A hybrid dispersion modelling approach for quantifying and assessing air quality in Germany with focus on urban background and kerbside concentrations

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AADT	Annual Average Daily Traffic
AirBase	European Air Quality database
BASt	Bundesanstalt für Straßenwesen *(Federal Highway Research Institute)*
BImSchG	Bundes-Immissionsschutzgesetz *(Federal Immission Control Act)*
CASES	Cost Assessment for Sustainable Energy Systems
CFD	Computational Fluid Dynamic
CI	Car International model
CLC2000	Corine Land Cover version 2000
CLRTAP	Convention on Long-Range Transboundary Air Pollution
CMB	Chemical Mass Balance
CO	Carbon monoxide
CO_2	Carbon dioxide
CORINE	Coordination of Information on the Environment
CRF	Concentration Response Function
DALY	Disability Adjusted Life Years
DEM	Digital Elevation Model
DIW	Deutsches Institut für Wirtschaftsforschung *(German Institute for Economic Research)*
EC	European Community
ECMWF	European Centre for Medium Range Weather Forecast
EEA	European Environmental Agency
EMEP	Co-operative Programme for Monitoring and Evaluation of Long-range Transmission of Air Pollutants in Europe
ETC-AQ	European Topic Centre on Air Quality
EU	European Union
EUROAIRNET	European Air Quality Monitoring Network
Eurostat	Statistical Office of the European Communities
EXTERNE	External Costs of Energy
FUND	Climate and Framework for Uncertainty, Negotiation and Distribution model
GENEMIS	Generation and Evaluation of Emission Data
GIS	Geographic Information System
GRACE	Generalisation of Research on Accounts and Cost Estimation
GWP	Global Warming Potential
HBEFA	Handbook Emission Factors for Road Transport
HDV	Heavy Duty Vehicles
HEATCO	Developing Harmonised European Approaches for Transport Costing and Project Assessment
IER	Institute for Energy Economics and the Rational Use of Energy
IFEU	Institute for Energy and Environmental Research
INFAS	Institut für angewandte Sozialwissenschaft *(Institute for Applied Social Sciences)*
IPA	Impact Pathway Approach
IPCC	Intergovernmental Panel on Climate Change
Km	Kilometres

K-S	Kolmogorov-Smirnov test
LCA	Life Cycle Assessment
LDV	Light Duty Vehicles
LE	Life Expectancy
LRS	Lower respiratory symptoms
LUBW	Landesanstalt für Umwelt, Messungen und Naturschutz Baden-Württemberg *(Regional Office for Environment, Measures and Nature Protection)*
LUCAS	Land Use and Cover Area frame sample Survey
LUR	Land-Use Regression
MB	Mean Bias
MC	Monte Carlo
MFB	Mean Fractional Bias
MFE	mean Fractional Error
MISKAM	Microscale Model
MLuS	Merkblatt über Luftverunreinigungen an Straßen *(Leaflet on air pollution along roads)*
NECD	National Emissions Ceilings Directive
NEEDS	New Energy Externalities Developments for Sustainability
NH_3	Ammonia
NMB	normalized mean bias
NME	normalized mean error
NMVOC	Non-Methane Volatile Organic Compounds
NO	Nitric oxide
NO_2	Nitrogen dioxide
NOX	Nitrogen oxides
NS	Not significant
NUSAP	Numeral Unit Spread Assessment Pedigree
O_3	Ozone
OECD	Organisation for Economic Co-operation and Development
PAREST	Particle Reduction Strategies
PDF	Probability Density Function
PEACE	Pollution Effects on Asthmatic Children in Europe
PM	Particulate Matter
PM_{10}	Particulate matter with an aerodynamic diameter of less than 10 µm
$PM_{2.5}$	Particulate matter with an aerodynamic diameter of less than 2.5 µm
PM_{coarse}	Particulate matter with an aerodynamic diameter between 10 and 2.5 µm
P-P plot	Probability-probability plot
PPB	Parts per billion
R^2	Coefficient of determination
RACM	Regional Atmospheric Chemistry Mechanism
RAD	Restricted Activity Days
RBS	Rural background monitoring station
RECORDIT	Real Cost Reduction of Door-to-door Intermodal Transport
RMSE	root mean square error
SIREAM	size-resolved aerosol model
SNAP	Selected Nomenclature for Air Pollution
SO_2	Sulphur dioxide

SOMO35	Sum Of Means Over 35 ppb
TERM	Transport and Environment Reporting Mechanism
TRAPOS	Traffic Pollution in Streets
TREMOD	Transport Emission Model
TU	Traffic urban monitoring station
U.S. EPA	United States Environmental Protection Agency
UBA	Umweltbundesamt *(Federal Environment Agency)*
UBS	Urban background monitoring station
UE	Urban Entity
UMZ	Urban Morphological Zone
UN	United Nations
UNECE	United Nations Economic Commission for Europe
UNFCCC	United Nations Framework Convention on Climate Change
UNITE	Unification of Accounts and Material Costs for Transport Efficiency
US	United States
USEPA	Unite States Environmental Protection Agency
USGS	United States Geological Survey
VBA	Visual Basic for Applications
VKT	Vehicle Kilometres Travelled
VOC	Volatile Organic Compounds
VOLY	Value of a Life Year
WHO	World Health Organisation
WLD	Work Lost Days
WTA	Willingness To Accept
WTP	Willingness To Pay
YLD	Years Lost due to Disability
YOLL	Years Of Life Lost

Abstract

Air pollution control strategies have helped to improve air quality over Europe over the last thirty years. Despite this success, the improvements have been insufficient to protect health of those who spend most of their time within urban areas and particularly near major roads. Considering that an urban street network is a structuring component of the city, a detailed analysis of its interaction with the environment and inhabitants is relevant for assessing policy measures aiming at improving urban air quality. However, given the inherent complexity of urban environments and the incomplete understanding of the physical and chemical processes involved in pollutant dispersion, it is a challenging task to estimate urban air quality.

The objective of this thesis was to develop a modelling approach to resolve not only the long-range pollution dispersion but also to capture the higher pollutant concentrations commonly found within urban areas and at kerbside for assessing the localized effects associated to vehicle-related pollutants. A major challenge was to provide estimates not only for specific streets and cities but for the major road network and all streets within major cities in Germany. For this purpose, a hybrid dispersion modelling approach was developed for predicting air quality across different spatial scales: from regional to urban and kerbside scale, accounting for the intrinsic and distinctive urban morphology of urban areas.

The hybrid dispersion modelling approach was used for estimating annual concentrations of PM_{10}, $PM_{2.5}$, and NO_2 for all urban areas with more than 50 000 inhabitants in Germany for the reference year 2005. The results showed that there are large differences on air quality levels across urban areas in Germany, which may be relevant when planning or evaluating emission control strategies. Furthermore, an empiric regression function was also developed to estimate the number of days exceeding the daily limit value of 50 $\mu g/m^3$ of PM_{10} by means of the annual mean PM_{10} concentrations.

The air quality reference scenario was also applied to estimate health and climate change impacts associated to road vehicle activities in Germany in the year 2005. The modelling approach enabled a differentiation not only by vehicle types and technologies but also across urban areas within a geographically referenced framework. The results indicate that the total health damages attributed to road vehicle operation in Germany in the year 2005 account for almost 60 thousand Disability Adjusted Life Years (DALYs). Furthermore, the urban areas with the largest total DALYs attributed to vehicle use are located in the Essen-Dortmund area, Cologne-Bonn, and Berlin, followed by Hamburg, Frankfurt, Munich, and Stuttgart.

The total health and climate change costs attributed to road vehicle operation in Germany in the year 2005 were estimated to be around 5.2 thousand millions $EURO_{2000}$. Whereas heavy duty vehicles did only 8% of the total mileage, they are responsible for 28% of the total costs. On the other hand, both diesel and petrol passenger account for about 86% of the total mileage and they are responsible for two thirds of the total costs.

Kurzfassung

In den letzten 30 Jahren haben Luftreinhaltungsstrategien entscheidend dazu beigetragen, die Luftqualität in Europa zu verbessern. Doch trotz dieses Erfolges sind die Verbesserungen noch unzureichend um die Gesundheit derer, die den Großteil ihrer Zeit in Ballungsgebieten und dort besonders in der Nähe von Hauptstraßen verbringen, zu schützen. Wenn man bedenkt, dass das städtische Straßennetz ein strukturbildendes Element einer Stadt ist, dann ist eine detaillierte Analyse, wie dieses Straßennetz mit seiner Umwelt und den dort lebenden Bewohnern interagiert, von Bedeutung um die politischen Maßnahmen zur Verbesserung der Luftqualität zu bewerten.

Das Ziel dieser Arbeit war es, einen Modellierungsansatz zu entwickeln, mit dem man nicht nur den Ferntransport von Luftschadstoffen abbilden kann, sondern auch die häufig in städtischen Gebieten und an Straßen zu findenden höheren Luftschadstoffkonzentrationen zu erfassen. Dieser Ansatz sollte eingesetzt werden um die zur Straßenverkehrsemissionen zugeordneten Effekte zu bewerten. Eine große Herausforderung war es, Abschätzungen nicht nur für bestimmte Straßen und Städte zu errechnen, sondern für das Hauptstraßennetz und alle Straßen in großen Städten in Deutschland. Zu diesem Zweck wurde ein hybrider Ausbreitungsmodellierungsansatz zur Modellierung der Luftqualität über unterschiedliche räumlichen Skalen entwickelt: von regionalen- zu städtischen- hin bis zu Straßenebene, unter Berücksichtigung der intrinsischen und charakteristischen urbanen Morphologie der städtischen Gebiete.

