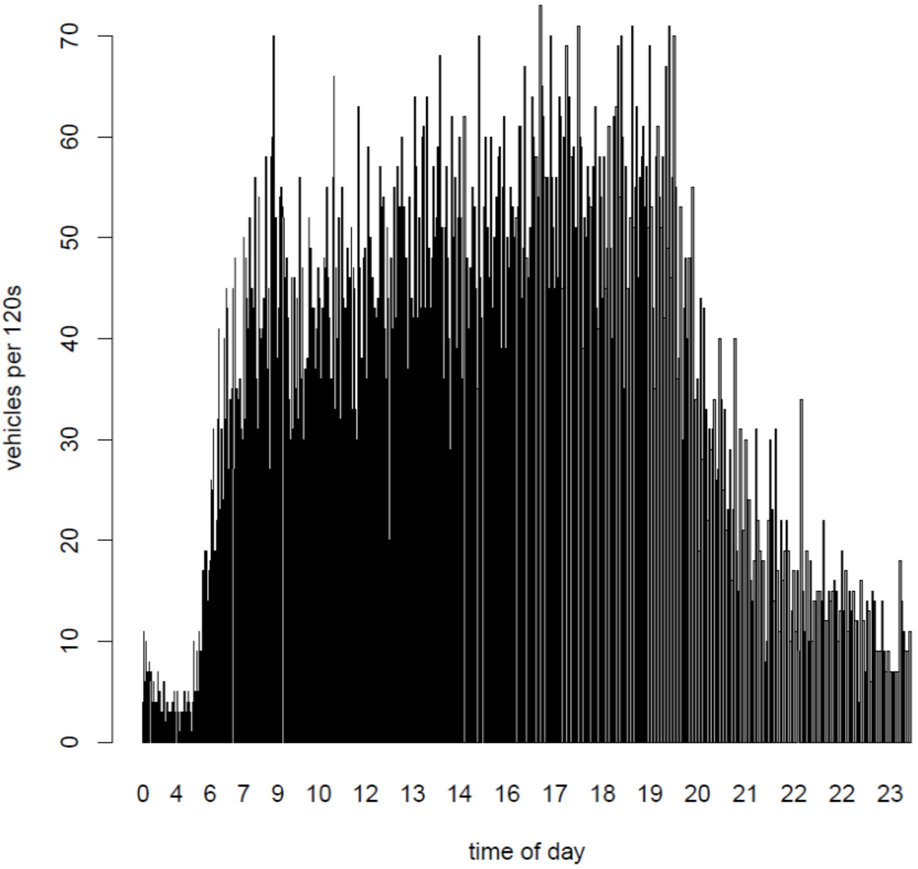


Figure 3.1: Inflow of vehicles onto the test road over time of day in 120 seconds intervals for July 07th 2009

Data for test vehicles were recorded by the Chair of Traffic Engineering and Control at Technical University of Munich (Chair of traffic engineering and control, TUM, 2009). It includes GPS data of the test vehicles driving through the city of Munich and recording information over time of day and for several days. Time-velocity profiles are of special interest in the case of emission modelling since driving patterns – including distance, travel time, acceleration and breaking between arbitrary locations – can be deduced. In a first step, this gives insights into the time-dependent traffic conditions in the network. In a second step, emissions can be calculated e.g. by the software tool PHEM and serve as benchmarks for the model. Thus, test vehicles are also generated as MATSim agents, setting their departure times equal to the real-world inflow times taken from the time-velocity profiles onto the test road. Due to the need of having data from counting stations and test vehicles available for the same days, the following eight days were selected and taken into account for analysing the simulation results: January 27th and 31st 2006, March 17th, 18th and 19th 2009 and July 07th, 08th and 09th 2009.

3.4.2 Goals and configuration

The two goals of analysing the test road are to find out (i) whether and under what conditions a plausible approximation of the link travel times is possible with MATSim and (ii) whether plausible results for emissions of diesel / gasoline cars can be obtained. For answering the first question, simulation data for the test vehicles is now compared to real-world data. The real-world data was taken from GPS tracks; it is shown in Figure 3.2a. Different configurations are tested for the simulation runs as shown in Table 3.1. For all of these configurations, the road is always assumed to have two lanes. In MATSim, where cars cannot overtake other cars, this mainly influences the storage capacity of the link and thus, in case of a traffic jam, the maximum travel time on the link. For example, when a car is driving onto a two lane link, there are double as many cars in front of it compared to a jammed single lane road. Thus, the maximum travel time is (as long as the flow capacity remains the same) exactly double as high as for a single lane road. All test scenario configurations are indexed with upper case characters (A to H) and are distinguished by (i) the flow capacity of the test road in vehicles per hour, (ii) the maximum velocity v_{max} in kilometres per hour and (iii) the distribution of departure times for all vehicles that is assumed within the two minutes time intervals of the counting stations.

Table 3.1: Overview of the eight different test scenario configurations; the selected configuration G is highlighted in green

Departure Times	**Initial flow capacity 1,900 veh/h**		**Initial flow capacity 1,400 veh/h**	
	vmax = 30 km/h	vmax = 60 km/h	vmax = 30 km/h	vmax = 60 km/h
Randomly distributed	A.	B.	C.	D.
End of interval	E.	F.	G.	H.

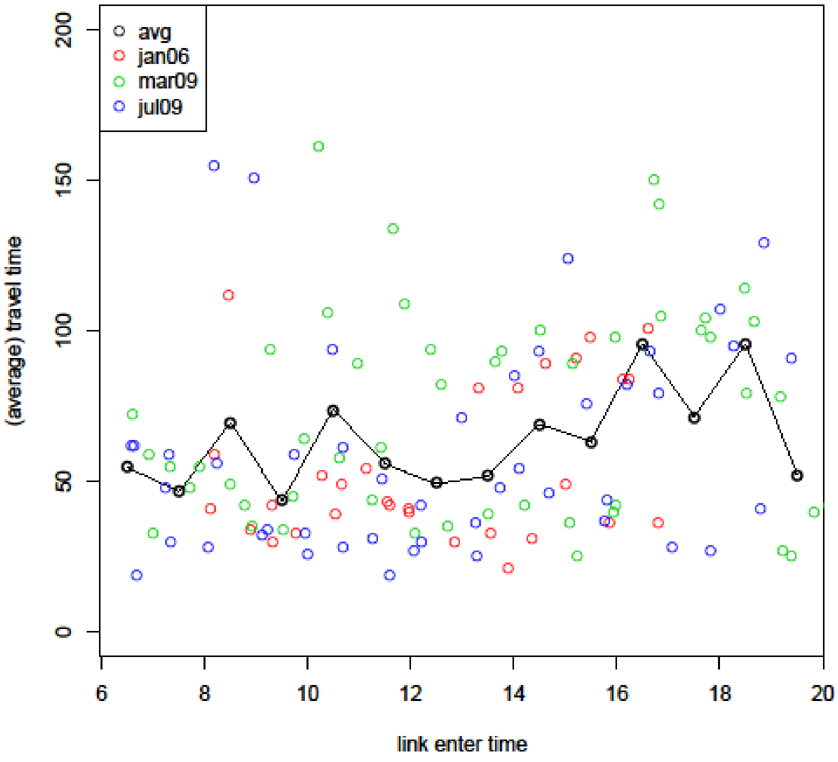
A discussion where the results of all configurations are compared to each other would exceed the scope of this work. Therefore, the main findings are summarised here:

1. The random distribution of departure times (configurations A to D) within the two minutes time intervals defined by the counting stations produces too little variations in the time-dependent link travel times. One reason is probably that cars in reality do not enter the link randomly distributed due to the upstream

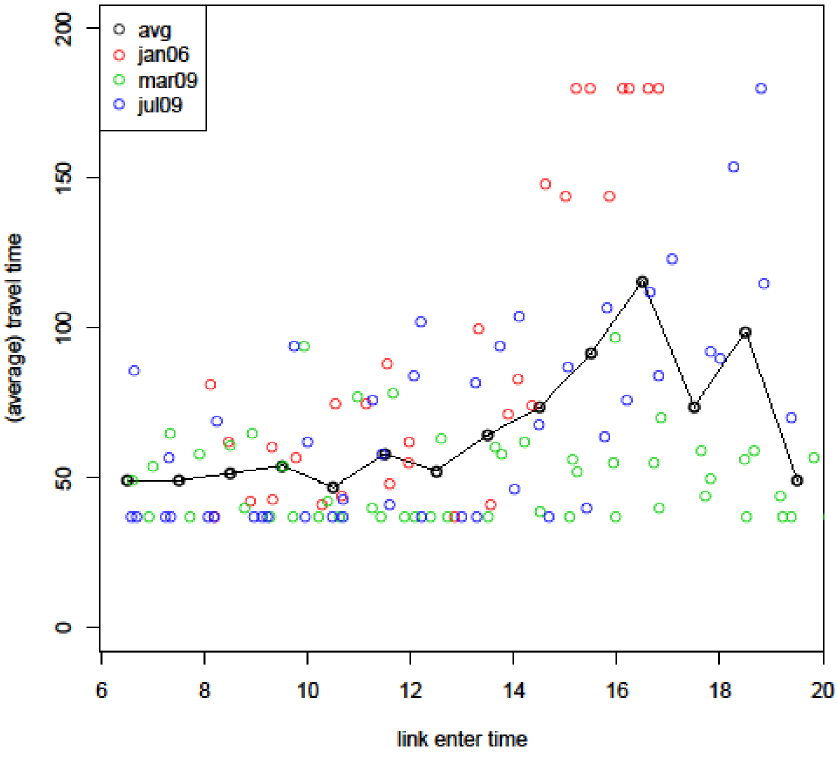
signaling systems. It is more likely that they enter the link as bulks dependent on the upstream signaling cycle. Therefore, setting departure times at the end of the time interval (configurations E to H) seems to be a plausible approximation of the upstream signaling cycles.

2. Setting the initial flow capacity of the test road to 1,900 veh/h with variations over the day also results in too little variation of the link travel times. Many agents leave the link after the minimal travel time of 19 s (for 60 km/h) or 38 s (for 30 km/h), respectively. There are two main reasons for this: on the one hand, MATSim does by default not implement time lags that occur when the first car of the queue leaves a link. On the other hand, capacities deduced from signaling plans only usually tend to be too high, since they assume that vehicles can leave the link if the signal is green. In reality, especially with mixed lanes (e.g. right and straight), cars that try to turn right might block the way of other cars wanting to go straight. This was actually observed during an inspection of this intersection. Therefore, a capacity of 1,400 veh/h was chosen.
3. The real-world data in Figure 3.2a suggest that the minimal travel time is indeed 19 s. However, due to the downstream traffic signal, the expected travel time with free flow road conditions is about double as high, e.g. when a car just misses the green phase, travel time directly adds up to about 60 s. This effect is often called phase failure which is not represented by the default MATSim setup. In order to meet the expected travel time for vehicles travelling in free flow conditions, the maximum velocity for the test road is set to 30 km/h.

For these reasons, parameter configuration G in Table 3.1 and the resulting link travel times are selected for emission modelling in the next Section. In Section 3.6.2, the question will be discussed whether and – if yes – how the above findings need to be considered when applying this model to a large-scale scenario.



(a) Travel times taken from GPS data



(b) Simulated travel times for scenario configuration G

Figure 3.2: Comparison of real-world and simulated travel times on the test road; black dots indicate the average travel times over all eight days for every hour

3.5 Results

This section compares emission levels based on MATSim output data to the emissions simulated by the emission model PHEM. Even though PHEM is a model itself and doesn't provide emission measurements there are two reasons why it is suited to be used in this analysis: it can compute the engine power demand in 1 Hz based on time-velocity profiles (Hausberger et al., 2009). Such modelling based on driving cycles provides a high level of detail since emissions per second are provided. The time-velocity profiles are segmented, according to the length of the test road, and can directly be used in PHEM. Beyond that, the emission factors of HBEFA 3.1 are mainly based on PHEM simulations. A validation of the emission calculation method applied in MATSim is therefore possible. PHEM uses driving cycles, driving resistance, losses in the transmission system and the road gradient as input parameters. The transmission ratios and a gear-shift model are used to simulate the 1 Hz course of engine speed. Transient correction functions are applied to adjust engine parameters, fuel consumption and emission levels. The HBEFA emission factors represent average values of vehicle categories and traffic situations and therefore PHEM creates models of “technology average” emission behaviour. The resulting emission maps differ by fuel type, emission EURO-class, traffic situation and road gradient (Hausberger et al., 2009).

In this study NO_x emissions are calculated for the emission EURO-class 3 (INFRAS, 2010) and for both, diesel fuel and gasoline. For EURO-class 3 passenger cars, an average rated power of 82 kilowatt is set in PHEM. Whereas PHEM simulates the emissions per second, the emission calculation tool of MATSim uses the HBEFA emission factors that measure emissions per distance. PHEM simulations are available for the driving cycles that are collected on three days, from July 07th to 09th, 2009, generating approximately one driving cycle for every hour between 6am and 8pm as described in Section 3.4.1.

Just by looking at the level of NO_x emissions based on PHEM and averaged over the three days (see Figure 3.3), it becomes obvious that at a few points in time the emission level deviates from expectations. A large deviation is found at 5pm, at which a higher traffic demand and therefore, a longer travel time resulting in a higher level of NO_x emissions is expected on average. A site inspection supports a high traffic demand at this hour. Thus, it can be stated that the NO_x emission level produced by PHEM for this hour is only based on an outlier in the data.

Emission levels based on MATSim output are calculated in two different ways:

1. Based on average speed (average speed approach)
2. Based on free flow and stop-and-go fractions (fraction approach)

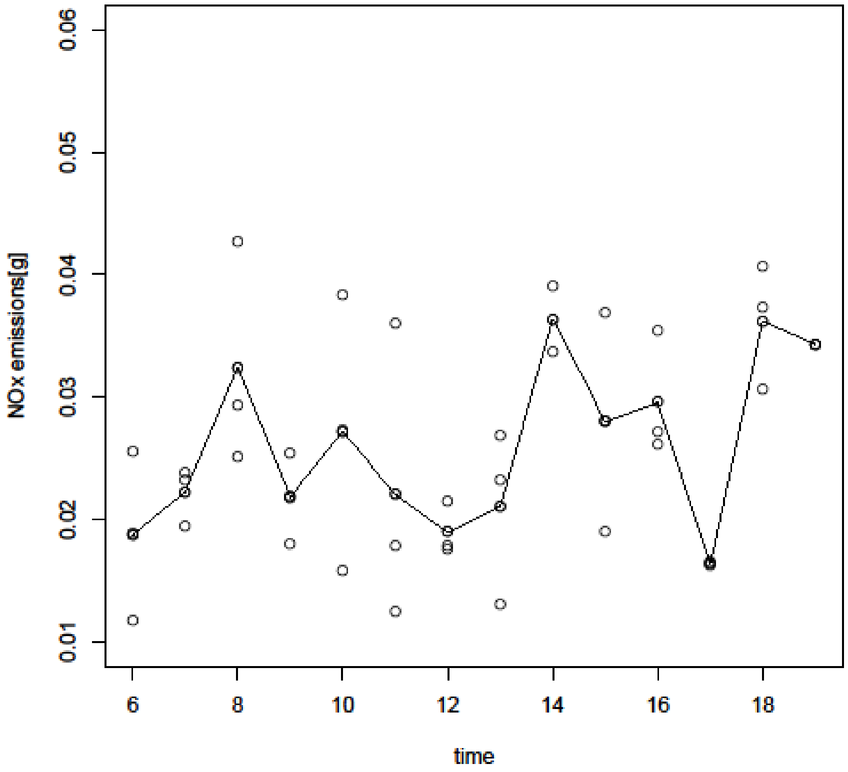


Figure 3.3: NO_x emission levels (gasoline) based on PHEM; average over three days