Der hybride Ausbreitungsmodellierungsansatz wurde zur Abschätzung der jährlichen Konzentration von PM_{10}, $PM_{2.5}$ und NO_2, für alle städtischen Gebiete mit mehr als 50 000 Einwohnern in Deutschland für das Bezugsjahr 2005, verwendet. Die Ergebnisse zeigten, dass es große Unterschiede hinsichtlich Luftqualität in städtischen Gebieten in Deutschland gibt, welche bei der Planung oder der Bewertung von Emissionsminderungsstrategien relevant sein können. Darüber hinaus wurde eine empirische Regressionsfunktion entwickelt um die Anzahl der Tage, an denen der Grenzwert von 50 µg/m^3 für PM_{10} überschritten wird, als Funktion des Jahresmittelwerts der PM_{10} Konzentration abzuschätzen.

Ferner wurde das Luftqualität Referenzszenario für das Jahr 2005 angewandt, um die Gesundheits- und Klimawandelauswirkungen, welche den Straßenverkehrsaktivitäten in Deutschland zuzuordnen sind, zu errechnen. Dieser Modellierungsansatz ermöglicht eine Differenzierung nicht nur nach Fahrzeugtypen und Technologien, sondern auch nach städtischen Gebieten innerhalb eines georeferenzierten Informationssystems. Die Ergebnisse zeigen, dass die durch die Straßenverkehrsaktivitäten in Deutschland im Jahr 2005 verursachten gesundheitlichen Schäden fast 60 000 Disability Adjusted Life Years (DALYs) betrugen. Darüber hinaus hatten städtische Gebiete wie Essen-Dortmund, Köln-Bonn und Berlin dann gefolgt von Hamburg, Frankfurt, München und Stuttgart die höchste Anzahl an DALYs. Die durch die Straßenverkehrsaktivitäten in Deutschland im Jahr 2005 gesamten Gesundheits- und Klimawandelkosten betrugen Schätzungen zufolge rund 5.2 Milliarden $€_{2000}$. Dabei entfallen auf schwere Nutzfahrzeuge 28% der Gesamtkosten bei nur 8% der gesamten Fahrleistung und zwei Drittel der Gesamtkosten auf Personenkraftwagen, die sowohl Benzin als auch Dieselfahrzeuge umfassen, bei 86% der Fahrleistung.

Chapter 1

Introduction

Environmental change occurs as a result of both human and natural activity. However, the pressure on natural resources resulting from unsustainable economic development has continuously increased over the last few decades. Although environmental pollution as it is usually understood today began with the industrial revolution in Europe, increasing international scientific concern began to be expressed at the end of the sixties of the past century. Since then, extensive research evidence has been gathered supporting the notion that air pollution is related to a number of adverse impacts on human health and the environment, such as increasing risk of cardiovascular and respiratory diseases (e.g., MacNee & Donaldson, 2000; Yang, 2000), decrease of life expectancy (e.g., Dockery et al., 1993; Pope et al., 1995; WHO, 2005a), and damages to buildings, crops, and ecosystems (e.g., Cowell & Apsimon, 1996; Tidblad et al., 2001).

In regard to the transport sector, the relationship between transport infrastructure, economic activity and population development is beyond question. Transport is an essential driver of economic development and growth, bringing tangible socioeconomic effects. However, according to a recent report from the Transport and Environment Reporting Mechanism (TERM), the environmental performance of transport has not improved and the message could be summarized in simple words: transport is becoming less and not more environmentally sustainable (EEA, 2009c). Road transport deserves special attention since it is the sector with the largest development and, at the same time, it remains the single main source of a number of harmful pollutants that largely contribute to poor air quality (EEA, 2008). Thus, energy efficiency and reducing transport emissions are among the greatest challenges faced by this sector.

1.1. Air quality in Germany, state and trends

In the Federal Republic of Germany, environmental awareness began early compared to other large economies in the world. In the 1960s, it was clear that the economy wonder had not only brought a stable economy but air pollution caused by industry and other activities as well. At that time, there were some initiatives and programs at all levels which addressed environment protection and environmental protection was implemented into policies in the seventies. This early engagement enabled Germany to be precursor on some aspects pertaining to the protection of the environment. The protection of human beings, animals and plants, soil, water, the atmosphere as well as cultural objects and other material goods against harmful effects on the environment is addressed in the Federal Immission Control Act (BImSchG, from its initials in German). This Act was promulgated in 1974 and since then it has been amended and modified several times.

As of 2009, emissions of several pollutants have markedly decreased in Germany and are no longer relevant for air quality policies (e.g., sulphur dioxide, carbon monoxide and lead). This should be seen as the consequence of large emission reductions achieved through systematic policies and instruments applied at a national and European level for this purpose. In fact, air pollutant concentrations in ambient air have receded significantly over the last few decades in almost all European countries, despite the growth in vehicle ownership and population. However, improvements can be mainly observed on the regional scale and control strategies are still insufficient in urban areas, where high levels of urban pollution can actually be observed across Germany (UBA, 2009). Hence, the high levels of certain pollutants, mainly particulate matter and nitrogen dioxide, within urban areas represent one of the most prominent issues on the environmental agenda in Germany and further measures are still needed to reduce pollutant concentration levels in order to guarantee that people, especially those living in urban areas, can breathe air that, by European standards, can be called acceptable for their health.

1.2. Problem statement – Setting the scene

In the light of current trends, transportation is the second-largest and the second-fastest-growing source of global greenhouse gases (OECD, 2008). In addition, road transport prevails as the single most relevant source of nitrogen dioxide and the second most important source of fine particulates (EEA, 2008). At the same time, people living in urban areas are likely to be the most affected by this development due to the higher pollutant levels commonly found within urban areas. This development put forward the task of improving the knowledge of the dispersion processes and adverse effects of vehicle-related pollution on human health and the environment.

Air quality modelling is an essential tool for most studies dealing with air pollution concerns. An air dispersion model attempts to describe how compounds of any nature disperse in the ambient atmosphere, providing estimates of pollutants concentrations for a defined spatial and temporal domain. They are developed to suit different purposes and, accordingly, their spatial resolution is mainly determined by the nature of the issue to be addressed. For instance, while a large scale can be the best option for studying the transboundary effects of pollutants in Europe, a medium scale may be better for forecasting regional air pollution, and an even smaller spatial scale could be needed for analysing flow and dispersion near a building.

However, road transport emissions may travel hundred of kilometres away from the source and, at the same time, significant effects on human health related to those emissions have been identified near their source. This fact poses a challenge when trying to assess vehicle-related pollution issues: on the one hand, models with a large spatial scale, which commonly ranges from dozens of kilometres down to a few kilometres, provide information about pollutant concentrations over extensive areas, allowing for considering regional and continental effects. Yet, their spatial resolution may not depict accurately pollutant concentrations at a local scale. On the other hand, models with a smaller spatial scale, which can range from several thousand metres to a few metres, are able to depict pollutant concentrations near their source but they cannot reproduce the long-range transport of such pollutants.

This dilemma clearly points out to the need for models able to depict concentration gradients over different spatial scales and, particularly when addressing vehicle-related air pollution, pollutant concentrations within urban environments and at the kerbside. An approach for tackling this problem is model nesting for addressing different scales. It basically consists of embedding high-resolution models within the domain of models with coarser resolution (e.g., Brücher, Kessler, Kerschgens, & Ebel, 2000; Kessler, Brücher, Memmesheimer, Kerschgens, & Ebel, 2001; Y. Tang, 2002). However, the applicability of this approach is limited to relatively small areas because the input data requirements and computational resources increase strongly with increasing domain size. For this reason, an application of nesting modelling for a detailed assessment, i.e. from regional to urban and kerbside scale, of the air quality in all large cities in Germany is not feasible.

Thus, it seems evident that existing models reflect only part of the true pollutant concentrations in ambient air, failing to describe the pollution increment found within urban areas and at kerbside. Considering that the majority of the German population lives in urban areas, this fact highlights the need for methodologies and tools for estimating more accurately the large concentration gradients. Here it is important to keep in mind that the information provided by air quality models is not only relevant for air quality managing purposes but it is also essential for addressing a wide range of relevant health policy issues, such as the impact of emission reduction policies, human exposure to vehicle-related emission at street level, urban climate, future strategic urban planning, and the quantification of the socio-environmental damage related to human activities (i.e., road transportation).

Over the last few decades, environmental issues have become economic issues as well. As a consequence, it seems unavoidable to address the concept of externalities when dealing with air quality issues. An externality of an activity can be simply defined as any external cost or benefit that it is not entirely borne by those responsible of it, i.e., the damages related to poor air quality are borne by all the individuals of a society, whether they are the polluters or not. Thus, given that air dispersion models are commonly integrated into impact assessment for estimating health damages and external costs, these issues are also addressed in this work.