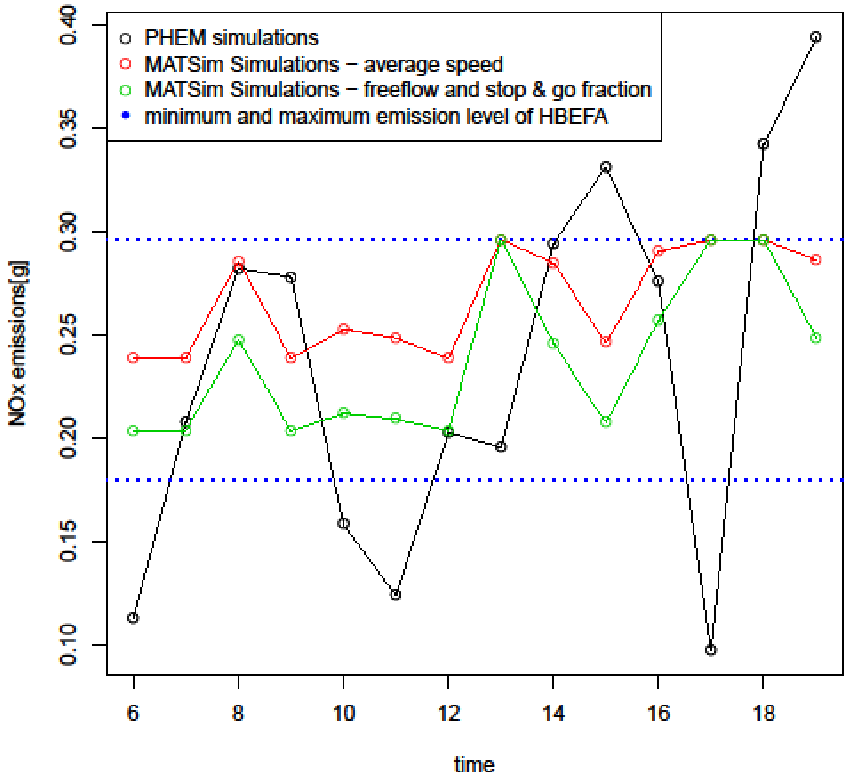
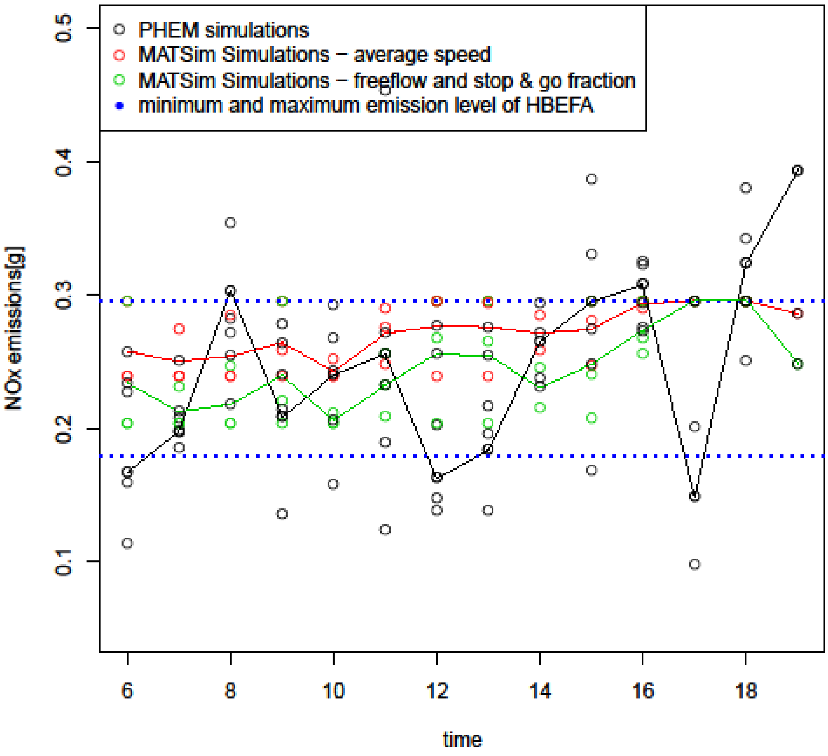
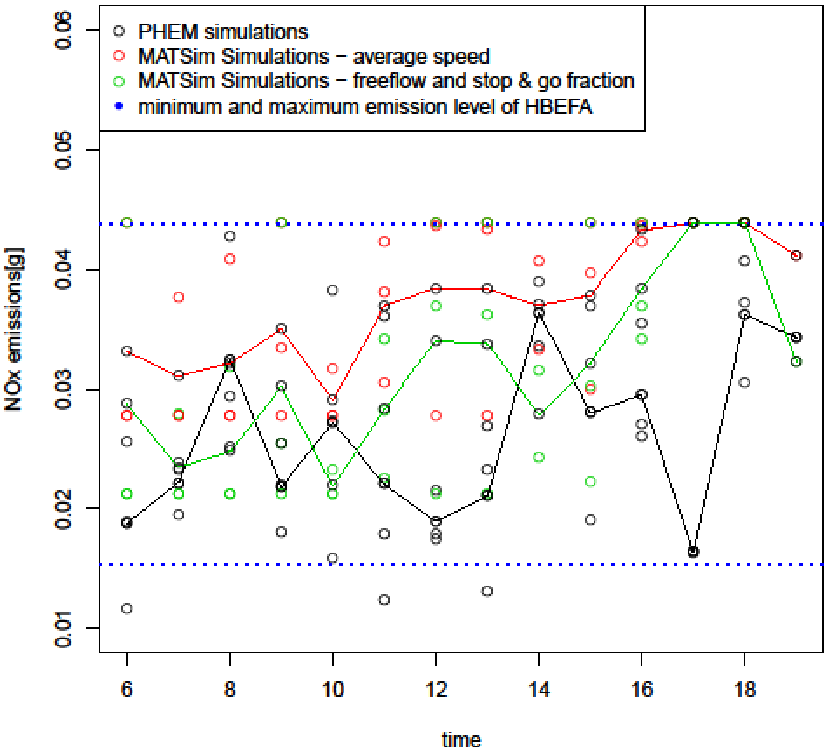


Figure 3.4: NO_x emission levels (diesel) for July 07th, 2009: in black PHEM data, in colour the two MATSim-based approaches

Figure 3.4 and Figure 3.5 show the NO_x emission levels modelled by PHEM and the emission levels calculated by the two MATSim based approaches for one day and for all three days, respectively. With respect to one day, the main reason for the deviations between the curves is the difference in travel time. Overall the course over day is similar picking up the morning peak with higher emission levels, a decrease during late morning and midday and an increase towards afternoon and evening. Figure 3.5 differentiates between emissions levels for diesel and gasoline. The points represent MATSim and PHEM simulations for each day and the curves show the average over three days. Additionally, the blue, dotted lower and upper lines represent the minimum and maximum emission levels, which can be calculated using the HBEFA emission factors. It is shown that it is not possible to simulate the emission levels that occur in reality with long travel times. Very low emission levels cannot be simulated as well. The reason is the distance based approach of HBEFA. A structural difference between the fraction approach and the average speed approach can be observed for both fuel types. The fraction approach generates on average lower emission levels than the average speed approach. Figure 3.5b shows that the fraction approach leads to a similar emission level as the PHEM results whereas the average speed approach generates on average higher emission levels than PHEM. This observation is partly supported by the course in Figure 3.5a. As it has been mentioned in Section 3.3, there is only a small difference between the emission factors of the free flow, heavy and saturated traffic situation. Therefore, it is important to determine the stop-and-go fraction, which relatively contributes the most to the overall emissions. It can be observed that the fraction approach – due to the higher resolution of traffic situations– better approximates the emissions than the average approach, which is based on one single emission factor for the entire link. Furthermore, the variations in the emission level are larger for gasoline than for the diesel fuel type. According to the HBEFA emission factors, the relative difference between emissions occurring in stop-and-go traffic situations and emissions resulting from the other three traffic situations is bigger for gasoline than for diesel.



(a) Diesel fuel type



(b) Gasoline fuel type

Figure 3.5: NO_x emission levels for PHEM and the two MATSim-based calculations (average speed and fraction approach); average over three days

Overall, the course of the emission level based on MATSim simulations shows a similar tendency as the PHEM simulations. The emission levels are generally lower during the morning peak. Towards late afternoon, where demand rises, an increase in the emission levels is found. These differences between PHEM and MATSim simulations can mainly be explained by similar deviations in travel times. In order to compare the course of the emission levels more in detail, the MATSim simulation needs to be applied to some more days. At the same time PHEM data or actual emission measurements must be available to validate such additional MATSim simulations. Here, it is shown that the emission calculation tool implemented in MATSim is able to approximate emission levels that look similar to PHEM data and shows similar tendencies over time of day.

3.6 Discussion

In this chapter, two approaches of how to link MATSim output data and HBEFA emission factors in order to calculate emission levels in a test scenario are proposed. It is shown that the resulting emissions are a possible approximation of those calculated by the very detailed model PHEM.

3.6.1 Extension of the emission calculation tool

The results have shown that it is difficult to validate simulated emission levels due to the difference in travel times when only selected driving cycles are analysed. A limitation of the emission calculation approach occurs which is based on the distance dependency of HBEFA emission factors. As a consequence it is not possible to picture the difference in emission levels between driving cycles from a certain critical value on at which stop-and-go prevails. As time-velocity profiles are available for some more days, there is actually scope for a more intensive analysis if PHEM data or actual emission measurements are available. There are still several possibilities to further differentiate the emission analysis. As described in Section 3.3.2, HBEFA emission factors and the agent’s attributes of the MATSim simulation differ both with respect to vehicle and fuel type, engine size as well as age and EURO-class, respectively. This is a major advantage of using MATSim output for emission modelling: it keeps the agent’s identity throughout the simulation. Thus, these additional attributes can be used in the post processing, the emission calculation tool. In this chapter only gasoline and diesel are differentiated because it is aimed at giving a general overview of the emission modelling. Beyond that, an interesting investigation would be to analyse the difference in emission levels with respect to the EURO-classes and cubic capacity, for example the impact of particle filters that are – for diesel vehicles – required for EURO-class 4 and newer.

Apart from warm emissions, cold-start emissions need to be assessed as they play a significant role especially in urban areas as the distances driven are short. The engine is sometimes not even warmed-up when the destination is reached leading to higher emissions throughout the travel than when the engine is already warmed-up. The emission tool will be extended in this direction.

3.6.2 Opportunities and challenges for large-scale real-world applications

When aiming at applying the approach presented in this chapter to a large-scale real-world scenario in the future, great opportunities open up in the context of policy analysis and in shifting towards a more sustainable transport and urban planning. However, there remain some challenges that need to be addressed.

When taking a closer look at the challenges, the assumptions made for the test road need to be discussed. It seems that for emission modelling in general, meeting the real-world link travel times is highly important. The need of reconstructing these in simulations of a single link test road, where agents cannot take any decisions about alternatives in terms of departure time, route or mode, led to three necessary adjustments: first, on the demand side, departure times had to be set to the end time of the counting stations intervals. Second and third, on the network side, flow capacity and maximum free speed had to be reduced in order to obtain enough heterogeneity in the link travel times. These adjustments are not applicable for large networks. Fortunately, the link travel times are correct if the system did convert to a Nash-equilibrium (Nash, 1951). Thus, these problems are expected to be minimised for large-scale applications. This will be verified for the test road in consecutive studies.

The opportunities of this approach can be characterised as follows: in a first step, it allows the mapping of emissions to households or individuals and additionally provides information *where* (on which link) and *when* (exact time of day) they are emitted. In a second step, desired policy measures can be simulated and the reactions of the whole population or different subgroups can be analysed. An example for such a policy could be raising distance based user costs for cars that are EURO-class 3 or older. It is then possible to identify winners and losers of the policy similar to Kickhöfer et al. (2010). At the same time, one could see the impact on the level of car emissions on every link over the day. Still, the overall system reaction can be calculated by aggregating the data. Furthermore, the approach presented in this chapter can easily be expanded to the modelling of external effects caused by noise emissions in urban transportation.

3.7 Conclusion

In this chapter, a methodology is developed of how to link the traffic flow simulation of MATSim to an emission calculation tool based on HBEFA. The tool uses two different approaches, one is based on average speed, the other on free flow and stop-and-go fractions. It was applied to a test scenario; it was shown that the simulated average travel times approximate the average travel times derived from driving cycles appropriately. Travel times were found to have a major impact on the total emission level. However, it is not possible to picture the emission levels that occur in reality with long travel times. The reason therefore is the distance based approach of HBEFA. The comparison between PHEM and MATSim simulated emissions shows a similar tendency of the emission level especially with respect to the late afternoon and evening hours.

The methodology developed in this chapter is a starting point to further refine the emission calculation by the integration of the test road into a large-scale application. Further emissions generated by other emission sources, such as cold-start emissions, can be added. In addition, different vehicle characteristics can be obtained from the agent's identity in the MATSim simulation. Thereby, a variety of opportunities is created to analyse several transport policies, determine the impacts on subgroups and urban quarters or canyons and be able to internalise such external effects.

4 Rising car user costs: comparing aggregated and geo-spatial impacts on travel demand and air pollutant emissions

4.1 Introduction

This chapter starts from the assumption that car user costs are about to increase in the forthcoming decades. This is likely to have impacts on aggregated air pollutant emissions and on the spatial distribution of emissions. The concentration of some air pollutants still exceeds the limiting values prescribed by the European Union, especially in urban areas. Thus, the main focus of this chapter is the question whether a decrease in car travel demand due to higher user costs would result in an overproportional reduction of air pollutant emissions. When it comes to the discussion of cost-related transport policies, large-scale transport models are needed. However, for the analysis of air pollutant emissions, a detailed investigation of the micro level is also necessary. In order to combine both objectives, a multi-agent transport model is used for our simulations. The multi-agent transport simulation MATSim is able to simulate large-scale scenarios. It is also particularly suitable for calculating air pollutant emissions on a detailed level as complete daily plans are modelled and the traveller's identity is kept throughout the simulation process. For illustration purposes of the impacts on air pollutant emissions, nitrogen dioxide is chosen. Furthermore, the transport sector is the main source of NO_2 emissions and NO_2 concentration limits are still often exceeded.

Section 4.2 describes the methodology. It starts with a presentation of the transport model in Subsection 4.2.1, followed by a description of the emission modelling tool in Subsection 4.2.2. Section 4.3 consists of three Subsections: first, a presentation of the Munich base scenario; second, a description of the simulation approach and a definition of four policy scenarios; and third, the validation of the base scenario with respect to modal split and traffic volumes. In Section 4.4 aggregated car user price elasticities of different subpopulations (inner-urban traffic, commuter, and inverse commuter) are calculated and discussed. Furthermore, car travel demand as well as NO_2 emissions are analysed on a spatially disaggregated level for all scenarios. The chapter ends with a conclusion in Section 4.5.

4.2 Methodology

This section (i) gives a brief overview of the general simulation approach of MATSim and (ii) shortly describes the emission modelling tool that is developed by the authors. In this present chapter, only general ideas will be presented. For further information, see Raney and Nagel (2006) and Appendix or Hülsmann et al. (2011).

4.2.1 Transport simulation with MATSim

In MATSim, each traveller of the real system is modelled as an individual agent. The approach consists of an iterative loop that has the following steps:

1. **Plan generation:** All agents independently generate daily plans that encode among other things their desired activities during a typical day as well as the transport mode for every intervening trip.
2. **Traffic flow simulation:** All selected plans are simultaneously executed in the simulation of the physical system.
3. **Evaluating plans:** All executed plans are evaluated by a utility function which encodes in this chapter the perception of travel time and monetary costs for the available transport modes.
4. **Learning:** Some agents obtain new plans for the next iteration by modifying copies of existing plans. This modification is done by several modules that correspond to the available choice dimensions. In this chapter, agents adapt their routes only for car trips. Furthermore, they can switch between the car and public transport modes. The choice between plans is performed with respect to a random utility model.

The repetition of the iteration cycle coupled with the agent database enables the agents to improve their plans over many iterations. This is why it is also called a learning mechanism (see Appendix). The iteration cycle continues until the system has reached a relaxed state. At this point, there is no quantitative measure of when the system is ‘relaxed’; the cycle is just allowed to continue until the outcome is stable.

4.2.2 Emission modelling tool

There are several sources of air pollution that can be assigned to road traffic: warm emissions are emitted when the vehicle’s engine is already warmed-up, whereas cold-start emissions occur during the warm-up phase. Warm emissions differ with respect to driving speed, acceleration and stop duration as well as vehicle characteristics including vehicle type, fuel type, cubic capacity and Euro-class (André and Rapone, 2009). Cold-start emissions differ with respect to distance travelled, parking time, average speed, ambient temperature and vehicle characteristics (Weilenmann et al., 2009). Furthermore, emissions also result from evaporation and air conditioning. Due to their small contribution to the overall emission level, this last source is not considered in the present chapter.

The calculation of warm emissions is composed of two steps: first, kinematic characteristics and vehicle attributes are deduced from the MATSim simulation output. Then, this information is used in order to extract emission factors from a database. MATSim exhibits activity chains for every agent over the entire day. Whenever an agent enters or leaves a road segment a time stamp is created. Thereby, it is possible to calculate the free flow travel time and the travel time in a loaded network for every agent and road segment. As MATSim keeps demographic information until the system is relaxed, information about each agent's vehicle is available at any time. Vehicle attributes are derived from survey data (see Section 4.3.1) and comprise vehicle type, age, cubic capacity and fuel type. They can, therefore, be used for very differentiated emission calculations. Where no detailed information about vehicle type is available, fleet averages for Germany are used.

Having identified the above kinematic characteristics for a road segment, specific travel behaviour resulting from such data is assigned by using the detailed handbook of emission factors called HBEFA. For some European countries including Germany, the handbook contains country specific emission factors that can vary by vehicle characteristics, road category, gradient and speed limit. The handbook provides further disaggregated emission factors depending on four traffic situations: free flow, heavy, saturated and stop-and-go. Such traffic situations are described by kinematic characteristics, which are deduced from driving cycles, i.e. time-velocity profiles. Typical driving cycles form the basis for calculating traffic situations and, thus, typical emission factors in HBEFA.

In order to assign emission factors to the traffic flows generated by MATSim, the driving behaviour of an agent on a certain road segment in the MATSim simulation is linked to the respective HBEFA driving cycle. Therefore, each road segment is divided into two parts representing stop-and-go and free flow traffic situations. A similar methodology was developed by Hatzopoulou and Miller (2010) who, in simpler approach, assume fixed exhaust emissions per time unit. This chapter uses a more detailed calculation based on different traffic situations: it is based on the assumption that cars role in free flow until they have to wait in the queue where a stop-and-go traffic situation applies. The length of the queue depends on the traffic demand on the road. If demand is higher than the capacity of a road segment, a queue emerges where stop-and-go is assumed. Another reason for the segmentation of a road segment into free flow and stop-and-go parts is due to the marginal difference between the emission factors of free flow, heavy and saturated. In contrast to these three traffic situations, the emission factors of stop-and-go are around twice as high. The difference between actual travel time and free flow travel time per road segment corresponds to travel time spent in stop-and-go. The average speed of stop-and-go that represents a kinematic characteristic of the typical stop-and-go driving behaviour can be obtained from the

HBEFA database. The stop-and-go average speed and travel time is used to calculate the queue length. The respective emission factors can be assigned to the resulting stop-and-go and free flow fractions. The implementation of the approach has been evaluated in a test scenario, which compared real traffic data with MATSim simulations for a single road segment. For a more detailed description of the emission modelling tool, please refer to Hülsmann et al. (2011).