Several assessment models have been designed for estimating external costs over the past decades. One of the pioneers in this area is the EcoSense model (e.g., European Commission, 1999, 2005). The assessment software EcoSense is designed for the analysis of single or multiple emissions sources (e.g., electricity and heat production) in Europe. However, considering that the dispersion models implemented within EcoSense assume that the emissions are released from point sources (such as industrial stacks) and at a certain height over the ground, the model is not able to depict accurately pollutant concentrations associated to road transport emissions, since they are better described as linear emission sources and are released at ground level. On account of this limitation, Vossiniotis et al. (1996) further developed the modelling framework into a suitable version for transport emissions – the EcoSense Transport model. This model presents several features designed to provide a better picture of vehicle-related emissions impacts. For instance, a Gaussian model simulates pollutant dispersion on a local scale specifically for lineal sources and a geographic referenced interface enables the analysis of spatially explicit user-defined routes and their corresponding emissions produced, making use of a comprehensive vehicle catalogue (Schmid, 2005; Vossiniotis & Schmid, 1999). The EcoSense Transport model has been used in several impact assessments (Bickel, Torras Ortiz, & Kummer, 2006; Preiss, Bickel, & Friedrich, 2004; Schmid, 2005). However, despite the improvements with respect to the previous EcoSense model, the transport version still fails to adequately depict pollutant concentrations at a local level. This is not surprising since the dispersion model integrated into EcoSense transport does not take into account urban morphology (i.e., land use, building geometry, and street patterns, among others), which is vital to analyse the higher pollutant concentration measured within urban environments. A further problem with the

EcoSense Transport model is the large amount of data required for analysing only one specific route and, thus, modelling a city with its entire street network is clearly not feasible. Finally, a validation against observational data has not been carried out, adding uncertainty and weakening the validity of the results obtained with this model. Other research efforts have been carried out over the last years to improve the evaluation of health-costs externalities of air pollution (e.g., Andersen et al., 2008; Jensen, Willumsen, Brandt, & Kristensen, 2008). Yet, the spatial resolution of existing models remains rather low, reflecting only part of the true pollutant concentrations in ambient air and, therefore, the additional health burden related to the pollution increment found within urban areas cannot be captured.

Summing up it can be said that there is a pressing need for methodologies and tools for estimating concentration gradients more accurately, especially when analysing vehicle-related pollutants in urban areas. These instruments are needed to address relevant health policy issues such as the effectiveness of emission reduction policy measures and their impact on air quality, the exceedances of mandatory ambient air quality limit values, and the human exposure to vehicle-related emission at street level.

1.3. Scope and objectives

The main goal of this thesis is to develop a modelling approach to capture the higher pollutant concentrations commonly found within urban environments and street canyons. For this purpose, a hybrid dispersion modelling approach is developed for predicting air quality across different spatial scales: from regional to urban and kerbside scale, accounting for the intrinsic and distinctive urban morphology of urban areas. The hybrid dispersion modelling approach should be used to build an air quality reference scenario for all large urban areas in Germany for the reference year 2005. The reliability and accuracy of the model should be evaluated comparing the results against observational data. Furthermore, a sensitivity and uncertainty analysis should be carried out in order to identify the parameters with the largest uncertainties and the strengths and weaknesses in the data generation process as well.

The air quality reference scenario will be applied to estimate human health impacts and their associated external costs of road transport in Germany for the year 2005. The results should enable a differentiation not only by vehicle types and technologies but also across urban areas within a geographically referenced framework. In this way, human health impacts and external costs for individual cities and technologies can be achieved, rather than generalised national values.

Given that, from the different impacts on the environment and living organisms attributed to road transport, human health and climate change are considered to be the most relevant, these are the impacts considered in this thesis. It is also relevant to note that an important premise guiding the development of the methodology presented here was to make use of freely available information, which normally already exists in every country or is easy to provide. The rationale behind this decision is to facilitate the application of the same methodology outside Germany, where data availability may be a relevant issue.

1.4. Outline of thesis

This thesis comprises six chapters, including necessary background, problem statement, scope, and objectives of the research presented in Chapter 1. The second chapter follows with a description of vehicle-related emissions. It discusses their main characteristics and their relevance to health-related damages. Moreover, a description of the European and German emission datasets used for dispersion modelling is provided, focusing on the spatial disaggregation of emissions in Germany and the definition of urban areas.

Chapter 3 is devoted to dispersion modelling. After a comprehensive review of the state of the art, the hybrid dispersion modelling approach developed in this work is presented. The conceptual basis of the hybrid approach along with a description of its components is given in this chapter. As an application of the modelling approach, estimations on urban air quality in all large urban areas in Germany are presented and a model to estimate the exceedances of the daily limit value for PM_{10} based on the annual mean PM_{10} concentration is introduced in this chapter as well

The evaluation of the modelling approach by means of a comparison of results against measured values is presented in Chapter 4. Sensitivity and uncertainty analysis of the model developed in this thesis can be found in this chapter as well.

In Chapter 5, the modelling approach developed in Chapter 3 is used to estimate human health and climate change impacts associated to airborne pollution generated by road transport in Germany. This chapter is devoted to describe the methodology chosen for estimating human health damages and their associated costs, focusing on the description of the Impact Pathway Approach. Furthermore, it is elucidated why monetary values can be used for evaluating non-market impacts and their advantages over other approaches. Finally, estimates of the human health and climate change costs attributed to road transport in Germany are presented in this chapter as well. Conclusions and recommendations for future research interest are presented in Chapter 6.

Chapter 2

Road vehicle emissions

Pollutant emissions can be defined as a discharge of chemicals, particulate matter or biological materials into the atmosphere by human and natural activities that cause harm or discomfort to humans and to other living organisms and materials (EEA, 2007a). Increasing pollutant releases have caused current and potential environmental problems like stratospheric ozone depletion, air quality decay global warming and climate change (IPCC, 2007b).

Several human activities can be accounted for as major contributors to air pollution, like energy production and industrial activities. However, in the light of current trends road transport is responsible for almost a fifth of the EU's greenhouse gas emissions (EEA, 2009a). In addition, road transport prevails as the single most relevant source of nitrogen dioxide and the second most important source of fine particulates (EEA, 2008). Whereas technological improvements in vehicles have led to significant reductions in emissions (e.g., carbon monoxide emissions have been largely reduced by increased engine efficiency and catalytic converters have significantly curbed tailpipe emissions of a number of pollutants), this development has not been enough to reduce emissions of several harmful pollutants.

This chapter outlines the intrinsic relationship between vehicle use and urban mobility. It presents a brief description of the main vehicle-related emissions in terms of their negative effects on human health and the environment. The chapter goes on presenting the emission datasets used for atmospheric dispersion modelling along with the methodology followed for their spatial disaggregation. Due to their relevance for this work, special attention is given to the definition of urban areas and their associated road transport emissions.

2.1. Urban Mobility – a paradox of modern time

Our vision of cities is changing. In the past, aesthetics and architecture prevailed in the traditional urban planning as the predominant concerns and, for most cases, scarce or little attention was paid to an efficient land-use distribution and transport planning. Over the last few decades, awareness has increased about an efficient organization of cities, the improvement in the quality of life and mobility of its inhabitants and, more recently, a sustainable urban development. In view of the complex and intrinsic relationships among its components, some authors even suggest that cities should be treated as organic creatures or even as whole ecosystems with their own dynamic, structure, and metabolism (Bradshaw, 2003; Pickett et al., 2001).

Urban mobility can be defined as the movement of goods and persons within cities using some kind of transport infrastructure. Since the 60s, increasing car ownership has been a relevant factor for growing fuel consumption in European cities. In Germany, car ownership has correspondingly grown, and as of 2008 only one out of five households did not have a vehicle and almost ten percent of them possessed more than one vehicle. Furthermore, data on daily mobility show that over 60 percent of all trips are made by car; although a newer survey reports a slight increase in trips by bicycle (INFAS & DIW, 2004, 2008).

As people and goods have become increasingly mobile, it is clear that this feature plays a relevant role in the sustainable city development and management. Yet increasing mobility has long-term impacts on the environment as motorization and energy use, mostly fossil fuels, rise as well. As a consequence, society seems to face two apparently opposite goals when citizens want to enjoy modern lifestyles that rely on a high level of personal and commercial mobility, but, on the other hand, they also demand clean air and reduction of vehicle-related pollutants in the places where they live, work, attend school or carry out leisure activities – a paradox in terms of urban mobility. In consequence, mobility plays an important role in a city's environmental performance and sustainable development, making reductions on vehicle-related pollutants an essential issue in the efforts to improve the quality of life of their citizens and reduce to a satisfactory degree the adverse effects of air pollution.

2.2. Environmental relevance of vehicle-related emissions

Considerable efforts have been made trying to shed light on determining the effects of harmful air pollutants on human health and the environment. Regarding vehicle-related emissions, accumulated scientific evidence points to a positive correlation between living near major roads and experiencing a significant higher risk of developing or worsening health problems (e.g., Ciccone et al., 1998; Holguin et al., 2007; Janssen, van Vliet, Aarts, Harssema, & Brunekreef, 2001). At the same time, vehicle exhaust is a mixture of thousands of gases and particles from which several has been identified as toxic. For instance, it has been demonstrated that chemicals in exhaust emissions can adversely affect lung function and may stimulate allergic reactions and airway narrowing (D' Amato, 1999; Koren, 1995; Yang, 2000). Considering that motor vehicles not only generate emissions through combustion processes but that they also produce a large amount of particles by the interaction between tires, road pavement and friction materials, these emission are also assessed in this work. In the following sections, a brief description of the main vehicle-related emissions from the point of view of their adverse effects on human health and the environment is presented.

2.2.1 Particulate matter

Particulate matter (PM) is a complex mixture. According to the definition of the World Health Organisation particulate matter consists of 'a mixture of particles that can be solid, liquid or both, are suspended in the air and represent a complex mixture of organic and inorganic substances' (WHO, 2005b). In addition to falling into different size ranges, particulate matter differs in chemical composition, formation mechanism and sources. According to their origin, particles emitted directly into the atmosphere are called primary particles, whereas particles resulting from atmospheric chemical processes are usually called secondary particles. Referring to their size, PM is normally classified according to its aerodynamic diameter into PM_{10} and $PM_{2.5}$ and, whereas PM_{10} have an aerodynamic diameter of less than 10 µm, $PM_{2.5}$ have an aerodynamic diameter of less than 2.5 µm.