Regarding cold-start emissions, HBEFA provides the relevant factors for passenger cars only. The application of the relevant cold-start emission factor depends on two attributes: distance travelled and parking time. The latter is calculated by subtracting the time stamp when the activity starts from the time stamp when the activity ends. The subsequent distance travelled is determined by aggregating the lengths of all road segments the agent drives along until the next activity is reached. The longer the parking time and the accumulated distance, the higher the cold-start emission factor.

In order to further process the warm and cold-start emissions, so-called emission events are generated and further segmented into a warm pollution and cold-start pollution emission event. The former describes the warm emissions for each person and road segment and adds a time stamp. Cold-start pollution is given for each person and the road segment on which the trip starts. The definition of emission events follows the MATSim framework that uses events for storing disaggregated information in XML-format (see Appendix).

4.3 Scenario: Munich, Germany

The methodology described in Section 4.2 is now applied to a large-scale scenario of the Munich metropolitan area with about two million individuals. For this purpose, a scenario needs to be set up based on network and survey data. The process is described in Subsection 4.3.1, followed by a specification of the simulation procedure in Subsection 4.3.2 and a validation in Subsection 4.3.3 where it is discussed to what extent the simulation reproduces reality.

4.3.1 Setting up the scenario

Network (supply side)

Network data was provided by the municipality of Munich (RSB, 2005). The data matches the format of the aggregated static transport planning tool VISUM.[10] It represents the road network of the federal state Bavaria, being more detailed in and around the city of Munich and less detailed further away. It consists of 92,259 nodes and 222,502 connecting edges (= links). Most road attributes, such as free speed,

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[10] Verkehr In Städten UMlegung’ developed by PTV AG, see www.ptv.de (accessed 09/04/ 2013).

capacity, number of lanes and so on, are defined by the road type. Only geographical position and length are attributes of each single link. This data is converted to MATSim format by taking length, free speed, capacity, number of lanes, and road type from VISUM data. VISUM road capacities are meant for 24-hour origin-destination matrices. Since the network is almost empty during night hours, peak hour capacity is set to VISUM capacity divided by 16 (not 24). This results in an hourly capacity of about 2,000 vehicles per lane on an urban motorway. In order to speed up computation, some road categories corresponding to small local roads are removed from the network. Furthermore, nodes with only one ingoing and one outgoing link are removed. The two resulting links are then merged, bringing the size of the network down to 17,888 nodes and 41,942 links. When merging, the two link lengths are summed up; free speed is calculated based on the minimal time needed for passing the original links; capacity is set to the minimum of the two links; the number of lanes is calculated based on the number of vehicles that fit on the two original links; and finally the road type – important input for emission calculations – is set to the one of the outgoing link.

Population (demand side)

In order to obtain a realistic time-dependent travel demand, several data sources are converted into the MATSim population format. The level of detail of the resulting individual daily plans naturally depends on the information available from either disaggregated stated preference data or aggregated population statistics. Therefore, three subpopulations are created, each corresponding to one of the three different data sources:

1. **Inner-urban traffic** (based on Follmer et al., 2004): The synthetic population of Munich is created on the base of very detailed survey data provided by RSB (2005), named ‘Mobility in Germany’ (MiD 2002). In the area of the Munich municipality, 3,612 households (with 7,206 individuals) were interviewed. The data consists of different data sets such as household data, person specific data and trip data. A detailed description of survey methods and data structure can be found in Follmer et al. (2004). Individuals were asked to report their activities during a complete day including activity locations, activity start and end times as well as the transport mode for the intervening trips. Due to privacy protection, not the exact coordinates of activity locations are available, but only the corresponding traffic analysis zones (1,066 zones in total). For the generation of the synthetic MATSim population, individual activity locations are distributed randomly within these zones. Furthermore, all incomplete datasets are removed, for example when the location or the starting times of one activity is missing in the survey. The train and bus transport modes are treated as public transport trips, motorbikes and mopeds are treated as car trips. The ride (= in car as passenger), bike and other (= unknown) transport modes are kept for the initial MATSim population. Overall, the data cleaning results in 3,957 individuals, the representative sample for demand generation. Finally, these

agents are ‘cloned’ while holding activity transport analysis zones constant but finding new random locations within these zones for every clone. This process is performed until the population reaches the real-world size of 1.4 million inhabitants. Thus, for this study the synthetic population living inside the Munich municipality boundaries consists of 1,424,520 individuals.

MiD 2002 also provides detailed vehicle information for every household. Linking this data with individuals makes it possible to assign a vehicle to a person’s car trip and thus, calculating emissions based on this detailed information. As of now there is, however, no vehicle assignment module which models intra-household decision making. It is, therefore, possible that a vehicle is assigned to more than one person at the same time.

2. **Commuter traffic** (based on Böhme and Eigenmüller, 2006): Unfortunately, the detailed data for the municipality of Munich does neither contain information about commuters living outside of Munich and working in Munich nor about people living in Munich and working outside of Munich. The data analysed by Böhme and Eigenmüller (2006) provide information about workers that are subject to the social insurance contribution with the base year 2004. Origin and destination zones are classified corresponding to the European ‘Nomenclature of Statistical Territorial Units’ (NUTS),[11] level 3. Thus, the origin-destination flows between Munich and all other municipalities in Germany are available. However, neither departure time nor transportation mode is provided. The total number of commuters tends to be underestimated since public servants and education trips are not included in this statistic. Therefore, every origin-destination relation is increased by a factor 1.29 (Guth et al., 2010). Initially, car trips are assumed to 67 % of the total commuter trips, public transport 33 % (MVV, 2007). Departure times are set so that people arrive at their workplace, according to a normal distribution with N (8 a.m., 2 hours) when routed on an empty network. Work end times are set to nine hours after the arrival at the working place. This results overall in 510,150 commuters from which 306,160 people have their workplace in Munich. All these MATSim agents perform a daily plan that encodes two trips: from their home location to work and back. Due to this simplification, they are the first contribution to “background traffic”, as it will be addressed from here on.

3. **Commercial traffic** (based on ITP/BVU, 2005): The second contribution to ‘background traffic’ is given by commercial traffic with the base year 2004. On behalf of the German Ministry of Transport, ITP/BVU (2005) published the origin-destination commodity flows throughout Germany differentiated by mode and 10 groups of commodities. Origin and destination zones inside Germany

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[11] See http://epp.eurostat.ec.europa.eu/portal/page/portal/nuts_nomenclature/introduction (accessed 18/02/2011).

are classified corresponding to NUTS 2 level, and outside Germany to NUTS 3 level, respectively. The number of trucks (> 3.5 tons) between two zones or within a zone is calculated based on the commodity flow in tons and the average loading of trucks.[12] The starting and ending points of the trips are – due to the lack of more detailed data – randomly distributed inside the origin and destination zones, respectively. The resulting MATSim agents obtain a plan that only consists of two activities with one intervening trip. Departure times are set so that the number of 'en-route vehicles' in the simulation matches a standard daily trend for freight vehicles.[13] For this scenario, trips are considered only if they are carried out at least once in Bavaria during the day. This results in 158,860 agents with one single commercial traffic trip.

Overall, the synthetic population now consists of 2,093,530 agents. To speed up computations, a 10 % sample is used in the subsequent simulations; other studies indicate that this seems to be an appropriate percentage in order to achieve results close enough to reality (see for example Chen et al., 2008). For background traffic, no detailed vehicle information is available. Emissions are, therefore, calculated with the help of fleet averages for cars and trucks from HBEFA.

4.3.2 Simulation approach

Choice dimensions

For the mental layer within MATSim, which describes the behavioural learning of agents, a simple utility-based approach is used in this chapter. When choosing between different options with respect to a random utility model, agents are allowed to adjust their behaviour among two choice dimensions: route choice and mode choice. The former allows individuals to adapt their routes on the road network when going by car. The latter makes it possible to change the transport mode for a subtour (see Appendix) within the agent's daily plan. Only a switch from car to public transport or the other way around is possible. Trips that are initially done by any other mode remain fixed within the learning cycle. From a research point of view, this approach can be seen as defining a system where public transport is a placeholder for all substitutes of the car mode.

Utility functions

In the calculations for the travel-related part of utility (see equation (A.1) in the Appendix), travel time and monetary distance costs are considered as attributes of

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[12] Estimations are based on personal correspondence with Dr Gernot Liedke from Karlsruhe Institute of Technology (10/2010).

[13] Estimations are based on personal correspondence with Dr Gernot Liedke from Karlsruhe Institute of Technology (10/2010).

every car and public transport (pt) trip. Due to the lack of data of the municipality of Munich, the utility parameters are taken from Kickhöfer (2009) who based the estimations on data from Switzerland provided by Vrtic et al. (2008). The initial formulation of the utility functions for these estimations is as follows:

$$V_{car,i,j} = \beta_0 + \beta_{tr,car} \cdot t_{i,car} + \beta_{cost,car} \cdot c_{i,car} \tag{1}$$

$$V_{pt,i,j} = \beta_{tr,pt} \cdot t_{i,pt} + \beta_{cost,pt} \cdot c_{i,pt} \ ,$$

where t_i is the travel time of the trip to activity *i* and c_i is the corresponding monetary cost. Travel times and monetary costs are mode dependent, indicated by the indices. The utilities $V_{car,i,j}$ and $V_{pt,i,j}$ for person j are computed in 'utils'. Estimating the parameters[14] $\hat{\beta}_{tr,car} = -2.26/h$, $\hat{\beta}_{tr,pt} = -2.36/h$, $\hat{\beta}_{cost,car} = -0.2/mU$, $\hat{\beta}_{cost,pt} = -0.0535/mU$, and splitting the time-related parameters into opportunity costs of time and additional disutility caused by travelling (see for example Kickhöfer et al., 2011), leads to the functional form[15] for the overall utility of an activity:

$$V_{car,i,j} = \frac{2.26}{h} t_{*,i} \cdot ln\left(\frac{t_{perf,i}}{t_{0,i}}\right) - \frac{0.2}{mU} \cdot c_{i,car} \tag{2}$$

$$V_{pt,i,j} = \frac{2.36}{h} t_{*,i} \cdot ln\left(\frac{t_{perf,i}}{t_{0,i}}\right) - \frac{0.0535}{mU} \cdot c_{i,pt} - \frac{0.1}{h} \cdot t_{i,pt} \ ,$$

In this chapter, $c_{i,car}$ and $c_{i,pt}$ are calculated for every trip by multiplying the distance between activity locations *i*–1 and *i* by a specific out-of-pocket distance cost rate for car and public transit (see below). For the functional form of the positive utility earned by performing an activity, see equation (A.2) in the Appendix. Because of the argument regarding the opportunity cost of forgone activity time when arriving early (see Appendix), the *effective* marginal disutility of early arrival is $\hat{\beta}_{early,eff} = -\hat{\beta}_{perf} \cdot t_{*,i}/t_{perf,i} \approx -\hat{\beta}_{perf} = -2.26/h$ which is equal to the effective marginal disutility of travelling by car $\hat{\beta}_{tr,car_{eff}}$. The effective marginal disutility of travelling by pt is, by the same argument, $\hat{\beta}_{tr,pt_{eff}} = -\hat{\beta}_{perf} \cdot t_{*,i}/t_{perf,i} - \left|\hat{\beta}_{tr,pt}\right| \approx -\hat{\beta}_{perf} - \left|\hat{\beta}_{tr,pt}\right| = -2.36/h$.

As a result of this simulation approach, it is possible to observe mode reactions to price increases and to derive price elasticities of demand.

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[14] Estimated parameters are in this chapter flagged by a hat. *h* is one hour and *mU* is a unit of money.

[15] The alternative specific constant β_0 (see for example Train, 2009) is estimated not significantly different from zero and is, therefore, not considered in the functional form of the utility functions. This essentially means that no general a-priori preference for one of the transport modes can be found in the data.

Simulation procedure

For 800 iterations, 15 % of the agents perform route adaption (discovering new routes), 15 % change the transport mode for a car or pt subtour in their daily plan and 70 % switch between their existing plans. Between iteration 801 and 1,000 route and mode adaption is switched off; in consequence, agents only switch between existing options. The output of iteration 1,000 is then used as input for the continuation of the base case and the four different policy cases:

1. Base case: car user costs remain constant at 10 ct/km
2. Policy case 1: increasing car user costs by 25 % to 12.5 ct/km
3. Policy case 2: increasing car user costs by 50 % to 15 ct/km
4. Policy case 3: increasing car user costs by 75 % to 17.5 ct/km
5. Policy case 4: increasing car user costs by 100 % to 20 ct/km

User costs for public transport are assumed to be constant at 17 ct/km for all policy cases. Note that the term ‘user costs’ is referred to as out-of-pocket costs for the users. All simulation runs are continued for another 500 iterations. Again, during the first 400 iterations 15 % of the agents perform route adaption while another 15 % choose between car and public transport for one of their subtours. The remaining agents switch between existing plans. For the final 100 iterations only a fixed choice set is available for all agents. When evaluating the impact of the car user cost increases, the final iteration 1,500 of every policy case is compared to iteration 1,500 of the base case.

4.3.3 Verification of the base case

Modal split

While converting the input data described by Follmer et al. (2004) into the MATSim synthetic population (see Subsection 4.3.1), some individuals were omitted due to a lack of coordinates or activity times. Therefore, Table 4.1 shows differences in the modal split over all trips comparing the input data with the synthetic subpopulation at iterations 0 and 1,500. Note that only the mode share of the subpopulation travelling within Munich is shown. As one can see, the initial synthetic population overestimates the percentage of walk trips by 2.55 % and of bike trips by 2.05 %, while underestimating the percentage of car trips by 3.52 % and of ride trips by 1.61 %. Public transport trips remain almost unchanged and the unknown mode is not discussed further due to the small number of trips. The error seems to be acceptable since no major differences occur.

When the system is in a relaxed state, car trips are even more underestimated, whereas pt trips are overestimated compared to iteration 0. Reasons might be the missing location choice module and the assumptions regarding the specification of the utility function. Overall, the additional increase in public transport and decrease in car trips amounts only to 1.6 %. Thus, the synthetic MATSim population seems to be a good starting point for analysing the change in travel demand and air pollutant emissions due to rising car user costs.

Table 4.1: Trips per transport mode as percentage of total trips; comparison between input data (Follmer et al., 2004) and the MATSim synthetic subpopulation

Mode	**Follmer et al. (2004)**	**Synthetic population it.0**	**Synthetic population it.1,500**	**Difference it.0**	**Difference it.1,500**
bike	10	12.05	12.05	+2.05	+2.05
car	26	22.48	20.88	–3.52	–5.12
pt	22	21.98	23.59	–0.02	+1.59
ride	13	11.39	11.39	–1.61	–1.61
undefined	0	0.55	0.55	+0.55	+0.55
walk	29	31.55	31.55	+2.55	+2.55

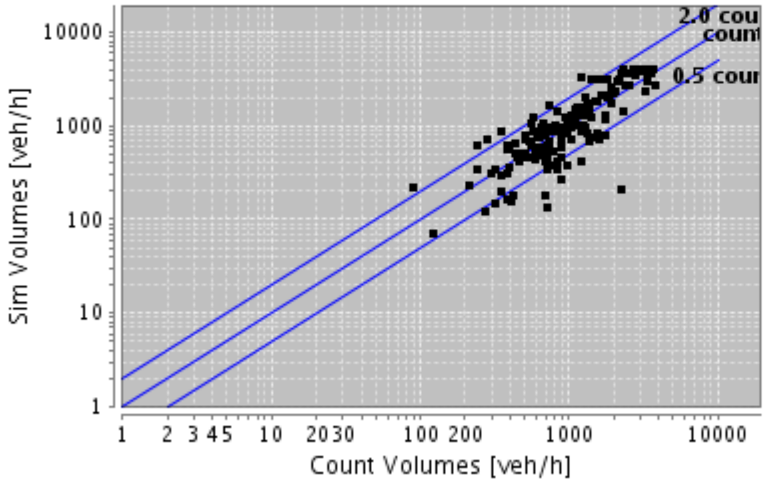
Comparison to counting stations

Before analysing demand and emission reductions, the realism of the executed plans in the simulation is verified. The interaction of individuals on the physical representation of the road network is simulated over 1,500 iterations as described in Subsection 4.2.1. After reaching a stable outcome, some kind of measurement must exist to determine the quality of the simulation output. For the Munich region, data from 166 traffic counting stations is available and aggregated for every hour over time of day.