Major sources of primary PM are motor vehicles, fossil fuel combustion by electric utilities, industry and, to a lesser degree, vegetation burnings and processing of metals. Besides the aforementioned sources, the smaller fraction of PM also contains the secondary particles which are created in the atmosphere by the oxidation of precursor gases or 'by other processes involving chemical reactions of free, adsorbed or dissolved gases' (U.S. EPA, 1996).

The most relevant secondary PM precursors are nitrogen oxides, non-methane volatile organic compounds and sulphur dioxide.

2.2.2 Nitrogen oxides

Nitrogen oxide (NO_X) is the generic name for a group of compounds of nitrogen and oxygen produced mainly by the burning of fossil fuels. Nitrogen oxides contained in exhaust gases from vehicles are nitric oxide (NO) and nitrogen dioxide (NO_2), both highly reactive compounds. NO is a precursor of tropospheric ozone and nitrates through photochemical processes and/or particle formation, and it also contributes to the deposition of wet and dry acidic components. NO_2 is a gaseous pollutant that has been associated with low birth weight (Ha et al., 2001) and respiratory difficulties among children (Chauhan et al., 2003). However, epidemiological evidence remains inconclusive as to whether the health risks observed are associated to NO_2 itself, its products (including particulate matter and ozone) or whether NO_2 is a marker of exposure to other vehicle-related pollutants not yet measured (WHO, 2004).

It should be noted that the use of oxidizing catalytic converters may also have contributed to increasing NO_2 and N_2O emissions (Scholz & Rabl, 2006; Wiedmann, Kersten, & Ballschmiter, 2000). Thus, considering that the latter is a greenhouse gas with a global warming potential 310 times larger than carbon dioxide (UNFCCC, 2003) and the former represents a burden to human health, they have become one of the main concerns on the European environmental agenda.

2.2.3 Ozone

Ozone is a powerful oxidizing agent and transboundary pollutant that represents a significant burden to human health. It is linked to aggravation of lung diseases, development of asthma, and premature mortality (e.g., Bell, Dominici, & Samet, 2005; Jerrett et al., 2009). Road transport contributes substantially to ozone, which is created in the atmosphere through complex chemical reactions driven by gases produced largely by transport, e.g., nitrogen oxides and non methane volatile organic compounds. After its release into the atmosphere, NO is rapidly oxidized to NO_2 by sunlight-driven chemical processes and available oxidants (WHO, 1997). The transformation rate is driven by complex non-linear photochemistry, which can even enhance ozone depletion at night time and in the immediate vicinity of large NO_X sources – known as the so-called titration effect.

2.2.4 Non-methane volatile organic compounds

Within the European regulatory context, volatile organic compounds (VOC) are ‘any organic compounds with an initial boiling point less than or equal to 250°C measured at a standard pressure of 101.3 kPa.’, (CEU, 2004). Due to its particular characteristics, methane is excluded from the analysis of other VOCs using the term non-methane VOC (NMVOC). Increasing NMVOC emissions from anthropogenic sources – such as burning fuels (gasoline, oil, coal, natural gas, etc.), solvent, paints and other products of daily use – have become a major health concern. They contribute to the production of photochemical oxidants by oxidizing nitric oxide in the presence of sunlight and are therefore an important precursor of ground-level ozone. Moreover, several NMVOCs are commonly found in vehicle exhaust and evaporation loses from vehicles, including benzene and 1,3-Butadiene – both well-known carcinogens, central nervous system disrupters, and respiratory irritants (U.S. EPA, 2002;

WHO, 1993). In order to address the potential hazard of benzene emissions, an air quality limit value for this pollutant will enter into force in the European Union in 2010.

2.2.5 Carbon dioxide

Looking at the worldwide increasing interest of society on environmental issues over the last few decades, it seems quite evident that one phenomenon attributed mainly to carbon dioxide (CO_2) has played a preponderant role in this development – the so-called global warming effect. Anthropogenic CO_2 is a major contributor to the enhancing of the natural greenhouse effect. The consequences of global warming have been largely discussed in the literature and since a detailed discussion of this subject is beyond the scope of this work, the reader is referred to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC, 2007a) for a more comprehensive discussion on the topic.

In this context, the road transport sector attracts special attention because of its share of overall CO_2 emissions, mostly driven by the constantly increasing demand for transport of passenger and goods, and the preference for road transport over other more environmental friendly transport modes.

2.3. Anthropogenic Emissions Inventories

When dealing with air pollution concerns, one of the basic questions needed to be answered is how large the amount of emissions released is. As in other areas of science, it is difficult to manage something when it cannot be measured. This premise also holds true for airborne emissions and, therefore, information on pollutant amount and their sources becomes crucial for any attempt to solve or even comprehend air pollution issues. In essence, a rather simple equation describing the direct influence of activity data and emission factors on the emissions produced is normally used for estimating anthropogenic emissions for all relevant sectors. This basic model can be written as follows:

$$\text{Emission} = \text{Activity data} \times \text{Emission factor} \qquad \text{Equation 2.1}$$

Although more complex models may be used for calculating emissions for some sources, kinds of emissions factors or activities can still be identified which parameterize these models. The simplicity of this equation, however, does not give the full picture of the complexity and large uncertainties inherent to estimating emissions. Quantitative data are required for a wide range of purposes: to identify activities and actors accountable for inadequate performance and, at the same time, to define objective environmental goals, priorities and limitations as well. Furthermore, strategies and policies performance can be measured and monitored to ensure that these instruments are effectively being implemented and to assess if air quality objectives are likely to be achieved.

In order to fulfil obligations specified in the different directives and regulations, emissions data for several relevant pollutants have to be reported to the Executive Body of the Convention on Long-Range Transboundary Air Pollution (CLRTAP). In 2001, the European Union introduced the National Emissions Ceilings Directive 2001/81/EC, also called NEC, which establishes national emissions ceilings in 2010 for sulphur dioxide, nitrogen oxides, non-methane volatile organic compounds and ammonia. In order to comply with the NEC directive Member States have to report their national emissions inventories, projections for 2010 and programs at the end of each year.

The emissions ceilings were set based on the share of each country in generating airborne pollutants and the associated costs. For Germany, this accounts for reductions of about 90% of SO_2, over 60% of NO_X, about 75% of NMVOC and 25% of NH_3 by 2010 compared to 1990 levels (EEA, 2009b). Germany has achieved large reductions in NMVOC and SO_2 emissions but it seems that additional reduction measures for NH_3 and NO_X, which are above 10% and 6% above their target values, respectively, are needed in order to comply with the NEC directive (UBA, 2007).

Given that road transport is the largest contributor to NO_X emissions in Germany, it seems clear that additional reduction measures in this sector are needed, such as curbing emissions through more limiting European standards for passenger cars and heavy-duty vehicles, or promoting purchase of low-emission heavy-duty vehicles. Furthermore, considering that NH_3 emissions are produced almost entirely by the agriculture sector, actions to reduce these emissions are being implemented mainly in this sector.

Whilst total national emissions are essential for starting any kind of analysis concerning environmental issues on a European level, the limited spatial resolution do not allow for going further and exploring the differentiated effects of air-borne pollution on human health at more local levels, such as within cities or near major roads. Thus, emissions datasets with a higher spatial resolution are needed. For this purpose, a reference scenario was assembled using two emissions datasets: one for the European domain and another with a higher spatial disaggregation for Germany. This reference scenario comprises all relevant sectors for the reference year 2005 and it is implemented as input for atmospheric dispersion modelling later in this work (Chapter 3). In the next section, the emissions datasets are described.

2.3.1 European anthropogenic emissions – The EMEP dataset

Annual emissions, activity data and projected total national emissions are officially reported by the Member States to the Co-operative Programme for Monitoring and Evaluation of Long-range Transmission of Air Pollutants in Europe (EMEP). Although the information is provided according to guidelines and harmonized estimation methodologies (e.g., Vestreng, 2003), the national information still contains inconsistencies or gaps, which have to be interpreted, corrected and/or gap-filled in order to guarantee Europe-wide unified emission estimations (Webdab, 2009). Thus, the EMEP inventory provides emission data for over 30 pollutants by sector of origin with a horizontal spatial resolution corresponding to the EMEP 50-by-50-km grid which can be obtained from the EMEP Centre on Emissions Inventories and Projections (CEIP) website and readily used for modelling purposes. The main pollutants considered for atmospheric dispersion modelling over Europe are primary PM10 and PM2.5, CO, NH3, SO2, NOX and NMVOC – all of them aggregated into eleven SNAP (Selected Nomenclature for Air Pollution) categories at the level one. A list of the categories is provided in the supplementary information.

A detailed description of this dataset and its components is beyond the scope of this work. For further details on the methodology implemented for each economy sector, spatial disaggregation and related data quality issues, the reader is referred to EEA (2007b) and the references therein.

2.3.2 German anthropogenic emissions – The IER dataset

The EMEP dataset presented in the last section provides emission data with a horizontal spatial resolution of 50 by 50-km. While this resolution may be acceptable for describing the atmospheric dispersion of pollutants over Europe, a higher resolution is required for a more detailed depiction of the dispersion processes in the domain of interest. Thus, a second emission inventory dataset with a higher spatial resolution was used for Germany.

Over the last decade and within the scope of a number of research projects, the Institute for Energy Economics and the Rational Use of Energy (IER from its initials in German), University of Stuttgart, has contributed to the development and continuous improvement of an emissions model. The model has been successfully applied for the generation of highly spatially and temporally resolved emission data for several national and EU projects, such as GENEMIS and ESPREME, to name a few (see Friedrich & Reis, 2004; Friedrich, Wickert, Schwarz, & Reis, 1999; Kühlwein, Wickert, Trukenmüller, Theloke, & Friedrich, 2002).