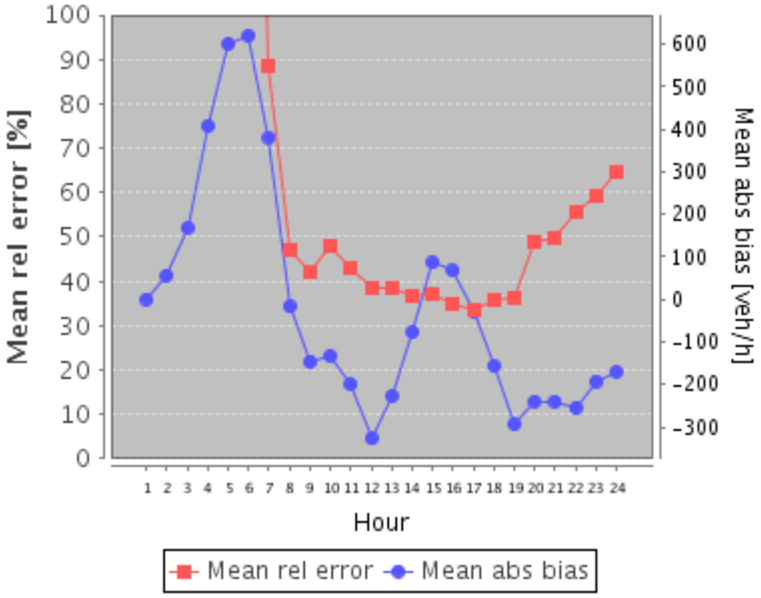
The best quality of these data is available for Thursday, January 10, 2008. It is now used to compare simulated traffic volumes to real-world values. Different statistical values can be calculated, such as mean relative error or mean absolute bias. Figure 4.1 shows two examples of standard reports that MATSim automatically generates: Figure 4.1a depicts the comparison for one hour and all counting stations. If all data points were on a 45 degree line, the simulation would nicely reproduce reality. However, as one can see, there are errors between simulated and real values. The mean relative error for every sensor is a good indicator for the overall fit of the simulation. It is calculated as:

$$MRE = \left|\frac{Q_{sim}-Q_{real}}{Q_{sim}}\right| \ , \tag{3}$$

where Q_{sim} indicates the simulated and Q_{real} the real-world vehicle flow over the corresponding counting station in the corresponding hour. Averages for a given hour are obtained by averaging over all sensors. In the example shown in Figure 4.1b, the simulation deviates strongly from reality during night hours that is from midnight until 7 a.m. During daytime, that is from 7 a.m. until the evening, the hourly mean relative error is between 30 % and 50 % with better values in the afternoon.



(a) Comparison for one hour (2 p.m to 3 p.m.)



(b) Hourly analysis over time of day

Figure 4.1: Realism of the simulation results at iteration 1,500; 166 traffic counting stations provide real-world traffic counts for the Munich municipality area

In order to reach this accuracy, some adjustments were done, for example, varying the parameters of the normal distribution that describe work arrival time peak and variance for commuters (see Subsection 4.3.1). For now, since this is meant to be a research scenario, the quality of the simulations seems to be adequate. However, by further optimising travel demand and network information, better values for the mean relative error can be obtained as Chen et al. (2008) or Flötteröd et al. (2012) showed for a scenario of Zurich, Switzerland.

4.4 The Relationship between car travel demand and air pollutant emissions

This section aims at investigating two research questions: (i) 'Are price elasticities of emissions higher than those for car travel demand?', and if yes, (ii) 'Can a spatial effect be observed?'. In Subsection 4.4.1, overall price elasticities of car travel demand are derived from the simulation and then compared to price elasticities of NO_2 emissions. In Subsection 4.4.2, first areas with high travel demand are identified in the city of Munich using a more disaggregated approach. In a second step, a spatial analysis of absolute changes in demand and NO_2 emissions is presented due to policy case 4. Then, the role of absolute changes in emissions per vehicle kilometre following the same spatial analysis is investigated.

4.4.1 Aggregated price elasticities

In this chapter, possible reactions of car users to increasing distance costs comprise either choosing shorter but eventually more time consuming routes or changing the transport mode to public transport, the placeholder for all substitutes to car.

Figure 4.2 shows the daily demand for vehicle kilometres travelled (vkm) over different distance cost factors (from 10 ct/km for the base case up to 20 ct/km for the highest policy case). The reduction in demand is presented for three different subpopulations (see Subsection 4.3.1): circles correspond to inner-urban traffic, triangles and plus signs to inverse commuter and commuter, respectively. The inner-urban demand for vehicle kilometres travelled drops from about 400,000 vkm in the base case by 18 % to roughly 333,000 vkm in the highest policy case. Much larger reductions in car travel demand are observed for the other subpopulations: car travel demand of inverse commuters drops from 1,650,000 vkm by 54 % to 754,000 vkm, and for commuters from 4,624,000 vkm by 72 % to 1,290,000 vkm. The big difference between inner-urban demand and (inverse) commuters is due to the much longer distances travelled by the last two groups where the car mode gets extremely unattractive. Travel demand reactions for freight traffic is not shown since this subpopulation is not allowed to change from car (or truck) to public transport. The figure also provides linear regression lines including their functional forms for every subpopulation. Even though, especially for commuter traffic, a linear regression obviously does not lead to the best fit (one can see the 'inverse-S-shape' produced by the logit model), it is still quite appropriate in order to derive constant price elasticities.

Choosing p_0=10 *ct/km* as the operating point, price elasticities of demand can directly be derived for every policy case *i*, using:

$$\eta_{q,p} = \frac{\frac{\mathrm{q_i - q_0}}{\mathrm{q_0}}}{\frac{\mathrm{p_i - p_0}}{\mathrm{p_0}}} \ , \tag{4}$$

where $\mathrm{q_i}$ is the travel demand at price level $\mathrm{p_i}$. In order to describe the overall relationship between user costs and car travel demand, a constant price elasticity can be derived using the regression functions:

$$\eta_{q,p} = \frac{dq}{dp} \cdot \frac{p_0}{\hat{q}_0} \ , \tag{5}$$

where $\frac{dq}{dp}$ is the gradient of the corresponding regression function and $\hat{q}_0$ is the estimated initial demand for car trips at p_0=10 *ct/km*. Applying equation (5) to the three subpopulations leads to the following estimated constant price elasticities of car travel demand:

$$\hat{\eta}_{p,q}^{Urban} = -0.173 \ , \ \hat{\eta}_{p,q}^{Inverse.Commuter} = -0.502 \ , \hat{\eta}_{p,q}^{Commuter} = -0.692.$$

These estimations indicate that, for example, a car user cost increase of 10 % (at the operating point p_0=10 *ct/km*) leads to a reduction in car trips by 1.73 % for inner-urban traffic, by 5.02 % for inverse commuter and by 6.92 % for commuter. Graham and Glaister (2002) present a wide range of fuel price elasticities collected from different studies. When summarising the different studies, the authors find short-term fuel price elasticities in the range from -0.2 to -0.5, for Germany around -0.45. However, the range within Germany goes from -0.25 to -0.86. The fuel price elasticities found in this chapter are somewhat smaller for inner-urban traffic and within the range for inverse commuter and commuter. Obviously, introducing more choice dimensions into the model, such as location choice or the possibility of dropping activities, is likely to influence the results. At this point, it can be stated that, overall, the model produces reasonable behavioural reactions to car user price increases.

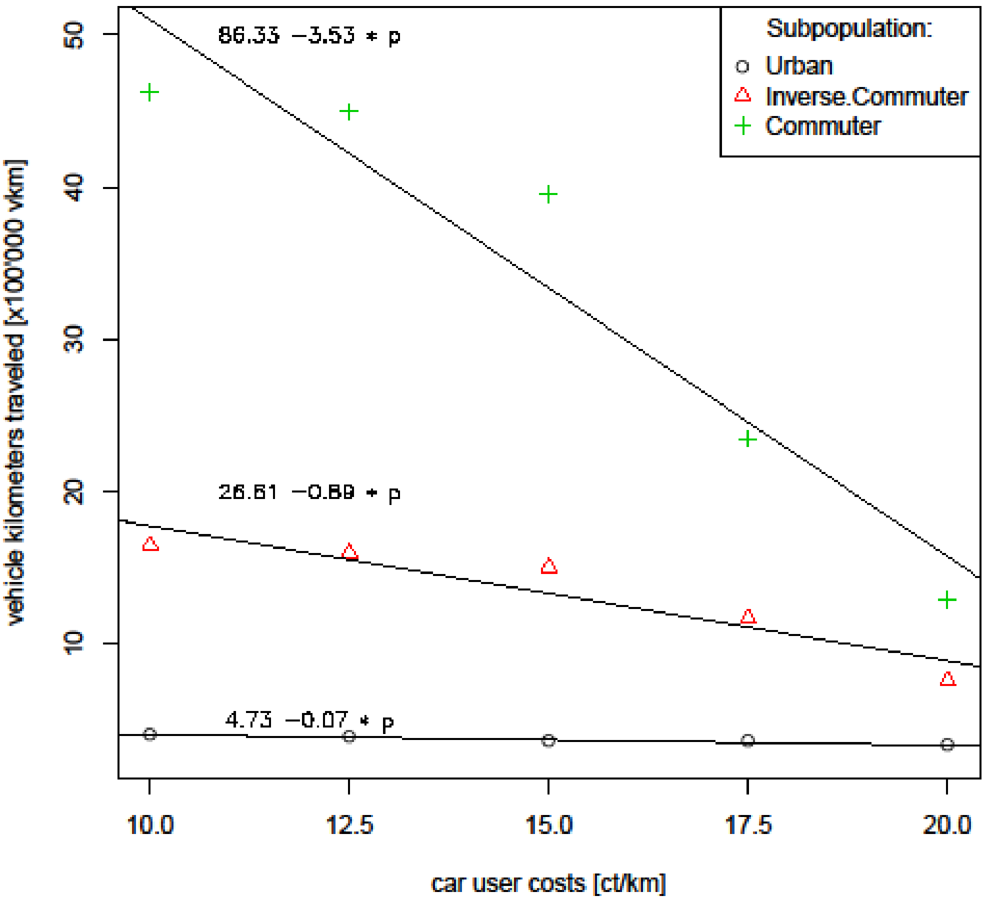


Figure 4.2: Overall daily vehicle kilometres travelled for the base case and the four policy cases by subpopulation: simulated values and estimations as linear regression functions (values for a representative 10 % sample)

Similarly to Figure 4.2, overall NO_2 emissions are shown in Figure 4.3, again for the base case and the four policy cases. Linear regression lines and functional form are also provided. In this figure, freight traffic emissions are indicated by crosses in order to show the big impact of freight traffic emissions on overall emission levels. Since freight demand is not allowed to change the mode to public transport, its emissions stay more or less stable for all policy cases. Only a small reduction can be observed, probably resulting from shorter distances chosen by the router module. Equally to the price elasticities of demand, price elasticities of NO_2 emissions are calculated:

$$\hat{\epsilon}_{p,q}^{Urban} = -0.219\ ,\ \hat{\epsilon}_{p,q}^{Inverse.Commuter} = -0.608\ ,\hat{\epsilon}_{p,q}^{Commuter} = -0.792.$$

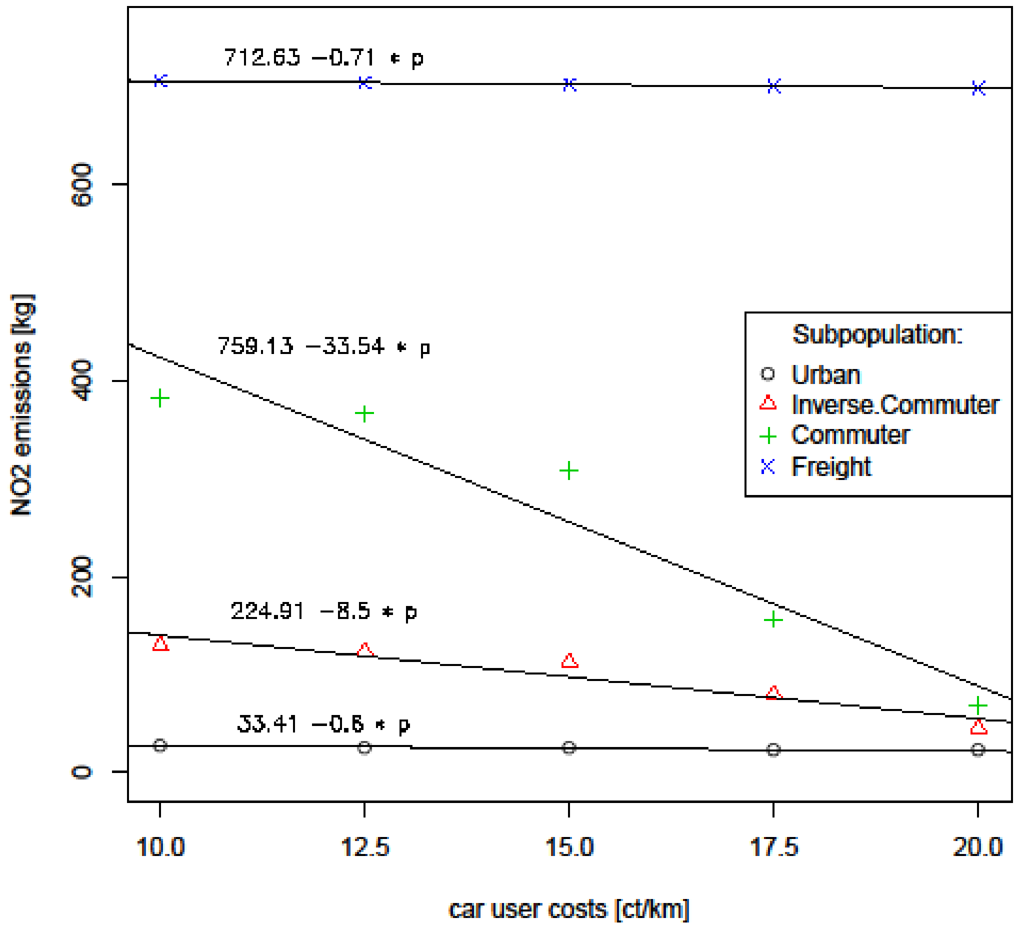


Figure 4.3: Overall daily NO_2 emissions in kilograms for the base case and the four policy cases by subpopulation: simulated values and estimations as linear regression functions (values for a representative 10 % sample)

The price elasticities are found to be roughly the same for other exhaust emission types under consideration (PM and SO_2). When comparing them to the price elasticities of car travel demand from above, one can notice a higher elasticity of emissions than of demand for all subpopulations. Thus, an increase in car user costs leads to a higher reduction in emissions than in demand. Two explanations come to mind:

1. An over-proportional fraction of travellers who performed long car trips with high speed levels now change from car to public transport ('biased mode switch effect').
2. Travellers are driving faster on formerly congested roads ('congestion relief effect').

Both explanations are based on the fact that emission levels are usually the lowest for speed levels around 60 km/h (see for example Maibach et al., 2008, 58). Emissions per vehicle kilometre increase for lower but also for higher speed levels, forming a "U-shaped" function with its minimum around 60 km/h. That is, when mainly trips with high speed levels are reduced (in this case by changing to another mode), overall emissions drop more than demand. The same is true when traffic flow becomes more fluid on formerly congested roads. It seems that the second effect can be observed since our model includes spillback effects, different traffic states, and individual vehicle characteristics. The following subsection will address this hypothesis by looking at spatial patterns of changes in travel demand and in air pollutant emissions.

4.4.2 Spatial analysis of changes in car travel demand and air pollutant emissions

This subsection analyses car travel demand and NO_2 emissions on a spatially disaggregated level. Using the features of the emission modelling tool, demand and NO_2 emissions can be aggregated per road segment and for any desired time interval. For visual presentation of the spatial effect within the urban area of Munich, emissions are spatially smoothed using a Gaussian distance weighting function with a radius of 500 m. Starting with the base case shown in Figure 4.4 one notices a high level travel demand (in vehicle kilometres travelled) for the inner ring road, the middle ring road, the main arterial motorways, and the tangential motorway in the north-west of Munich (see Figure 4.4a). Travel demand is highly correlated with the level of exhaust emissions (see Figure 4.4b).[16] The population exposure of NO_2 emissions near these road sections is critical; this is also found by the air pollutant concentration levels at monitoring stations, for example, at Landshuter Allee (LfU, 2011).

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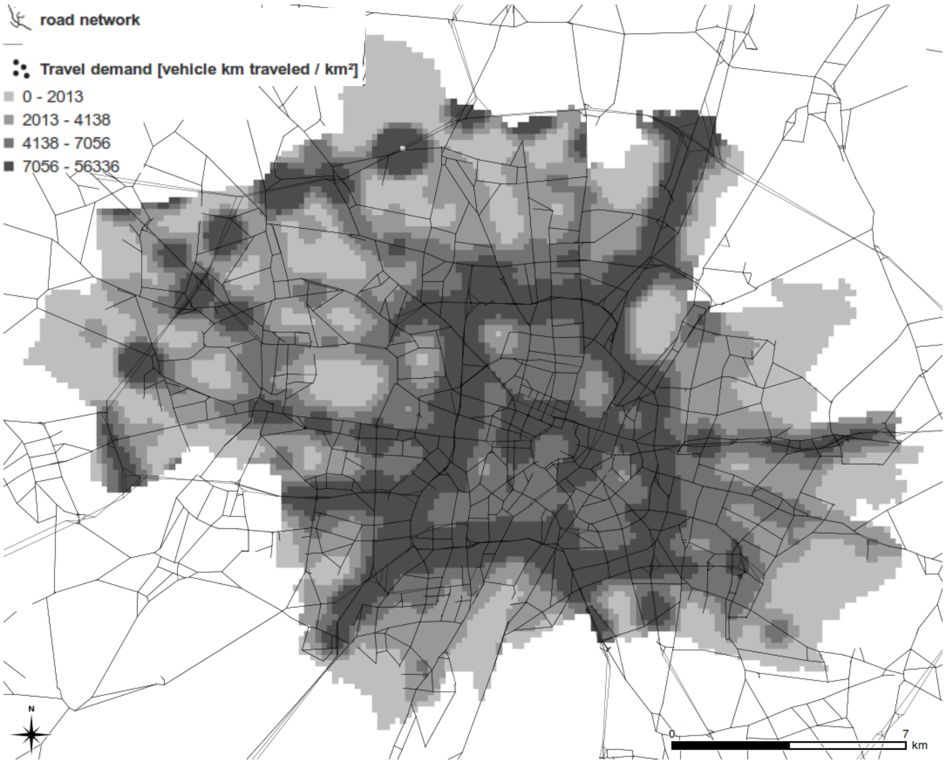
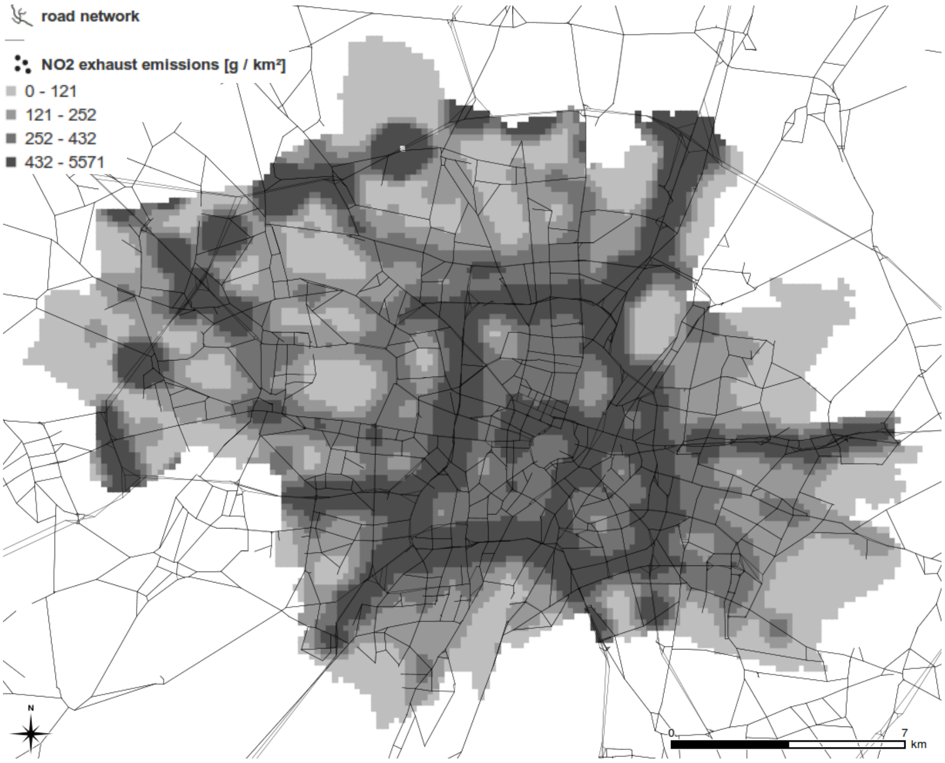
[16] This method currently localises all emissions on a road segment at the center coordinate. This explains why the tangential motorway in the north-west of Munich is shown as a sequence of filled circles rather than an uninterrupted line.



(a) Vehicle kilometres travelled in vkm/km^2

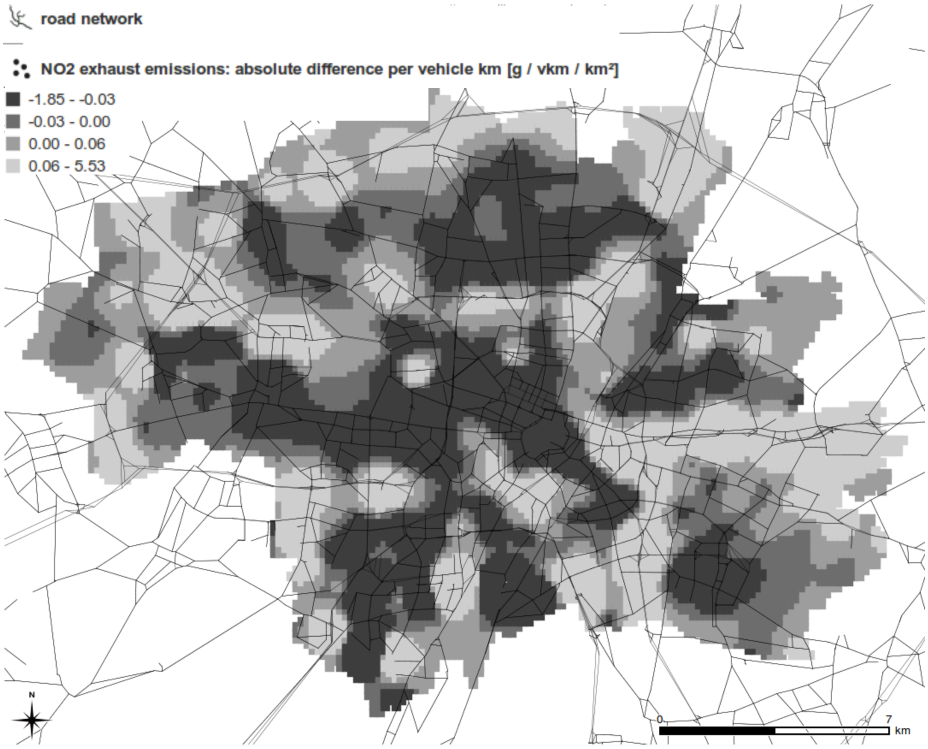


(b) NO_2 emissions in g/km^2

Note: Plots based on spatial averaging for all road segments. Values for a representative 10 % sample.

Figure 4.4: Base case: areas with high car travel demand and areas with high NO_2 emissions

(a) Absolute change in NO_2 emissions in g/km^2



(b) Absolute change in NO_2 emissions per vehicle kilometre in g/vkm/km^2

Note: Plots based on spatial averaging for all road segments. Values for a representative 10 % sample.

Figure 4.5: Absolute changes in NO_2 emissions between the base case and the 100 % price increase (policy case 4)

Figure 4.5 shows the absolute change in NO_2 emissions between the base case and the 100 % price increase (policy case 4). As already presented in Subsection 4.4.1, the increase in car user costs leads to an important reduction in emission levels. This finding is now confirmed by Figure 4.5a, which decomposes the overall effect in a spatial distribution. The lesson learned when comparing that picture to Figure 4.4 is that roads with the highest potential for emission reductions are located along the corridors with the highest travel demand (and therefore the highest emissions). Figure 4.5a also shows that potential gains are considerably larger at the medium- and high-speed roads than, for example, in the inner-urban area. Our approach allows to show such effects on a detailed single-street level while still being applicable to large-scale scenarios. This allows both the identification of relevant corridors ('hotspots') and the spatially disaggregated analysis of the consequences of policy measures.

In order to answer the question whether spatial patterns of higher emission elasticities compared to demand elasticities can be observed, Figure 4.5b is analysed. Similar to Figure 4.5a, it depicts the absolute difference in emission levels between the base case and the 100 % price increase (policy case 4), but now the absolute change in *emissions per vehicle kilometre travelled*. Values above zero imply that vehicles produce more emissions per km travelled, whereas values below zero indicate that vehicles emit fewer emissions for the same distance. Again, two effects can be observed that correspond with those presented in Subsection 4.4.1:

1. The 'biased mode switch effect' is most important for the main arterial motorways and the tangential motorway in the north-west of Munich: Figure 4.5a indicates that overall emissions (and demand) go down on these road segments. But following Figure 4.5b, average emissions per vehicle kilometre go up (light grey areas).
2. The 'congestion relief effect' seems to be less coherent in Figure 4.5b than the first effect. However, dark grey areas indicate that average emissions per vehicle kilometre go down. This means that a reduction in travel demand leads to lower emissions per vehicle kilometre.

The first effect can be interpreted as follows: in the base case, average speeds on motorways were closer to the (emission) optimal speed of 60 km/h. Fewer vehicles on these roads lead to higher emissions per vehicle kilometre, since travellers drive faster. That is, congestion relief leads to higher emissions per vehicle kilometre. A similar finding was obtained by Newman and Kenworthy (1989), who state that the average traffic speed is correlated positively, and not negatively, with gasoline consumption per capita. The second effect might be interpreted as follows when combining the aggregated and the disaggregated observations: it is likely that due to the reduction in demand, average travel speeds in the corresponding areas get closer to the (emission) optimal speed of 60 km/h. Emissions along a congested urban road are about twice as high as when traffic is flowing. When car travel demand is reduced and, thereby, the traffic situation on the road segment changes from stop-and-go to saturated or even heavy, emissions are more reduced than the flow on that road segment. That is, congestion relief leads to lower emissions per vehicle kilometre especially in urban contexts.

4.5 Conclusion

In this chapter, a real-world scenario of the Munich metropolitan area was set up and travel demand of a 10 % sample (around 200,000 individuals) with a large-scale multi-agent simulation simulated. The simulation was coupled with detailed emission factors from HBEFA, considering the kinematic characteristics derived from the simulation and vehicle attributes obtained from survey data. Since the simulation keeps track of the approximate position and attributes of every traveller's vehicle during every time step, it was possible to map the kinematic characteristics to different traffic situations such as free flow or stop-and-go. Thereby, emissions were calculated every time a traveller leaves a road segment, or starts his/her engine. The mapping of demand (in vehicle kilometres) or emissions back to the road segments was therefore quite straightforward.

Then four policy cases were introduced, where user costs for car are rising from 10 ct/km in four steps up to 20 ct/km. Aggregated price elasticities of demand were found to be in a reasonable range for all subpopulations. Commuters reacted more sensitively to the price increase than inner-urban travellers, for example by changing from car to public transport. Price elasticities of NO_2 emissions turned out to be higher than those of demand. Two possible explanations were given: first, it might happen that an overproportional fraction of travellers who performed long car trips with high speed levels changed from car to public transport. The authors called this the 'biased mode switch effect'. Second, it seems that travellers are driving faster on formerly congested roads, referred to as the 'congestion relief effect'.

A spatially more disaggregated analysis allowed to identify so-called 'hotspots' that have high potential for emission reduction: absolute emissions dropped most in many, but not all, areas where travel demand was high. Furthermore, the spatial analysis showed that the 'biased mode switch effect' was most important for high-speed arterials and tangential motorways since absolute emissions (and demand) go down on these road segments, but average emissions per vehicle kilometre go up. Due to higher speeds, fewer vehicles — in this case — lead to higher emissions per vehicle kilometre. The 'congestion relief effect' was found to be less coherent in terms of the type of road segment. Nonetheless, some areas showed a reduction in emissions per vehicle kilometre caused by a reduction in demand. Due to higher speeds, fewer vehicles — in this case — lead to lower emissions per vehicle kilometre. Possibly, both effects stem from the fact that the emission optimal speed is usually around 60 km/h. Measures that allow travellers to drive faster than that will result in higher emissions per vehicle kilometre. However, the relief of congestion seems to bear some potential to reduce emissions on urban roads.

This work can add valuable information to the transport planning and policy making process by providing insights into a new emission calculation model for large-scale scenarios. In future studies, it is planned to account for more choice dimensions than just route and mode choice. This is likely to influence the results. Also, the robustness of the results needs to be tested by performing sensitivity analysis. A possible extension would be the modelling of air pollutant concentration, which could be used to validate simulation results with measured concentration values.

5 Modelling traffic and air pollution in an integrated approach – the case of Munich

5.1 Introduction

For a detailed policy-sensitive assessment of air quality in street canyons, the challenge is to, on the one hand, involve the complex interactions of travel behaviour to determine traffic demand and air pollutant emissions and, on the other hand, to include air pollution processes to calculate air pollutant concentrations. An air pollution model is required that considers transport and dispersion as well as chemical processes based on meteorological conditions, street geometry and background pollution to simulate air pollutant concentration at individual receptor points. The majority of air quality models refers to emission inventories when calculating air pollutant concentrations. Traffic flow models can simulate air pollutant emissions per street section and vehicle. Traffic demand is optimised by allowing for changes in travel behaviour such as mode choice and route choice. Air pollutant emissions per street section can be calculated by considering the vehicle type, driving dynamics and number of vehicles.

Some types of air quality models are able to model air pollution using street section based air pollutant emissions as individual sources. Microscopic dispersion models such as LASAT[17] and MISKAM[18] can be used with line sources. LASAT is based on the 3-dimensional Lagrangian particle model. MISKAM uses a 3-dimensional microscopic flow and dispersion model. These models provide a high resolution, but are not applicable to large-scale scenarios because of the high computational requirements (Bachler, 2010; Eichhorn and Kniffka, 2010). Both models are generally applied to a defined small area and are based on static vehicle emissions. Hatzopoulou and Miller (2010) applied the regional and urban dispersion model CALPUFF[19] to the multi-agent

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[17] Lagrangian Simulation of Aerosol-Transport, see http://www.janicke.de/en/lasat.html (accessed 15/10/2013).

[18] 3-Dimensional non hydrostatic flow model and an Eulerian dispersion model, http://www.lohmeyer.de/en/content/about-us/work-methods/numerical-models/miskam (accessed 15/10/2013).

[19] Advanced non steady-state meteorological and air quality modelling system, see http://www.src.com/calpuff/calpuff1.htm (accessed 15/10/2013).

transport model MATSim[20]. CALPUFF calculates emissions per agent and street section, which is used as input data for the dispersion modelling. The necessary spatial resolution to examine air pollutant concentrations along single street canyons is, however, too low when using CALPUFF. Street canyon modelling is often based on semi-parametric approaches that can be applied locally. Two examples are the CPBM and the OSPM[21]. In contrast to microscopic models such as MISKAM and LASAT, this approach is not able to consider complex building structures and intersections, and simplifies the dispersion processes by empirically determined constants. Instead, street canyon modelling has shorter calculation times, fewer uncertainties and is often well validated. Accuracy and availability of the input data are, besides the purpose of a study, vital determinants for choosing the appropriate model for any application (Vardoulakis et al., 2003).

The challenging task is to keep a high spatial resolution using detailed time dependent line sources, but still apply the approach to an urban area. This chapter presents an innovative approach: the optimised traffic demand and resulting emissions obtained from the large-scale transport simulation tool, MATSim, are linked with traffic-related air pollution modelling in street canyons, i.e. OSPM. The aim of this study is to combine both detailed emission calculation with large-scale scenarios, and a traffic model with an air quality model to simulate policy-sensitive scenarios in one run. Such an integrated tool is capable of determining environmental exposure and costs and the full cause-and-effect chain to consider all interactions caused by transport policies.

The remainder of the study is organised as follows: in Section 5.2 the integrated approach is described including the simulation of traffic demand and air pollutant emissions as well as the processing of the input data and parameters required for the air quality model. A base case for Munich, Germany, is presented in Section 5.3. The data sources used for the integrated modelling approach, the simulation approach as well as the study area are described. For validation purposes simulations are compared to measured air pollutant concentrations and statistical performance measures are applied. The results in Section 5.4 show air pollutant emissions and concentrations in the investigated area and a study of a street canyon. The impact of a change in transport policies on air quality is further illustrated and explained. The chapter ends with concluding remarks in Section 5.5.

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[20] Multi-agent transport simulation, see http://www.matsim.org/ (accessed 15/10/2013).

[21] Operational street pollution model, see http://envs.au.dk/en/knowledge/air/models/ospm/ (accessed 15/10/2013).

5.2 Integrated air pollution modelling approach

5.2.1 Overview

This section describes the developed policy-sensitive air pollution modelling approach, which integrates the generation of transport activities with air pollutant emission and concentration modelling. The air pollution modelling approach is able to cover a large area with a highly resolved grid of receptor points, at which concentration of different air pollutants are simulated. Several models are described in the literature, which simulate large-scale scenarios, but the spatial resolution is often not detailed enough if the air pollutant concentration along street canyons is examined. In this study, the spatial resolution of air pollutant concentrations can be directly linked to the spatial resolution of the emissions, which are street section based. At the same time, the integrated tool allows for the simulation of a base case and different policy scenarios in a reasonable timeframe.

The street canyon approach refers to the dispersion and chemical processes of the OSPM model. The OSPM follows a semi-empirical approach, which is based on a parameterisation of the most important dispersion processes close to the street including the influence of the traffic-produced turbulence created by movements of the vehicles, the influence of buildings along street canyons on dispersion (street canyon effect) and the chemical transformation between nitrogen monoxide – ozone – nitrogen dioxide. For the pollutants, nitrogen oxides (NO_x = sum of NO and NO_2), carbon monoxide and particulate matter, the local contribution from the street is directly proportional to the emission rate since they are considered as non-reacting at this short time scales inside the street canyon. Measured background concentration is added to determine total concentration. Computed total NO_x and measured O_3 background concentration and global radiation are passed to the OSPM module on chemical processes to transform NO_x to NO_2 concentrations. OSPM has been tested and applied in many places worldwide (Kakosimos et al., 2010). For more information about the dispersion and chemical processes of the OSPM and validation with measurements see Berkowicz et al. (1997) and Ketzel et al. (2012). The dispersion and chemical processes of the OSPM are transcribed into an OSPM module written in JAVA and integrated into the Java environment, in which MATSim and the emission modelling tool are embedded. The resulting integrated tool combines the generation of the transport activity, the emissions and air pollutant concentration (see Figure 5.1). By doing so the required traffic and emission data and parameters can be directly accessed without generating a complex interface between different programming languages or software programmes.