More recently, a comprehensive update of the German dataset was accomplished in the framework of a collaborative project with several research centres and federal agencies. The project PAREST (Particle Reduction Strategies) aims at identifying the reasons for the extensive PM_{10} exceedances in the country and suitable mitigation measures in order to comply European air quality regulations. Seeing that the European Commission is considering to include the fine portion of particulate matter in the air quality directive, plausible limit values for this pollutant are also explored in this project (Builtjes, Stern, & Theloke, 2008). Using a top-down approach, major improvements in the dataset were achieved within this project including a higher horizontal resolution (a 1-by-1 arc-minute grid), updated activity data and emission factors for the transport sector, a more detailed point sources inventory and enhanced spatial distribution parameters. Furthermore, release height was assigned following Pregger and Friedrich (2009).

As one of the main sources for several pollutants, special attention was given to the transport sector. Due to its relevance for this work, a description of the main data sources for estimating emissions totals and parameters used to spatially allocate the emissions are outlined in the next sections. The methodology and distribution parameters implemented for the other sectors are discussed in depth in Thiruchittampalam et al., (2009) and the references therein.

2.3.2.1 Estimation of road transport emissions

Data regarding road transport exhaust emissions were provided by the Transport Emission Model (TREMOD). This model has been developed and improved since 1993 by the Institute for Energy and Environmental Research (IFEU) on behalf of the German Federal Environmental Agency. TREMOD estimates energy consumption, modal split and exhaust emissions of the motorised traffic in Germany. The model considers not only the road traffic on public roads within Germany (excluding agriculture and military), but also other transport modes like rail (public transport), air (traffic from German airports to the first stopover), and inland water transport as well. The model has been continuously improved and updated with good-quality data provided by federal agencies and it constitutes an important tool for complying with international emissions reporting directives. The model provided national emission totals differentiated by road type and vehicle category, using emissions factors mostly taken from the Handbook Emission Factors for Road Transport (HBEFA). A detailed model description can be found in Knörr et al. (2005) and the references therein.

As TREMOD does not provide data on non-exhaust emissions, other sources are used for estimating these emissions. Emission from brake, vehicle tyre and road surface wear are estimated using emission factors from EMEP/CORINAIR Emission inventory guidebook (EEA, 2007b). Concerning resuspension, this parameter was estimated within the framework of PAREST following the assumptions presented in Schaap et al. (2009).

Road transport contributions to the total national emissions for the reference year 2005 are presented in Figure 2.1. From this figure, it is evident that this sector has an important share in the total CO, NO_X, PM_{10}, and $PM_{2.5}$ national emissions.

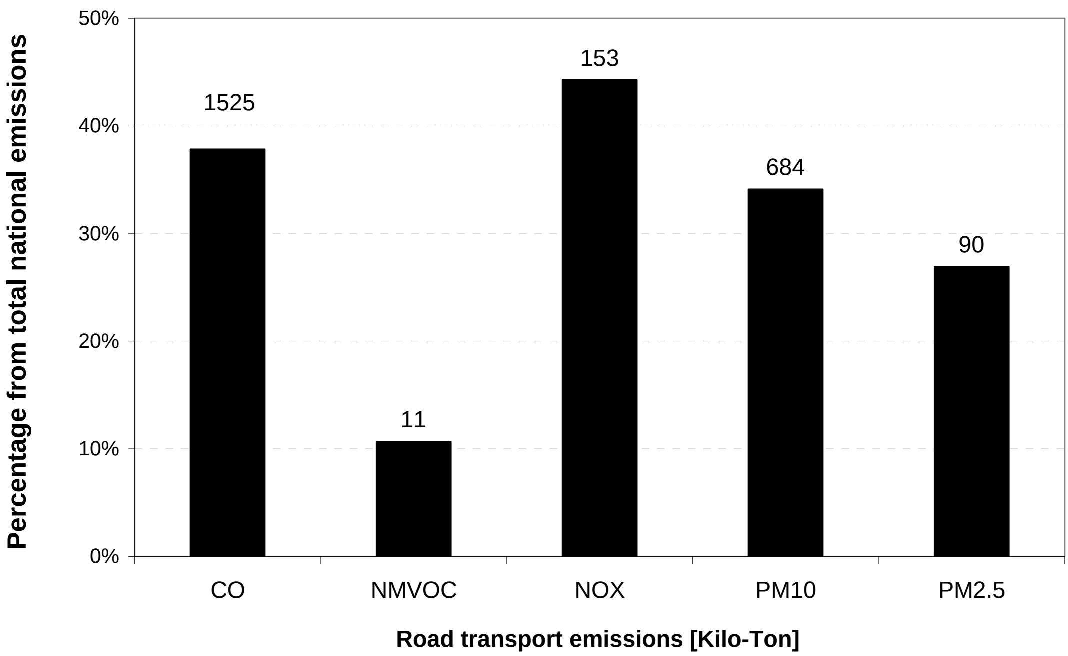

Figure 2.1 Road transport emissions and contribution to total national emissions.

Regarding the emissions regulated under the NEC Directive described in section 2.3., it is important to note that the road transport emissions of NMVOC and NO_X presented here differ slightly from the ones officially reported for the year 2005 (see EEA, 2007c). The reason for this discrepancy lies in the fact that energy balance is the basis for the international emission reporting. This means that road transport emissions are calculated and reported on the basis of fuel sold in the country concerned. Whilst parties might report their emissions based on the kilometres actually driven by vehicles on the corresponding geographic area, the energy balance method has proven to be easier to apply because the results are consistent with energy balances reported to other international agencies (e.g., Eurostat or the International Energy Agency) and, hence, it is preferred to the alternative method. Whereas this decision may not represent large differences for several countries, the growing fuel tourism phenomenon, i.e. when domestic car drivers get their fuel from over the border due to given price differences, is a cause of concern in Germany since this phenomenon substantially undermines the desired effects of environmental fuel taxes and creates additional vehicle-related pollution near the country borders as well.

Although the exact amount of additional vehicle kilometres driven using foreign fuel has proved to be difficult to estimate, it is presumed that significant differences exist between the emissions estimated based on fuel consumption and the emissions actually emitted by vehicles within the country boundaries. For instance, the Austrian Environmental Agency reports that increasing CO_2 emissions in this country can be explained by lower fuel prices in comparison with neighbouring countries. The agency further estimates that the share of fuel tourism accounts for about a third of the total emissions estimated using the energy balance method (Gugele, Rigler, & Ritter, 2006). In Germany, cost-benefit analyses have shown that even small differences in fuel prices constitute a strong incentive for filling up on fuel outside Germany (Michaelis, 2003). Therefore, it should be evident that for addressing air quality issues it is vital to consider the emissions that are actually being released within the geographical domain considered. Once total national emissions have been estimated, their spatial allocation is carried out according to several parameters. This issue is discussed in the next section.

2.3.2.2 Spatial disaggregation of road transport emissions

An important issue to be addressed by any emission inventory is the way in which the emissions are distributed over the inventory domain. This issue becomes more relevant when trying to assess the adverse effects of those emissions when they are released into the atmosphere. In this context, the physical location of emissions has to be determined as accurately as possible. In Germany, roads can be classified into the following categories:

- Motorways
- Federal roads
- State roads
- District roads
- Urban roads.

In this thesis, the first two road types are referred as the main German road network. This network comprises over 50 000 kilometres distributed across the thirteen German States and three independent cities (see Figure 2.2). Road emissions for the main German road network were allocated following a top-down approach using data from three sources: data from the automatic traffic counting system (Fitschen & Koßmann, 2007); manual road traffic counts provided by the Federal Highway Research Institute (BASt from its initials in German) (BASt, 2007); and a georeferenced digital road network (GfK Geomarketing, 2007). Taking advantage of available detailed vehicle mileage data, emissions were disaggregated according to this parameter for motorways and national roads (Köble, Thiruchittampalam, Theloke, & Kummer, 2009).

From Figure 2.2 it becomes evident that not all existing roads in Germany are included in this network. The main reason for this is the lack of a nationwide georeferenced database depicting vehicle mileage for state, district, and urban roads. As a result, other disaggregation parameters had to be used for the remaining road transport emissions. For state and district roads, their associated emissions were spatially allocated using total area as distribution parameter following a top-down approach.

Concerning emissions associated to urban roads, one important parameter used for their spatial disaggregation was the CORINE (Coordination of Information on the Environment) Land Cover database. This database provides a comprehensive digitalised inventory on land cover obtained through satellite image interpretation (EEA, 2002). The updated version for the reference year 2000 (abbreviated in the following as CLC2000) includes data for all 25 EC State Members and other European countries with an accuracy of at least 100 metres and using 44 land cover classes. A table with the description of the cover classes is provided in the supplementary information (Table E.2).

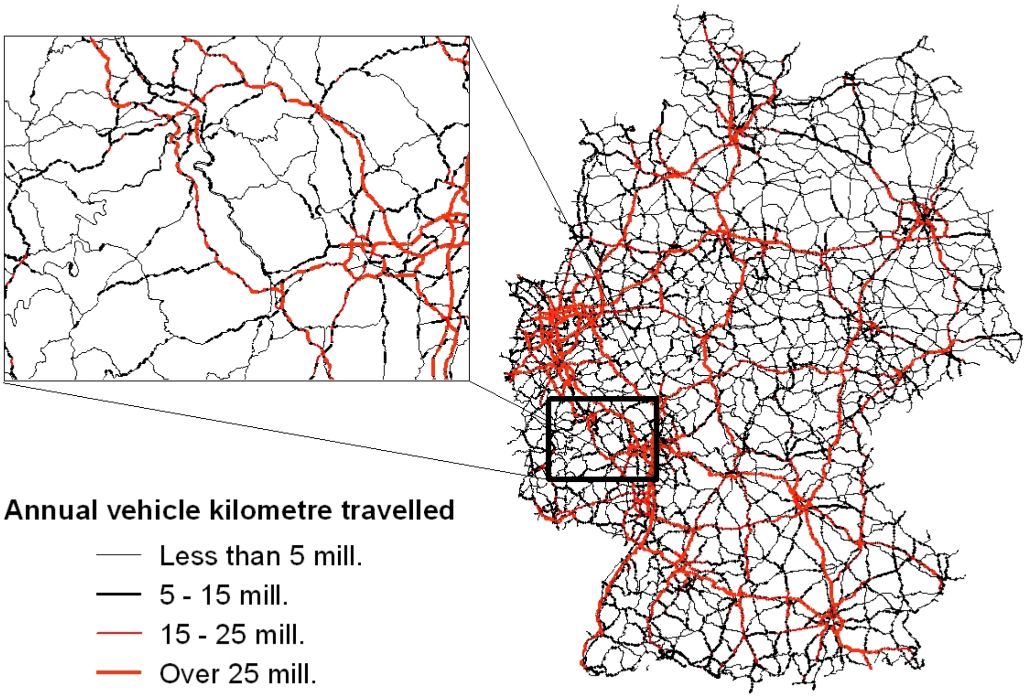

Figure 2.2 German main road network and mileage.

Even though field data collection was not implemented for building this database, it has been compared for testing its thematic accuracy with the LUCAS (Land Use and Cover Area frame sample Survey) database (e.g., Eiden et al., 2004; Eurostat, 2003). Since LUCAS is based on statistical sampling of points where field photographs were used for digitally registering land use and land cover in situ, this database has a higher accuracy than the CLC2000. In fact, the LUCAS database was the first option for this research, yet due to use restrictions and smaller domain (only 13 European States) the CLC2000 was chosen instead. Nevertheless, a comparison study found that the total reliability of CLC2000 is near 90% for all classes, depicting a higher reliability (> 95%) for artificial surfaces such as urban fabrics, industrial, commercial and transport units (EEA, 2006a).

Thus, the IER dataset is able to provide spatially and temporarily resolved emissions from brake, tyre and road surface wear, exhaust, cold start, fuel evaporation and resuspension.

2.4. Urban areas – definition and vehicle mileage

In the last section, the main characteristics of the IER dataset were provided, focusing on the parameters for the spatial allocation of road transport emissions. Despite its completeness, however, two important issues need to be addressed before using the dataset as input for dispersion modelling. Firstly, the extension of urban areas is not explicitly defined and secondly, information about vehicle activity within urban areas is rather scarce. Both issues arise as a consequence of the objectives pursued in this work, which aims to capture the higher pollutant concentrations commonly found within urban environments and street canyons. Thus, in the next section both issues are addressed and discussed.

2.4.1 Urban areas definition – The UMZ dataset

Relevant to any discussion involving urban areas is to define what areas are considered as such. Due to significant definition differences among countries, there is no international agreement upon the definition of rural and urban areas (UN, 2007). However, the Statistical Office of the European Communities (Eurostat) in collaboration with the member states developed a typology for a harmonized classification of the urbanization degree. According to this typology, population density is used for distinguishing urban, semi-urban and rural areas, with the following definitions:

Urban area: a population density greater than 500 persons/km^2;

Sub-urban area: a population density between 500 and 100 persons/km^2;

Rural area: a population density less than 100 persons/km^2.

This definition is quite straightforward and it can be easily applied to estimate the population distribution in a country using administrative units (e.g., municipalities or districts) as spatial entities. Following this definition, 85 percent of the German population are living in urban and sub-urban areas, and only 15 percent are living in areas defined as rural (Federal Statistical Office, 2005). Yet, these data do not provide information about the actual extent of the urban sprawl since they are computed based on rather large administrative units. To illustrate this issue, consider Figure 2.3. The scattered and heterogeneous land-use distribution within the boundaries of the German district of Stuttgart gives insight into how difficult it can be to define urban boundaries. This distinction is vital for addressing the difference between pollution levels within urban areas with respect to rural levels – The so-called urban increment. This concept is particularly relevant for estimating detailed pollutant concentration levels within urban areas and their associated adverse effects on human health, one of the main foci of this thesis.

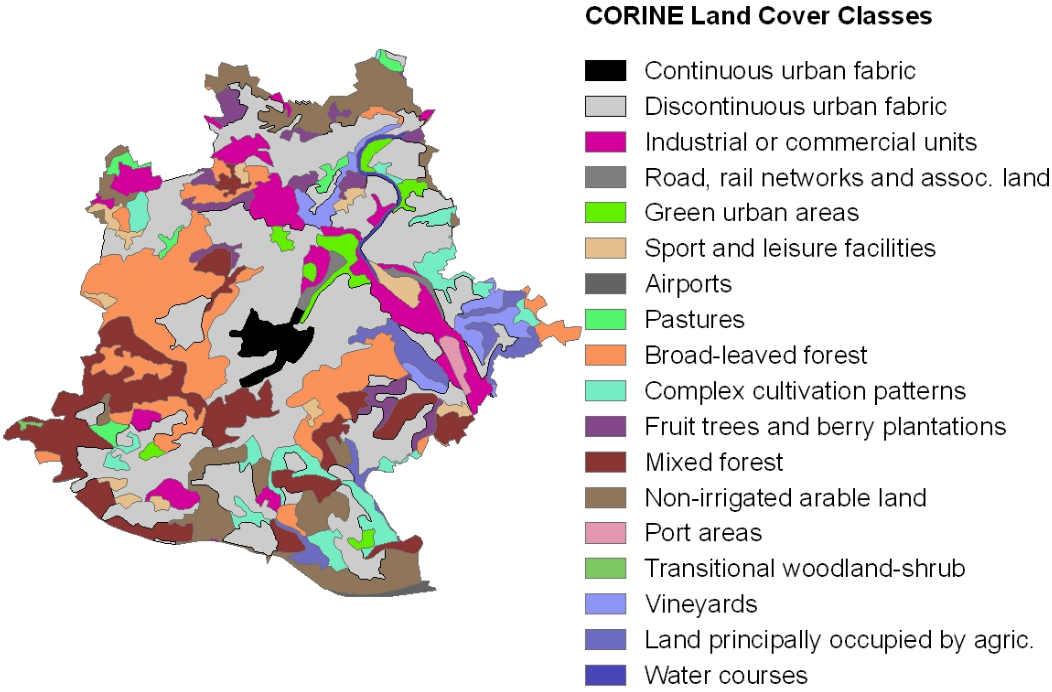

Figure 2.3 Land use in the German district of Stuttgart according to the Corine Land Cover database in its version 2000.

Thus, in recognition of the importance of defining urban boundaries when addressing urban pollution, the methodology for defining Urban Morphological Zones (abbreviated in the following as UMZ) proposed by Milego (2007) is adopted in this work. The methodology merges land-use classes contributing to the urban tissue and function. A summary of the CLC classes considered for this classification, along with the criteria for its inclusion in the UMZ is provided in the supplementary information (Table E.3).

The geographically referenced UMZ dataset (EEA, 2007d) for Germany is depicted in Figure 2.4. According to this classification schema, there are nearly 20 000 UMZ with a population density ranging from 22 to over 6000 inhabitants per square kilometre.

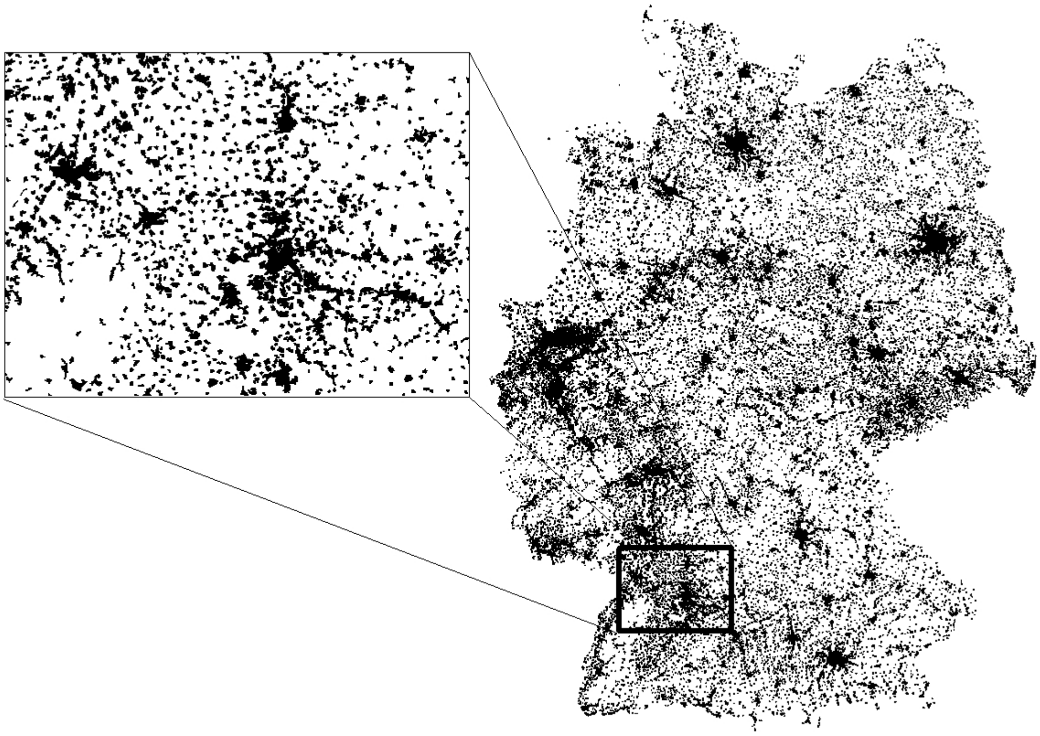

Figure 2.4 Urban Morphological Zones (UMZ) in Germany.