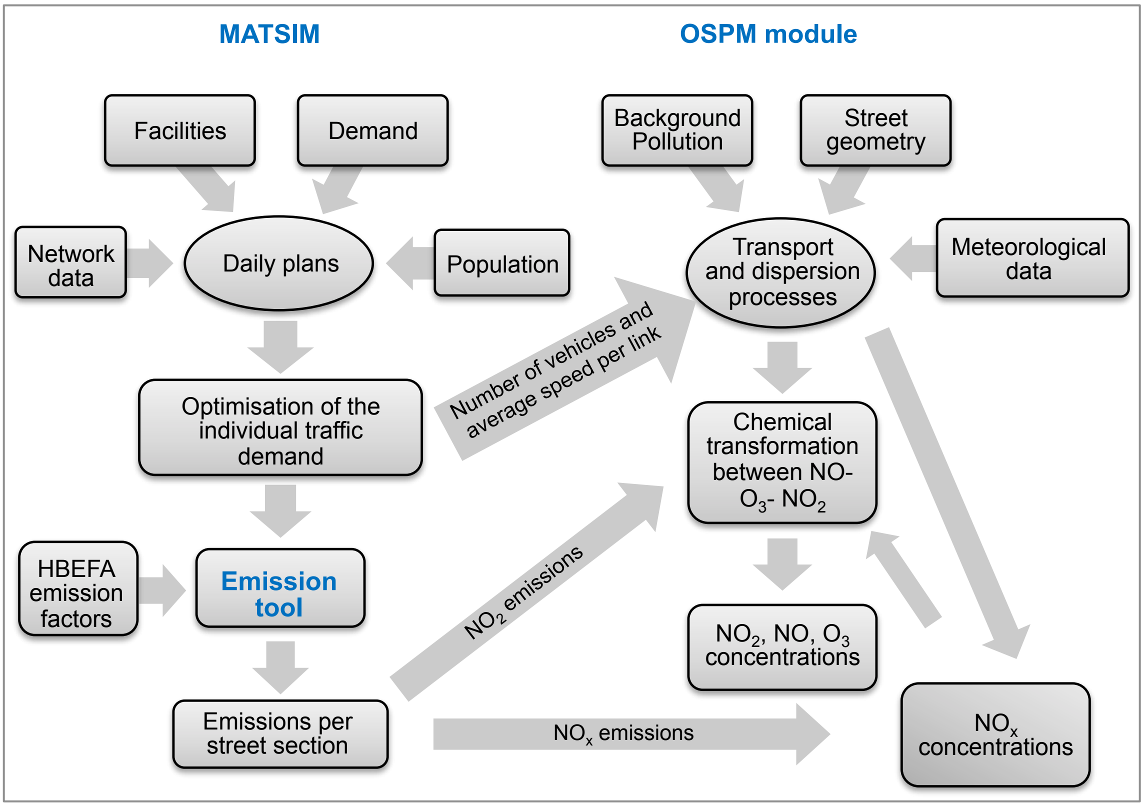

Figure 5.1: Integrated air quality model – scheme

The data and parameters required for the integrated modelling approach can be divided into five input categories:

- Traffic data: number of passenger cars and heavy duty vehicles and average speed per link,
- Emission factors,
- Meteorology: wind speed, wind direction, ambient temperature, global solar radiation,
- Background concentration,
- Street and building geometry, receptor points.

Hourly urban background concentration and data on meteorology are based on measured data (see Section 5.3). The calculation of the other input data is described in more detail in the following sections.

5.2.2 Traffic in the street canyon

The number of passenger cars and heavy duty vehicles as well as average speed is simulated by the multi-agent transport simulation, MATSim. In MATSim, each traveller of the real system is modelled as an individual agent. The approach models an entire day and consists of an iterative loop that is characterised by the following processes: plans generation, traffic flow simulation, evaluating plans and a learning mechanism.

Each agent is assigned a daily activity plan, which shows each trip and mode chosen over a day. Based on the utility gained from choosing a certain activity plan, some agents change plans from one iteration to another. Agents adapt their routes only for car trips. Furthermore, they can switch between the modes car and public transit (pt). Further information on traffic flow simulation and the modelling of route and mode choice using MATSim can be found in Raney and Nagel (2006) and Hülsmann et al. (2011).

The main features that are relevant from this simulation are the street section (link) and agent-based information for each time step, which are generated when the system has reached a relaxed state, meaning the outcome is stable. As a result, for each second of the day the location of an agent in the network is known. This allows for an aggregation of vehicles differentiated by vehicle type per link and the determination of the average speed driven on a link in a certain timeframe. This study aggregates passenger cars and heavy duty vehicles on each link per hour.

5.2.3 Exhaust emissions

The emission modelling tool essentially calculates warm and cold-start emissions for passenger cars and heavy goods vehicles.[22] The former are emitted when the vehicle's engine is already warmed whereas the latter occur during the warm-up phase. Warm emissions differ with respect to road type, driving speed, driving dynamics and vehicle characteristics. Cold-start emissions differ with respect to distance travelled, parking time, and vehicle characteristics. For the majority of air pollutants it is found, that during cold-start conditions in comparison to warm engine conditions more emissions are generated. This is largely relevant for NO_2, but some exceptions of vehicle types (specific combinations of fuel type and Euro-class) exist resulting in lower emissions during the first part of trip. This relation of cold-start and warm emissions can be also found in IFEU (2010). The emission factors are taken from the handbook on emission factors for road transport (HBEFA) (INFRAS, 2010). The vehicle characteristics are derived from survey data (see Section 5.3.1), comprise vehicle type, age, cubic capacity and fuel type and are, thus, assigned to the synthetic population, which is the input data for MATSim traffic demand.

MATSim generates daily plans with activity chains for every agent over the entire day. The time is recorded whenever an agent enters and leaves a link. Using this information and the link length it is possible to calculate the free flow travel time and the travel time in a loaded network for every agent and link. MATSim driving dynamics are

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[22] Public transit is in the present chapter assumed to run emission free.

mapped to two traffic situations of the HBEFA database: free flow and stop-and-go.[23] As MATSim keeps the vehicle specific characteristics such as fuel type, Euro-class, etc. until the system is relaxed, i.e. an outcome is generated, information about each agent's vehicle is available at any time. Therefore, very differentiated emission calculations are applied. Where no detailed information about the vehicle type is available, fleet averages for Germany are used.

Cold-start emissions are only applied to passenger cars. The exact locations of departure and activities are not known for heavy duty vehicles and these locations are mostly outside the urban area. HBEFA cold-start emission factors are applied to each passenger car based on two attributes: the distance travelled and the parking time. The latter is calculated by knowing the time stamp of all activities starting and ending. The travelled distance following an activity is determined by adding up the distance of each link the agent drives along until the start of the next activity.

In conclusion, so-called ''emission events'' including warm and cold-start emissions are generated. These events provide information about the vehicle, the time, the link and the absolute emitted mass by air pollutant. The definition of emission events follows the MATSim framework that uses events for storing disaggregated information as objects in JAVA and as XML in output files (see Appendix in Hülsmann et al. (2013)).

In a second step, for the calculation of air pollutant concentration, these emission events are summed up per time period and link, resulting in a line emission source with a time resolution of one hour. If a street cross section consists of two or more links the emissions on those links are summed up. Street canyon modelling includes all emissions generated in both directions of a street section.

5.2.4 Street geometry and placement of receptor points

The OSPM model simulates air pollutant concentration at receptor points, which can be located along any street segment. The dispersion processes depend on the location of the receptor point, the width, length and orientation of the street section and the building heights or gaps within this section (Berkowicz et al., 1997). Receptor points are placed at the facade of the buildings along street canyons. In order to cover the urban area with receptor points to capture the most polluted areas, receptor points are placed in a 20 m grid format along the building facades. This density of receptors is chosen to keep the calculation time for the entire modelling approach reasonable. A higher spatial resolution would increase model calculation time considerably whereas with a lower spatial resolution it is not possible to cover the variety in concentration levels due to street geometry and meteorology. Receptor points are not placed at

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[23] The section of a link driven with free flow and the section driven with stop-and-go are determined by using MATSim and HBEFA driving dynamics. Emission calculation is, therefore, not only based on average speed per link as it is done by most transport models, but on a distribution between traffic situations and consequently includes congested traffic situations more accurately.

intersections because the more complex dispersion processes at intersections cannot be modelled with this approach. Additionally, open spaces are not included because they are less relevant with respect to population exposure.

With an extension of ArcGIS, the so-called AirGIS, three shapefiles – street, building and receptor points – are joined. From the position of a receptor, the street orientation, street width, building height and all gaps in the building structure (including the respective height) are calculated (Jensen et al., 2001; Ketzel et al., 2011).

5.3 Munich base case development

In this section, a short introduction to the large-scale real-world scenario of the Munich metropolitan area is given and the scenario setup for the transport model and the emission calculation tool are described. These subsections are followed by a description of the base case simulation and the validation of the approach.

5.3.1 Scenario setup for the transport model MATSim and emission calculation tool

The information on network and population refers to Kickhöfer et al. (2013). Only a brief summary is given here. The road network consists of 17,888 nodes and 41,942 street segments. It covers the federal state of Bavaria, with more detail in and around the city of Munich and less detail further away. Every link is characterised by a maximum speed, a flow capacity and a number of lanes. This information is stored in the road type, which for the emission calculation is always assigned to a corresponding HBEFA road type. Overall, the synthetic population consists of 2,093,530 agents. Three ‘subpopulations’ exist, each corresponding to one of the three different data sources:

- Urban population (based on Follmer et al., 2004): The synthetic population of Munich is created on the basis of very detailed survey data provided by RSB (2005), named ‘Mobility in Germany’ (MiD 2002). The synthetic urban population of Munich consists of 1,424,520 individuals, for which each trip between two activities is simulated.
- Commuter population (based on Böhme and Eigenmüller, 2006): A total of 510,150 synthetic commuters are created from which of 306,160 work in Munich. All commuters perform a daily plan that encodes two trips: from their home location to work and back.
- Freight population (based on ITP/BVU, 2005): This study provides origin–destination commodity flows throughout Germany differentiated by mode and ten groups of commodities. This population consists of 158,860 agents with one single commercial traffic trip.

Regarding the total population 68 % can be assigned to the urban population, 7.6 % to heavy duty vehicles and 24.4 % to commuters. For passenger cars, information about vehicle type and attributes exists and vehicle specific emissions can be calculated. For commuters and freight traffic, no detailed vehicle information is available. Emissions are, therefore, calculated based on fleet averages for cars and trucks from HBEFA.

5.3.2 Scenario setup for the air quality model

As mentioned above, the integrated air quality model combines information from MATSim, the emission modelling tool, data on street and building geometry, and meteorological data. The data on street and building geometry is provided by the city of Munich (RSB, 2005). The study area for this work is the Munich inner city bounded by the ring road Mittlerer Ring with a length of 28 km (see Figure 5.2). This area accounts for a large share of the most densely populated areas in Munich and exhibits mixed residential, retail, institutional and office land uses as well as dense residential areas only.

Several receptor points are distributed on both sides of each street canyon within the study area including the Mittlerer Ring, resulting in a total of 7,900 receptor points. Background concentration for this study is taken from an air quality monitoring station, located in the northeast of Munich and operated by the Bavarian Environment Agency. This station measures hourly urban background concentrations of NO, NO_2 and O_3 (DWD, 2008). In addition, hourly meteorological data including wind speed and direction, temperature, and relative humidity are measured at one location in Munich, where the German meteorological service is located (LfU, 2008). Data on global radiation are available per month for a grid cell of 1 km (LfU, 2008).

Figure 5.2: Map of Munich city area showing the receptor points placed in the study area surrounded by the ring road Mittlerer Ring

5.3.3 Base case simulation

To speed up computations, a base case using a 1 % sample of the population in Munich is simulated as described in Section 5.2.2. The link storage capacity, which limits the number of agents on the link, is reduced to fit to the 1 % sample. MATSim is run for 1,000 iterations.[24] For a more detailed description of the MATSim simulation used in this chapter please refer to Kickhöfer et al. (2013). The output of the last iteration is used to calculate emissions per link and agent. As the emissions are generated for 1 % of the population as an outcome of MATSim they need to be extrapolated for the entire population. The emissions are further processed from gram per km to milligram per meter and second, which are used in the air quality model to determine NO_2 concentrations for each receptor point. Hourly NO_2 concentrations are calculated for the entire year of 2008.

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[24] In each of the first 800 iterations, 15 % of the agents are forced to discover new routes, 15 % change their transport mode for a car or public transit sub-tour in their daily plan and 70 % switch between their existing plans. Between iteration 801 and 1,000, route and mode choice are switched off; in consequence, agents only switch between existing options. In order to include a transport policy in the MATSim simulations, the policy is introduced at iteration 1,000 and the simulation continues for another 500 iterations resulting in the final iteration of 1,500 for both, the base case and policy scenario (Hülsmann et al., 2013).

5.3.4 Comparison of the base case simulation with measurements

The air quality model is validated using an air quality station located at Landshuter Allee – an 8-lane major urban arterial road and part of the Mittlerer Ring. As the arterial road is also used by transit traffic, the traffic density is high with approximately 140,000 vehicles per day. The street is north–south oriented and about 56 m wide with 20 m high buildings on both sides. An air quality monitoring station, located at the western side of the street and operated by the Bavarian Environment Agency, is measuring hourly concentrations of NO, NO_2, CO and PM_{10}.

Comparing simulated with measured NO_x concentrations

In order to validate the integrated model, the simulated air quality data are compared to measurements collected at the station. For the modelled air quality, in a first step, traffic demand of three weekdays, Tuesday, Wednesday and Thursday, is generated from traffic counts using MATSim. The traffic demand is then used as input data for the emission modelling tool described in Section 5.2.3. The average emissions per hour are calculated based on these three days. Emission factors as well as urban background concentrations, hourly meteorological data including wind speed and direction, temperature and global radiation are obtained from the sources described in Section 5.3.2. Simulated hourly mean NO_x concentrations are then compared to the average measured concentration data of the same three days (see Figure 5.3). The OSPM simulates NO_2 concentration based on NO_x concentrations, chemical processes with ozone and NO_2 as background concentrations. NO_x seems to be most appropriate for assessing the quality of the MATSim transport simulations, the emission modelling tool, the processing of the street geometry and the meteorology. The simulation of NO_2 out of NO_x within the OSPM model based on NO_x concentrations, chemical processes with ozone and NO_2 as background concentration has been validated in several studies such as Kakosimos et al. (2010) and Ketzel et al. (2012). A statistical performance analysis for NO_2 concentrations follows later in this section.

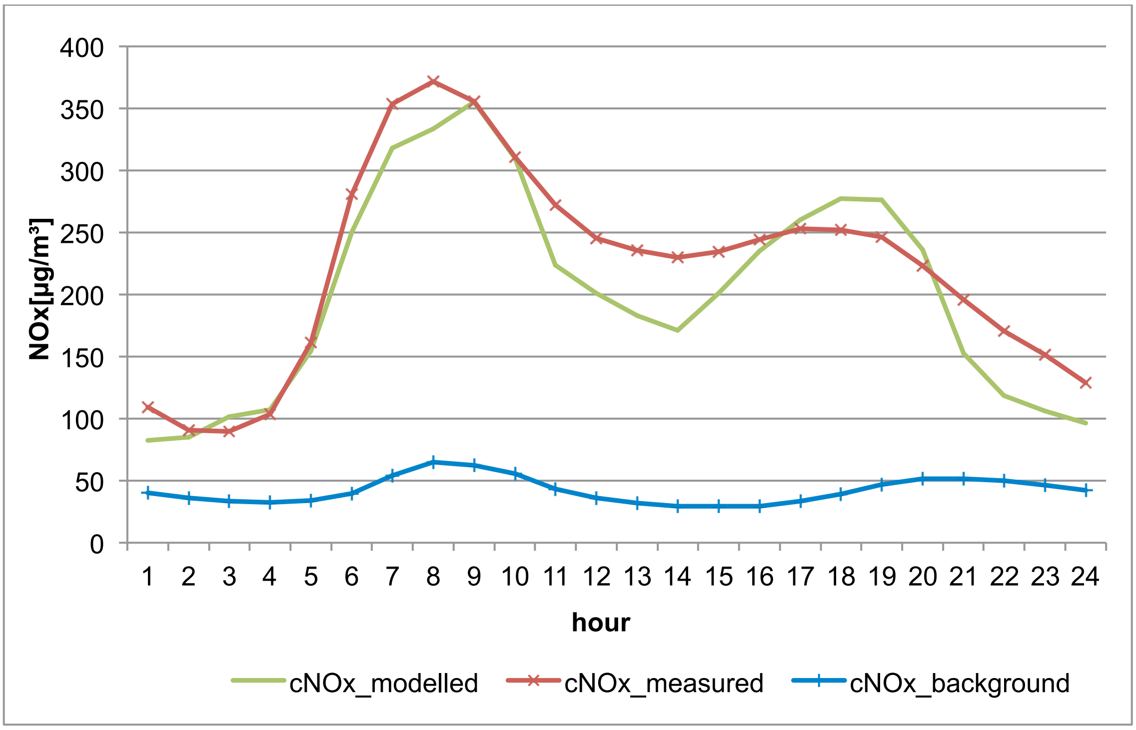

Figure 5.3: Measured and simulated NO_x concentration based on the average emissions of three weekdays, Tuesday, Wednesday and Thursday, in 2008 at Landshuter Allee, Munich

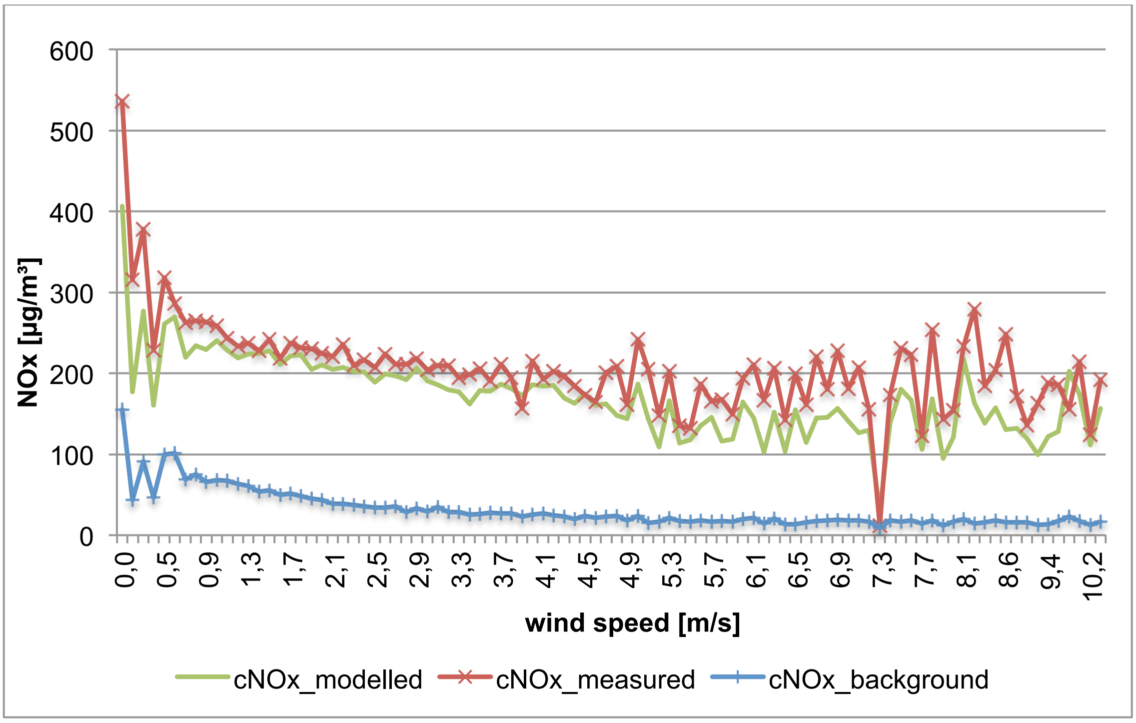

Figure 5.4: Relation between hourly measured and simulated NO_x concentrations and wind speed modelled for all Tuesdays to Thursdays, in 2008 at Landshuter Allee, Munich

In Figure 5.3 a similar diurnal pattern can be observed for modelled and measured NO_x concentrations showing peaks for the morning and afternoon rush hour. NO_x concentrations depending on wind speed are shown in Figure 5.4. For the analysis on the relation between concentrations and wind speed, hourly NO_x concentration is modelled for each Tuesday, Wednesday and Thursday in 2008. The average modelled and measured concentration is calculated for each level of wind speed and compared with the respective measured NO_x concentrations. In Figure 5.4 measured and modelled NO_x concentrations follow the same decreasing trend when wind speed is increasing with high concentrations at very low wind speeds and fluctuating values for high wind speeds. The latter appears to be stronger for measured NO_x concentrations. Similar patterns between measured and modelled concentrations can be identified to some extent.