Assuming that additional pollution levels generated by smaller UMZ are low or negligible, only urban areas with a population larger than 50 000 inhabitants are analysed more in detail. Applying this criterion, there are 114 such entities in Germany comprising about one third of the total population. Once the urban areas were identified, the geographically referenced dataset was combined via spatial location with the IER dataset in order to obtain the Urban Entities (abbreviated in the following as UE) depicted in Figure 2.5. The entities defined in this way represent the basic spatial unit for analysing urban air quality, providing emissions disaggregated at a city level for all sectors. In Chapter 3, the UE provide the basic input data for developing a mathematical model to estimate urban increments. A comprehensive list of the administrative units included in each urban entity is provided in Annex A.

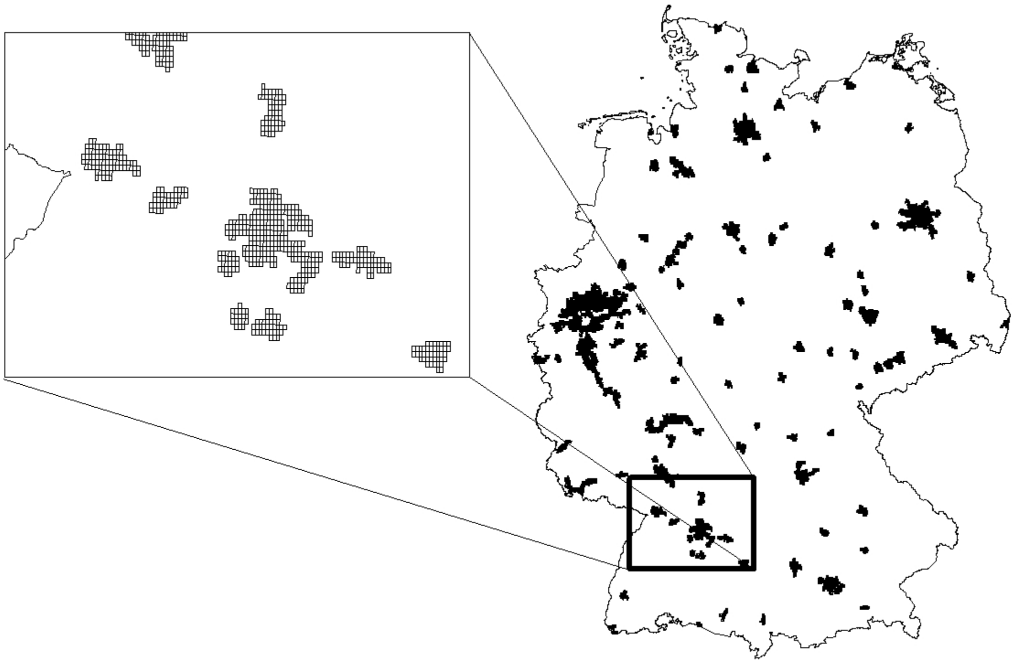

Figure 2.5 Urban entities with over 50 000 inhabitants in Germany.

2.4.2 Vehicle mileage in urban areas

The spatial allocation of emissions needed for estimating urban increments, i.e., the difference between pollution levels within urban areas with respect to rural levels, has been covered in the last section. Later in this work, this information is used for assessing average urban background pollutant concentrations for the urban entities under examination. However, pollutant concentrations are not evenly distributed within urban environments, but they are actually higher in places where stagnant meteorological conditions give rise to contamination hotspots, such as heavily travelled streets or street canyons. In fact, pollutant concentrations measured near traffic lines may be several times higher than the value measured at roof level, which represents the urban background pollutant concentration. This issue gains more importance when addressing adverse effects of vehicle-related air pollution since people living near busy roads may experience more short-term and long-term health effects attributed to air pollution than people living further away (WHO, 2005a).

On account of this, road transport emissions with an even higher spatial resolution than city level are needed in order to accurately depict pollutant concentrations within urban streets. Ideally, emissions should be computed using detailed vehicle flow and fleet composition data for every segment of an urban street network or for the main streets at least. In reality, only large cities are able to maintain and manage state-of-the-art traffic administration systems from which comprehensive vehicle flow and composition datasets can be generated. Thus, this information remains scarce or is not publicly available as the collection of reliable data entails large investments in traffic survey systems, which may comprise the installation of video cameras, automated counters and the use of traffic flow models.

In view of the difficulties in obtaining vehicle fleet composition and comprehensive vehicle flow information for each of the urban areas under analysis, another approach had to be developed to further disaggregate urban transport emissions. So far, total transport emissions released by each UE have been estimated. By definition, these emissions can be viewed as the result of vehicle flow, in this case expressed in total vehicle kilometres travelled (abbreviated in the following as VKT) within an urban entity, multiplied by an emission factor. This emission factor could be then interpreted as representative of the vehicle fleet and driving conditions for a specific urban entity. In this way, road transport emissions for any street within an UE could be calculated, providing that the VKT for such street are also known. In the following, the methodology applied for estimating average emission factors is depicted. As the computation of VKT of individual urban streets is strongly connected with the development of a model to estimate pollutant concentrations in urban streets, this issue is addressed in Chapter 3.

For estimating the average emission factor, Equation 2.1 can be rewritten as follows:

$$EF_{UE}^{i} = \frac{E_{UE}^{i}}{VKT_{Urban}}$$ Equation 2.2

where

EF^{i}_{UE} = Average annual emission factor for pollutant i (in grams per kilometre).

E^{i}_{UE} = Total annual emissions of pollutant i released within an urban entity (in grams).

VKT_{Urban} = Total annual vehicle kilometres travelled within an urban entity (in millions).

Regarding total urban VKT, Schmitz (1990) carried out a statistical analysis using detailed data from several German districts, finding a strong positive correlation between population and urban mileage, which was used to develop an empirical function to predict total urban VKT. Later, Schmitz et al., (1997) updated the aforementioned function using detailed mileage data from 67 German districts, obtaining a high correlation (R^2 = 0.97). The model depicting the relationship of VKT and population is formulated as follows:

$$VKT_{Urban} = 10^{\alpha} \times P^{\beta}$$ Equation 2.3

where

VKT_{Urban} = Annual urban vehicle kilometres travelled (in millions).

P = Number of inhabitants in a certain area.

α and β = Exponents equal to -2.5888 and 1.0527, respectively.

It is worth noting that the parameters of the function are based on mileage and population data from the eighties. Therefore, it is possible that the relationship between population and mileage may have changed over time. In order to account for this change, the exponent β was updated using total vehicle activity and population data of the German State of Baden-

Württemberg generated by the (LUBW, 2006, 2009)[1]. The exponent α was assumed to remain constant for simplicity. Thus, the Equation 2.3 can be rewritten as follows:

$$VKT_{Urban} = \sum_{i}^{n} 10^{-2.5888} \times P_i^{\beta} \qquad \text{Equation 2.4}$$

where

VKT_{Urban} = Total annual urban VKT in Baden-Württemberg (in millions).

P_i = Number of inhabitants in each of the municipalities in Baden-Württemberg.

β = Exponent to be updated.

Once the total urban VKT is known, this equation can be solved iteratively for the exponent β. Yet, data available provide information only by road category, without making a clear distinction between urban and non-urban VKT (see Figure 2.6). Thus, two important issues remain to be elucidated. First, it is a fact that several federal roads pass through urban areas but their share in the total VKT cannot be separately identified using these data alone; and second, whereas it can be reasonably assumed that VKT for area sources refer to urban areas, this is not valid for state, district, and local roads. In order to address the first issue, own detailed data for federal roads were used for determining the urban VKT associated to this road category. The second issue was dealt with by assuming an equal distribution between urban and non-urban VKT for state, district, and local roads. This assumption is taken from an study from another German State, Saxony (Gerike, Seidel, Becker, Richter, & Schmidt, 2006), which has the same state/district roads length ratio as Baden-Württemberg (BVBS, 2007) and, therefore, it was considered to have roughly similar urban and non-urban VKT split for state, district, and local roads.

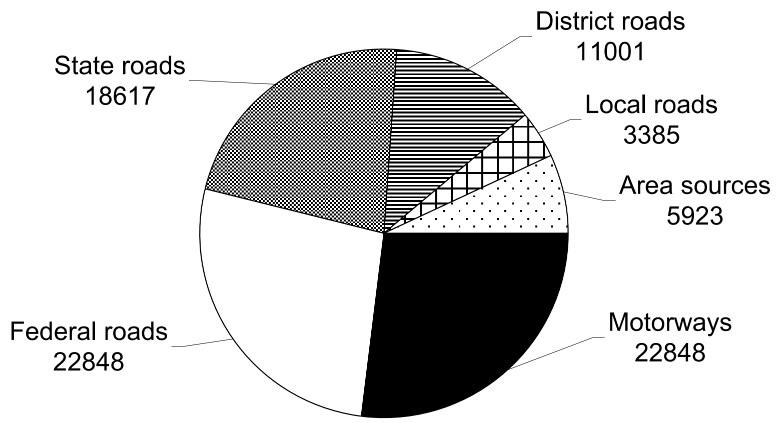

Figure 2.6 Total annual vehicle kilometres travelled for the German State of Baden-Württemberg (in millions).