Statistical performance measures based on NO_2 concentration

The simulated and measured NO_2 concentrations are evaluated using statistical performance measures. In Hanna and Chang (2012) a range of important statistical performance measures is given. The following measures are calculated in this study: fractional bias (FB), normalised mean-squared error (NMSE), normalised absolute difference (NAD) and the fraction of modelled concentrations within a factor of two of the measured concentrations (FAC2). For the statistical analysis simulated and measured hourly NO_2 concentration data at Landshuter Allee measurement station for each day of the entire year 2008 are used.

Table 5.1: Statistical performance for the base case

Statistical performance measure	**Base case – statistical performance**	**Acceptance criterion for urban areas (see Hanna and Chang, 2012)**
|FB|	0.50	<~0.67
NMSE	0.56	<~ 6.0
FAC2	0.57	>~0.30
NAD	0.66	<~0.50

The acceptance criteria FB, NMSE and FAC2 are satisfied according to Table 5.1 if the criteria for urban areas are applied (Hanna and Chang, 2012). However, the measure NAD exceeds the acceptance criterion, which indicates that the absolute level of NO_2 concentrations overall differs between simulated and measured. This could be an indication of lower emission levels simulated with the integrated approach compared to real-world emission levels.

5.4 Air pollutant concentration in an urban context

In this section, air pollutant emissions and concentrations are illustrated for the base case. The cause-and-effect chain of the integrated model is then depicted by introducing a speed limit of 30 km/h and applying this speed limit to all streets in the study area.

5.4.1 Air pollutant emissions

In Figure 5.5, the NO_2 emissions for one typical weekday are illustrated for the area of Munich on a spatially disaggregated level. NO_2 emissions are aggregated per road segment over a day. The emissions are spatially smoothed for visualisation purposes.[25] The emission level is high along the major ring road Mittlerer Ring, the neighbouring roads and motorways leading from and to the ring road as well as along the inner ring road Altstadtring, which surrounds the city centre.

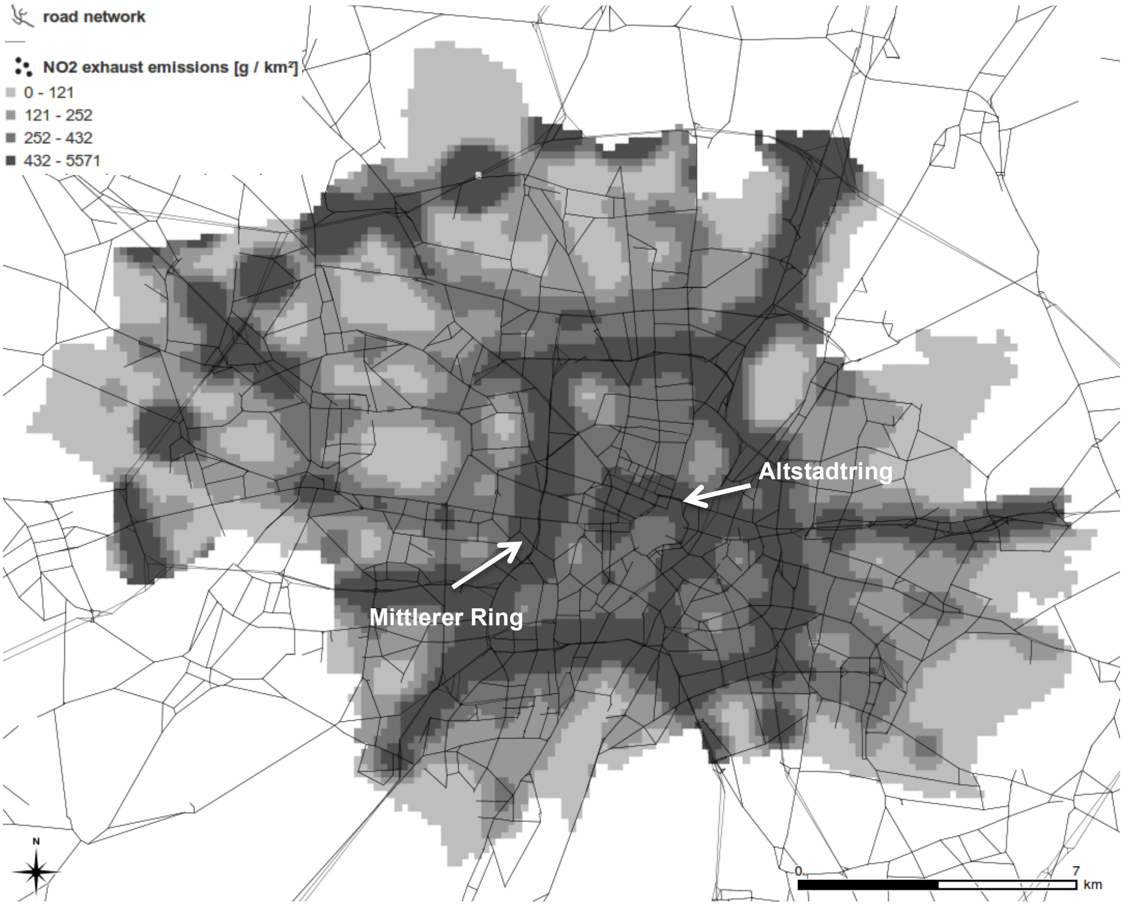

Figure 5.5: NO_2 exhaust emissions spatially smoothed for the base case and the entire area of Munich (Kickhöfer et al., 2013)

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[25] Spatially smoothing is done by using an Gaussian distance weighting function with a radius of 500 m (see further explanations of the emission calculation and visualisation in Kickhöfer et al. (2013)).

5.4.2 Air pollutant concentrations

In Figure 5.6 the modelled annual mean NO_2 concentrations based on weekdays in 2008 are presented.[26] The concentrations are illustrated for each receptor point and vary depending on the relation of traffic demand, street geometry, wind direction and speed, temperature and urban background concentration on an hourly basis.

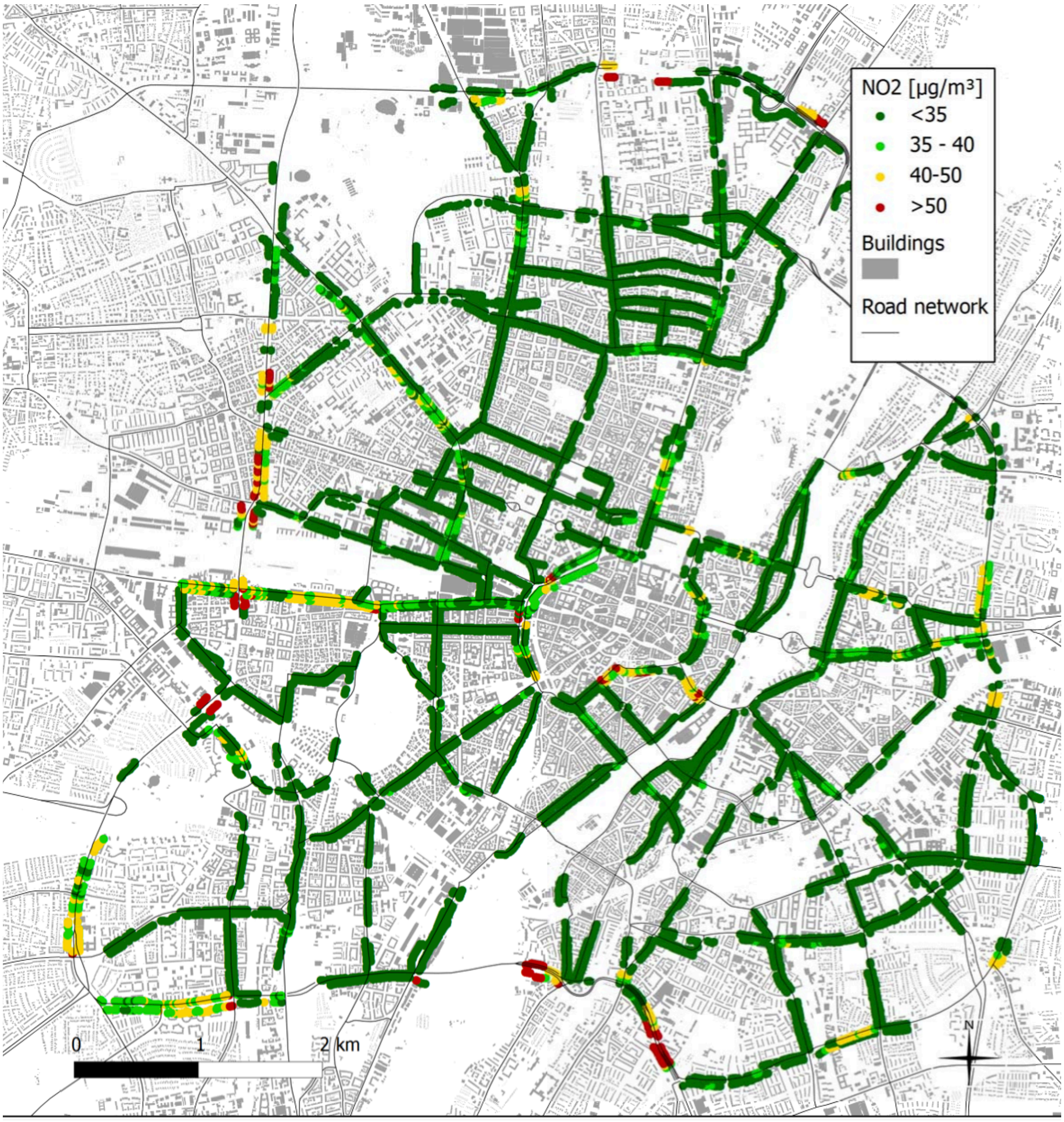

Figure 5.6: Annual mean NO_2 concentrations along the entire road network bounded by the Mittlerer Ring

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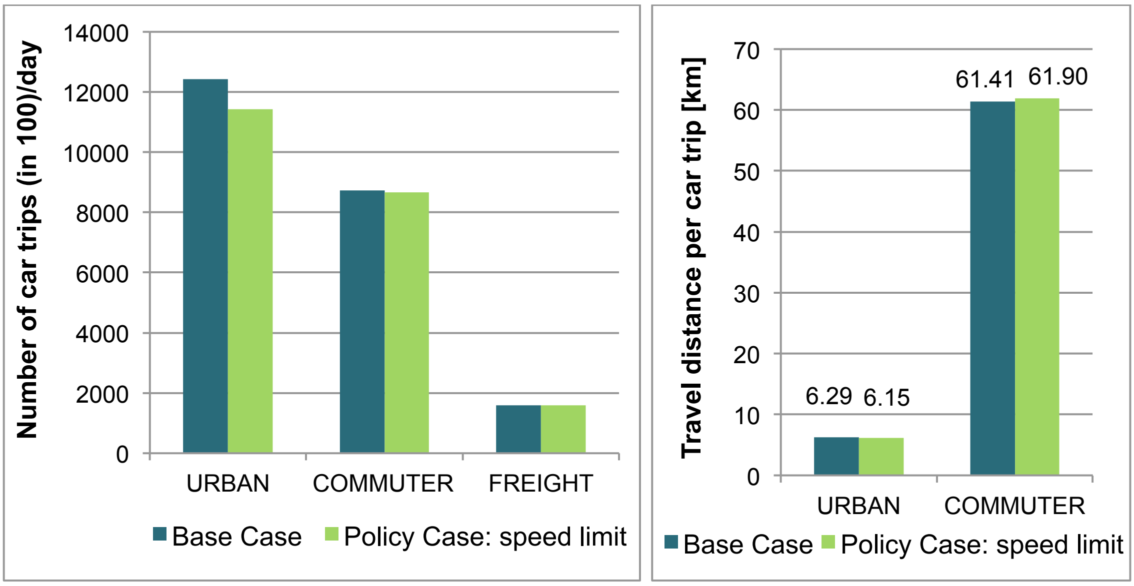
[26] The calculation of annual mean NO_2 concentration is based on emissions generated on each day of the week including weekday and weekend. As the emissions are simulated for a representative weekday with MATSim, this discrepancy should be considered, when analysing policies with respect to concrete limit values. A temporary solution to adjust the concentrations based on emissions of the entire week can be found in Hülsmann et al. (2013).

The simulated receptor points show NO_2 concentrations between 40 and 50 µg/m^3 at several locations and along some street canyons within the Munich road network. At some locations annual mean NO_2 concentration is even higher than 50 µg/m^3. For comparison, the EU limit value for annual mean NO_2 concentration is 40 µg/m^3 (EC, 2008). The simulations show that NO_2 concentrations within a street canyon can be different between the sides of the street canyon (see Figure 5.8). This is mainly caused by the wind direction, the street and building geometry.

In order to show the effect of a changed traffic demand on air pollutant concentration, a policy scenario is developed. A speed limit of 30 km/h is implemented on all streets within the study area, which is bound by the Mittlerer Ring. In Figure 5.7a and b the number of trips and distance travelled considering all trips in the Metropolitan area of Munich are illustrated. The change in the number of trips by car for each group, urban population, commuters and freight traffic, between the base and policy case shows that with the introduction of a speed limit fewer trips are done by car (see Figure 5.7a). This is especially relevant for the urban population of Munich. Freight traffic is hardly changing with the introduction of a speed limit. However, according to Figure 5.7b, the distance travelled by car increases for commuters and decreases for the urban population. Commuters may take a detour not entering the area bound by the Mittlerer Ring, which increases the travelled distance.



(a) (b)

Figure 5.7: Number of trips by car (a) and the distance travelled per trip for each group of travellers (b), entire area of Munich

The impact of a speed limit on NO_2 concentrations is a result of different effects. How NO_2 concentrations change depends on the following: NO_x emissions per vehicle and kilometre are higher for a speed limit of 30 km/h in the policy case compared to a speed limit of 50 km/h in the base case (see HBEFA emission factors). On the other hand, the number of car trips is reduced because other transport modes become more attractive and commuters reduce routes leading along road sections with speed limits (see Figure 5.7a). Fewer car trips involve lower emission levels. As a result of higher NO_x emissions per vehicle and kilometre and less traffic, NO_2 concentrations decrease to some extent (see Figure 5.8).

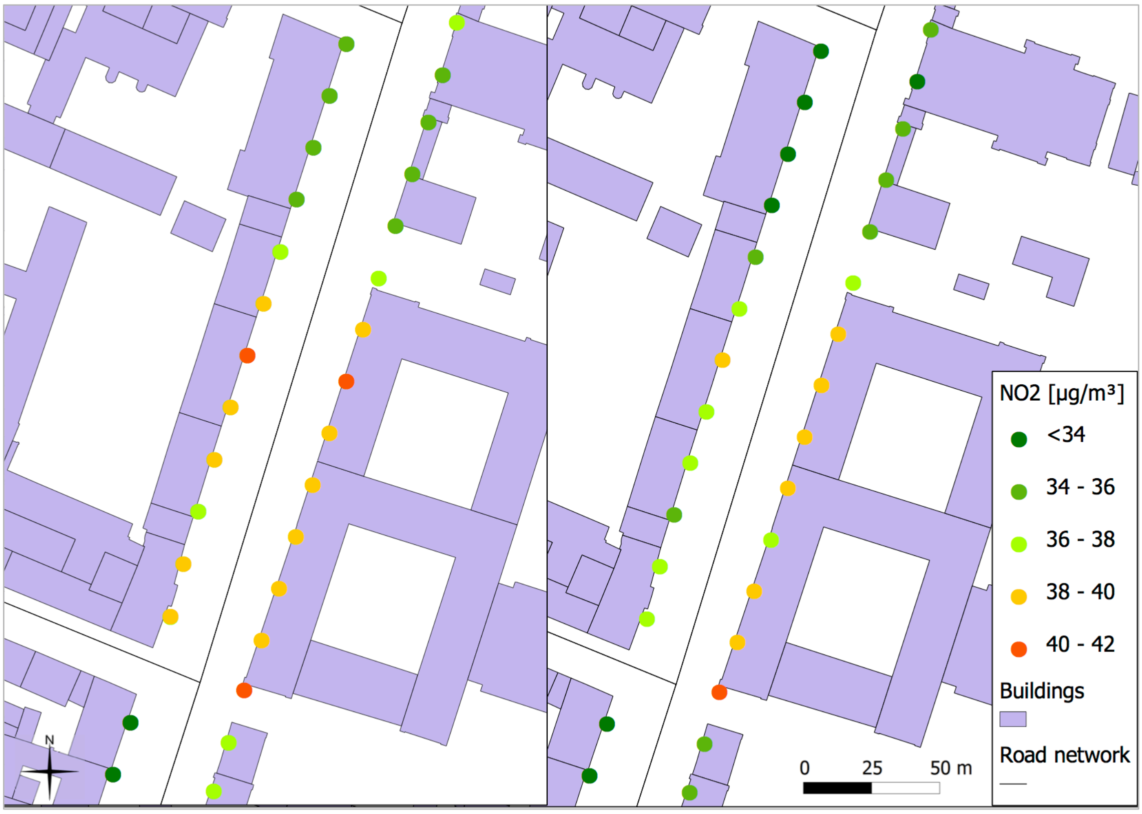


Figure 5.8: Annual mean NO_2 concentrations along a street canyon for the base case (left) and the policy case with a speed limit (right)

5.5 Conclusion

The developed integrated approach allows for modelling the complete cause-and-effect chain from the agent-based traffic activity to the population exposure to air pollution. The impact of different transport policies on traffic demand, air quality and population exposure to air pollution can be analysed on a microscale. These transport policies can range from local to citywide measures. This approach can be seen as a tool that allows policy-sensitive studies of air quality for an entire metropolitan area. NO_2 concentrations are determined for individual receptor points and vary depending on street and building geometry, meteorological conditions and road traffic-related emissions. The integrated approach can also be applied to other air pollutants such as PM.

Uncertainties remain especially due to input data availability and quality as well as parameters derived from samples to be used for the total population. Among these are, for example, the model assumptions made and the use of only weekdays when generating traffic demand in MATSim. More spatially disaggregated measurements of the local conditions in the study area including background pollution and meteorological data could improve the quality of the results. Further work should include the implementation of different policy scenarios to identify effective air pollution reduction strategies. Additionally, the integrated air quality model can continuously be improved if new and more data is available, for example, to differ between weekdays and weekends and to improve the assumptions of emission calculation regarding heavy duty traffic.

6 Concluding remarks

This chapter summarises the main findings of this thesis in Section 6.1 by referring to the objective of the work and describing important methodological developments. Further research is needed with respect to the integrated air pollution modelling approach discussed in Section 6.2. The concluding remarks end with an outlook of this work.

6.1 Summary of results

The objective of the thesis was to develop an integrated air pollution model that simulates the complete cause-and-effect chain from changes in transport behaviour and vehicle technology to the impact on air quality. In order to identify the polluter, the final level of air pollution and analyse locally and citywide effective transport policies, several subthemes and challenges had to be addressed and solved.

This work shows that the main influencing factors of air pollutant emissions, driving dynamics and vehicle attributes, can be considered within MATSim. In Chapter 3, the traffic demand was mapped to individuals to identify the agent's identity and to integrate emission specific vehicle attributes such as vehicle type, age, engine size and fuel type. Travel times were simulated with MATSim for a test road and compared with travel times from driving cycles. It could be shown that they follow measured travel times, especially when the system converts to a Nash-equilibrium. A relationship between MATSim and PHEM simulated emissions using measured driving cycles was depicted. Therefore, driving dynamics in terms of stop-and-go and free-flow traffic situations and vehicle attributes are generated by MATSim to calculate emissions by using HBEFA emission factors. As a result, the emission level is linked to the agent causing it and to the street section where the emission level was caused forming the basis for policy-sensitive analyses.

Chapter 4 describes the methodology of the emission calculation tool for the large-scale multi-agent transport simulation and how a real-world scenario of the Munich metropolitan area was developed. Based on this, the link-based emission calculation tool was projected on a citywide modelling approach. The Munich base case was developed by using survey data to generate agents with activity chains travelling in the Munich road network. Whenever an agent was leaving a link, the information about travel time and speed, as well as the vehicle attributes were used to calculate emissions by comparing them with the typical driving dynamics and vehicle attributes given in HBEFA 3.1. This approach allows for analysing a variety of transport policies and their impact on air pollutant emissions. An example of a change in travel behaviour and the analysis of the cause-and-effect relationship were provided in this work by introducing increased user costs for cars. Such increased car user costs can, for example, result from higher fuel taxes or a congestion charging scheme. The individual decision making of travellers was influenced by higher costs for every driven kilometre. Aggregated price elasticity of subpopulations with respect to traffic demand and emissions show that the impact of higher user costs varied between subpopulations: traffic demand reduced more for commuters than for inner-urban travellers. This investigation was followed by a spatially disaggregated analysis to determine emission hotspots and areas with increasing and decreasing emission levels. It was found that an overall change in traffic demand does not always linearly translate into changes in the emission level. Since it was not only costs that were optimised but also travel time, both, travel costs and time, and their mutual influence on each other have an impact on traffic demand. The results show that overall traffic demand and emissions are reduced, mainly due to commuters by changing from car to public transport. Along major arterials or motorways an increase in emissions per vehicle kilometre was determined due to higher vehicle speeds above the emission minimising speed level. The congestion relief effect was identified for some formerly congested areas: fewer vehicles and, thus, less stop-and-go lead to lower emissions per vehicle kilometre. In conclusion, the effects of car user costs can vary spatially, can even reduce emissions more than traffic demand in case of congestion, but can also result in higher emissions per vehicle kilometre when changing from free-flow vehicle speeds to even higher speeds.

Chapter 5 shows the coupling of an atmospheric dispersion model with MATSim and the emission calculation tool by maintaining the level of detail with respect to the spatial resolution. The emission level can be an indicator of air pollution in a certain area or at a specific location. However, what the population is exposed to exactly can be more precisely represented by the air pollutant concentration modelled in the fifth chapter. The completely integrated air pollution modelling approach is depicted with a focus on dispersion modelling. Information from both, MATSim and the emission calculation tool were used for air pollution modelling. The street canyon approach of the OSPM used these link-based emissions to simulate air pollutant concentrations from several receptor points in a street canyon. Due to the trapped air pollution in street canyons, these canyons are often locations which show high air pollutant concentrations. Therefore, such street canyons cover most air pollution hotspots in a city. In addition to transport mechanisms, chemical processes were simulated to calculate NO_2 concentrations. This work projects air pollution modelling of a single street canyon to a large area, the inner city, in Munich. As a result, air pollutant hotspots were identified within this area. The methodology was validated by showing that simulated NO_x concentrations of a street canyon, which were modelled based on traffic counts, follow nearly the same course and reach a similar level compared to measured NO_x concentrations. Additionally, a statistical performance analysis of NO_2 concentrations was conducted based on survey data satisfying three of the four statistical acceptance criteria. The chapter concluded with studying the effects of a regulatory transport policy. It could be shown that a speed limit introduced in the inner city of Munich reduces air pollutant concentrations in a selected street canyon resulting in different impacts on air pollution within the street canyon. With respect to the entire urban area the speed limit results in overall fewer car trips, especially for the urban population, but longer car distances travelled by commuters. This analysis depicts the cause-and-effect chain of the introduction of a speed limit and determines the impact on local air quality, but also the aggregated impact on traffic demand for the large-scale scenario, which – in this case – results in possible detours made by commuters.

Beyond the specific transport policies analysed in this thesis, a variety of further transport policies can be investigated with the integrated air pollution modelling approach. This includes, amongst others, modelling the effects of a congestion charging zone on air pollutant emissions and concentrations with respect to the area concerned and the surrounding area. By including emission costs in the decision making function of travellers, internalisation strategies can be developed and evaluated. Apart from transport policies affecting the transport behaviour, changes in vehicle technology can be simulated. The developed approached is able to show, for example, at what share of electric vehicles in the vehicle fleet air pollution hotspots would disappear due to significantly reduced air pollution. Overall, the developed approach addresses a variety of research fields and methodologies to bridge between multi-agent transport and air quality modelling for large-scale scenarios. The integration of the different models along with simultaneously keeping valuable features of each model during this integration is a major strength of this thesis.

6.2 Further research needs and outlook

This work provides valuable information to the transport planning and policy decision making process. With respect to further work, a multitude of options exist due to the fact that the developed approach includes three different fields of research related to transport, emission and atmospheric dispersion modelling.

The multi-agent transport simulation MATSim considers route and mode choice when optimising traffic demand. Beyond these two choices, it could account for more choice dimensions, for example, destination choice or choice in departure times. Along with more choice options additional modules that address possible future developments, which change travel behaviour significantly, could become important. An example would be autonomous driving, which will most likely change travel behaviour in the future enormously. In addition to the consideration of more changes in travel behaviour for passenger cars, the transport behaviour of heavy duty vehicles could be simulated in more detail. The knowledge of heavy duty vehicle types is also beneficial and could be related to the available emission factors of HBEFA. A more precise determination of the contribution of heavy duty traffic to air pollution is important, as freight traffic is a big contributor to air pollution. However, the inclusion of heavy duty traffic depends largely on the input data, which is more difficult to obtain for heavy duty traffic than for passenger transport. Additionally, decision making processes of freight traffic are different from the ones of passenger cars and also different with respect to the transported goods. The analysis of freight traffic, therefore, represents an important, but at the same time challenging future research field.

With respect to the emission calculation tool, the emission factors should always be re-evaluated to include changes in vehicle technology, for example, in the case of new filtering systems or updated Euro-classes in the future. The street canyon model simulates street canyons, because they often show the highest air pollution concentrations in cities. As a number of people lives close to intersections with a high volume of traffic passing by, it would be beneficial if intersections were included in the integrated approach. Considering the complexity of modelling air pollution at intersections and the need for a microsimulation, intersections should only be included in future modelling to such an extent that the simulation time remains reasonable and large-scale scenarios are still possible.

The integrated approach models air pollutant concentrations for every street section. In order to determine at what location air pollution causes the most damage to human health, the population exposed to air pollutant concentrations could be included in the modelling approach. As a result, air pollution hotspots, which are most relevant with respect to population exposure, as well as what policy is most effective in reducing air pollution at such locations can be identified. This could be supplemented by an analysis of human health and environmental impacts.

Overall, the simulation speed of the integrated approach should be steadily improved to be able to calculate policy scenarios in a short timeframe and to give policy makers and the public the opportunity to evaluate transport strategies and proposed measures directly.

Apart from methodological issues reliable data is most important to yield results that can be used for political decision making. If a city has undergone several changes in infrastructure or broader societal changes such as demographic developments or changes in preferences, new survey data or other data sources to model individual travel behaviour should be applied. The availability and reliability of data are also relevant for the validation of the results, which usually requires measured data or available sophisticated approaches to compare it with. Measurements of air pollutant concentrations are one example. In conclusion, the maintenance and installation of new measurement stations at locations with high traffic demand should be aimed for.

With this work, the methodological prerequisites for urban air pollution modelling and the evaluation of transport policies have both been developed. The effects of selected transport policies are exemplarily evaluated for the city of Munich. Beyond Munich, this approach is aimed at application in other cities, which also need to reduce air pollutant concentrations and could benefit from using the developed methodology and integrating the respective city specific data. A one-to-one implementation will most likely not be possible as cities differ from each other. Thus, some changes in setting up a base and policy case would be required. Nevertheless, the developed integrated air pollution modelling approach, as developed and applied in this thesis, provides the tools and framework for such analyses.

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Appendix: Simulation details

This Appendix presents more information about the MATSim simulation approach that is used in chapter 4. Every step of the iterative loop in Section 4.2.1 is illustrated in more detail in the following.

Plan Generation

An agent's daily plan contains information about his/her planned activity types and locations, about duration and other time constraints of every activity, as well as the mode, route, the desired departure time, and the expected travel time of every intervening trip (= leg). Initial plans are usually generated based on microcensus information and/or other surveys. The plan that was reported by an individual is marked as 'selected' in the first step.

Traffic Flow Simulation

The traffic flow simulation executes all selected plans simultaneously in the physical environment and provides output describing what happened to each individual agent during the execution of its plan. The *car traffic flow simulation* is implemented as a queue simulation, where each road (= link) is represented as a first-in first-out queue with two restrictions (Gawron, 1998; Cetin et al., 2003). First, each agent has to remain for a certain time on the link, corresponding to the free speed travel time. Second, a link storage capacity is defined which limits the number of agents on the link; if it is filled up, no more agents can enter this link. The *public transport simulation* simply assumes that travelling takes twice as long as travelling by car on the fastest route in an empty network[27] and that the travel distance is 1.5 times the beeline distance between the activity locations. Public transport is assumed to run continuously and without capacity restrictions (Grether et al., 2009; Rieser et al., 2009).

All other modes are modelled similar to public transport: travel times are calculated based on mode-specific travel speed and the distance estimated for public transport. However, the attributes of these modes are not relevant for the present chapter since agents are only allowed to switch from car to public transport and the other way around. Trips from the survey that are no car or public transport trips, are held fixed during the learning cycle, thus not changing mode share in any direction.

Output of the traffic flow simulation is a list that describes for every agent different *events*, for example, entering or leaving a link, arriving or leaving an activity. These

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[27] This is based on the (informally stated) goal of the Berlin public transport company to generally achieve door-to-door travel times that are no longer than twice as long as car travel times. This, in turn, is based on the observation that non-captive travellers can be recruited into public transport when it is faster than this benchmark Reinhold (2006).

events are written in XML-format and include agent ID, time, and location (link or node ID). It is, therefore, quite straightforward to use this disaggregated information for the calculation of link travel times or costs (which is used by the router module), trip travel times, trip lengths, and many more.

Evaluating Plans

In order to compare plans, it is necessary to assign a quantitative measure to the performance of each plan. In this work, a simple utility-based approach is used. The elements of this approach are as follows.

First, the total utility of a plan is computed as the sum of individual contributions:

$$V_{total} = \sum_{i=1}^{n} \left(V_{perf,i} + V_{tr,i} \right) \ , \tag{A.1}$$

where V_{total} is the total utility for a given plan; *n* is the number of activities; $V_{perf,i}$ is the (positive) utility earned for performing activity *i*; and $V_{tr,i}$ is the (usually negative) utility earned for travelling during trip *i*. Activities are assumed to wrap around the 24-hours-period, that is, the first and the last activity are stitched together. In consequence, there are as many trips between activities as there are activities.

Second, a logarithmic form is used for the positive utility earned by performing an activity:

$$V_{perf,i}\left(t_{perf,i}\right) = \beta_{perf} \cdot t_{*,i} \cdot ln\left(\frac{t_{perf,i}}{t_{0,i}}\right) \ , \tag{A.2}$$

where $t_{perf,i}$ is the actual performed duration of the activity, $t_{*,i}$ is the “typical” duration of an activity, and β_{perf} is the marginal utility of an activity at its typical duration. β_{perf} is the same for all activities, since in equilibrium all activities at their typical duration need to have the same marginal utility. $t_{0,i}$ is a scaling parameter that is related both to the minimum duration and to the importance of an activity. As long as dropping activities from the plan is not allowed, $t_{0,i}$ has essentially no effect.

Third, the disutility of travelling used for simulations is estimated from survey data which is explained in Section 4.3.2.

In principle, arriving early or late could also be punished. For this work, there is, however, no need to do so, since agents are not allowed to reschedule their day by changing departure times. Arriving early is already implicitly punished by foregoing the reward that could be accumulated by doing an activity instead (opportunity cost). In consequence, the effective (dis)utility of waiting is already $-\hat{\beta}_{perf} \cdot t_{*,i}/t_{perf,i} \approx -\hat{\beta}_{perf}$. Similarly, that opportunity cost has to be added to the time spent travelling.

After evaluating daily plans in every iteration, a certain number of randomly chosen agents are forced to re-plan their day for the next iteration. This learning process is, in the present chapter, done by two modules corresponding to the two choice dimensions available: a module called ‘router’ for choosing new routes on the road network and a module called ‘subtour mode choice’ for choosing a new transport mode for a car or public transport trip. The router module bases its decision for new routes on the output of the car traffic flow simulation and the knowledge of congestion in the network. It is implemented as a time-dependent best path algorithm (Lefebvre and Balmer, 2007), using generalised costs (= disutility of travelling) as input. The subtour mode choice module changes the transport mode of a car subtour to public transport or from a public transport subtour to car. A subtour is basically a sequence of trips between activity locations. However, the simulation needs to make sure that a car can only be used if it is parked at the current activity location. Thus, a subtour is defined as a sequence of trips where the transport mode can be changed while still being consistent with the rest of the trips. For example, it is assured that a car, which is used to go from home to work in the morning, needs to be back at the home location in the evening. If the car remains, for example, at the work location in order to use it to go for lunch, then the whole subtour of going to work and back needs to be changed to public transport.