[1] The reports mentioned here refer to the years 2004 and 2006. For the year 2005, it was assumed that the vehicle activity changed linearly during this period.

Results of the top-down approach to estimate total urban VKT for the German State of Baden-Württemberg are presented in Table 2.1. It can be seen from this table that, in comparison with the LUBW data, there is a small difference in the total VKT. A reason for this difference may be that urban VKT is commonly not attributed to federal roads but to area sources in the LUBW inventory.

Table 2.1 Total annual vehicle kilometres travelled in Baden-Württemberg in millions.

Road type	**Total annual VKT** (LUBW, 2006 and 2009)	**Total annual VKT disaggregated**		
		Non-urban	Urban	Total
Motorways	**22848**	22696	0	**22696**
Federal roads	**22848**	16238	8710	**24948**
State roads	**18617**	9308	9308	**18617**
District roads	**11001**	5500	5500	**11001**
Local roads	**3385**	1692	1692	**3385**
Area sources	**5923**	0	5923	**5923**
Total	**84621**	**55435**	**31135**	**86570**

Source: own data and LUBW, 2006.

Using the total urban VKT estimated above and detailed population data comprising over 1 100 municipalities of the German State of Baden-Württemberg, the Equation 2.4 was iteratively solved for the exponent β, which was found equal to 1.0125. Equation 2.4 can be then rewritten as follows:

$$VKT_{Urban} = 10^{-2.5888} \times P_{UE}^{\ \ 1.0125} \qquad \text{Equation 2.5}$$

where

VKT_{Urban} = Annual VKT within an urban entity in millions.

P_{UE} = Number of inhabitants in an urban entity.

It is, however, recognized that the actual mobility patterns and energy consumption related to transport varies among cities, depending on factors like land-use spatial distribution, road infrastructure, perception of value of time, existent public transport modes, among others. In order to explore how large the deviation of the estimates using the updated Schmitz function could be, detailed mileage data available for the German cities of Berlin (Senate Department for Urban Development - Berlin, 2007) and Bremen (Ingenieurgruppe IVV, 2008) were used to evaluate the performance of the updated Schmitz function. The results of this comparison are presented in Figure 2.7.

A more complex model proposed by Cameron (2004) was also considered for comparison. This model includes several relevant parameters, such as vehicle stock and urban population density, which is one of the better ways of numerically taking into account urban morphology or patterns in land-use changes. This refers not only to the way commercial, industrial or residential areas are spatially distributed with respect to each other but also their interaction with the development of the transport infrastructure network which logistically makes these patterns possible (Zeibots, 2002). The model developed by Cameron can be written as follows:

$$\alpha_k = 115552\ \beta_p^{0.74}\ \lambda_a^{0.26}\ S \qquad \text{Equation 2.6}$$

where

α_k = Total annual VKT by passenger vehicles

β_p = Population of the urban area

λ_a = Built up area in km2

S = vehicle saturation factor, equal to:

$$S = \left(\frac{1}{\left(1 + \exp\left(-3.4 \left(\frac{\alpha_c}{0.85\beta_p} \right) \right) \right)} \right)^{3.4} \qquad \text{Equation 2.7}$$

where

αc = Number of motor vehicles on register

The parameters required by the Cameron's model were retrieved from the Urban Audit database (European Commission, 2004). A comparison between the updated Schmitz function, Cameron's model and the inventory data is presented in Figure 2.7.

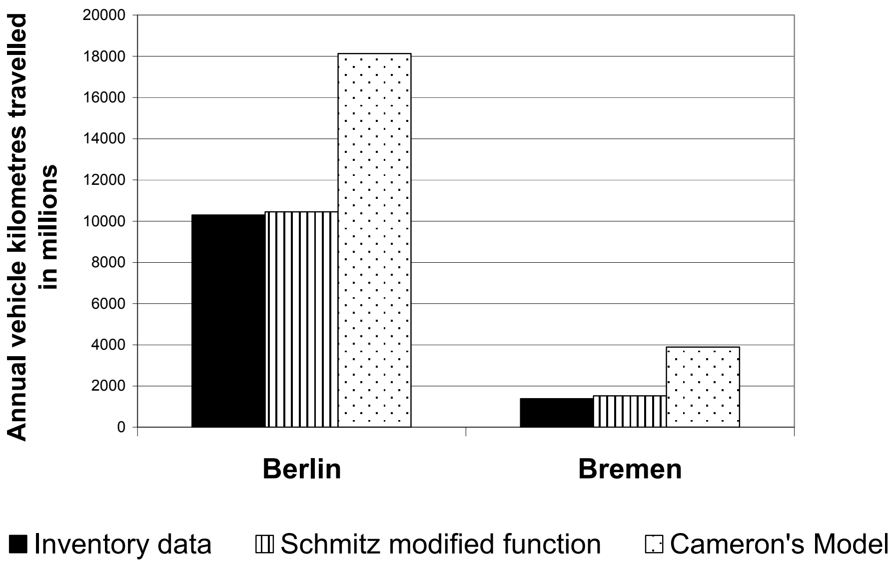

Figure 2.7 Comparison of inventory data against annual urban VKT calculated with the updated Schmitz function and Cameron's Model.

Looking at the results, it is clear that the Schmitz modified function is able to predict the urban VKT for both German cities fairly well. On the other hand, Cameron's model largely overestimates VKT for both cities. A reason for this difference may be that Cameron's model is based on data from over 30 cities around the globe and, therefore, factors influencing urban mileage have been averaged over cities with very different urban mobility characteristics. In this way, the model is not able to take into account specific characteristics of German cities, such as a good public transport infrastructure and availability of alternatives to vehicle use (e.g., walking and cycling).

On account of the results presented above, the modified Schmitz function was used for estimating urban VKT for each urban entity and, using Equation 2.2, for computing average emission factors. These emission factors are implemented later in this work to develop a model for estimating pollutant concentrations in urban streets.

2.5. Results – Road vehicle emissions mapping

In the last sections, the main characteristics of the emission databases used in this work were described. Furthermore, special attention was paid to the methodologies utilized for the spatial allocation of the emissions. With this information, an emission reference scenario was created comprising all relevant sectors for the reference year 2005. In this way, the reference scenario integrated into a geographically referenced framework can be readily used for dispersion modelling purposes – a topic discussed at length in the next chapter.For illustration purposes, Figure 2.8 shows the PM_{10} transport emissions associated to the main road network and to the urban entities.

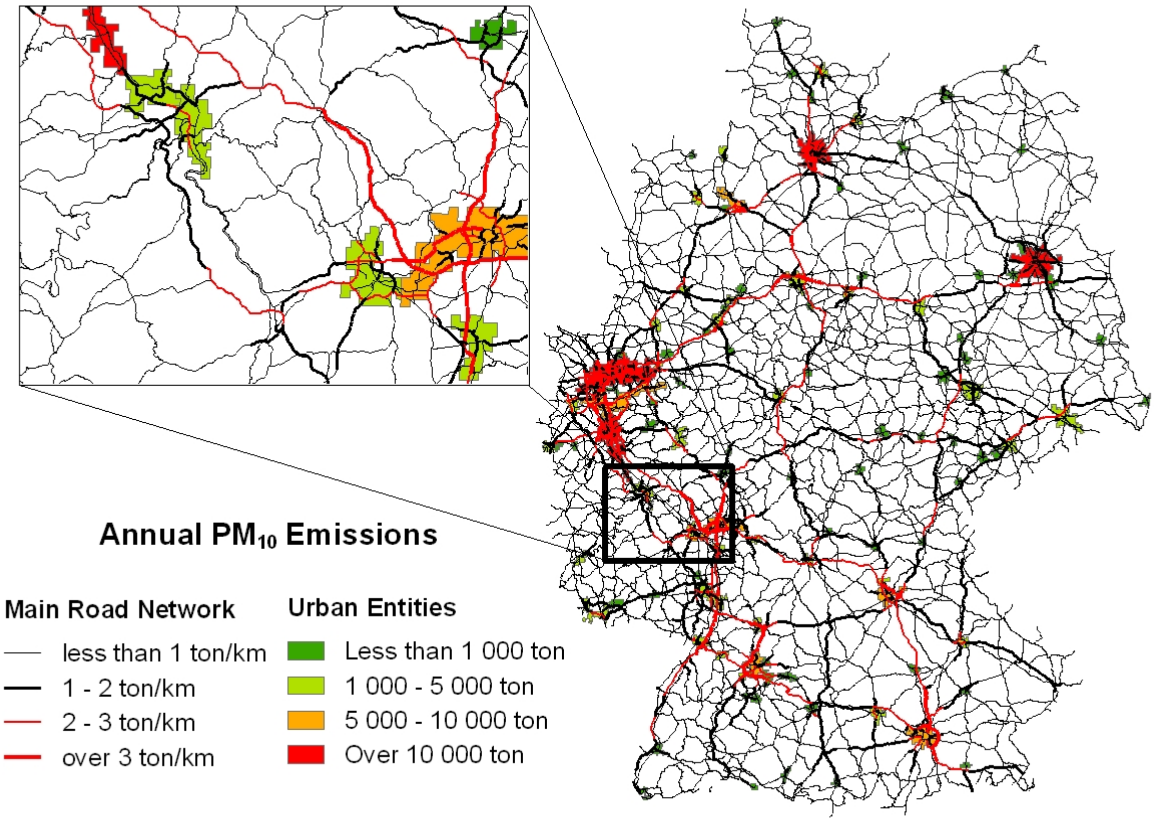

Figure 2.8 PM_{10} road transport emission for the reference year 2005 in Germany.

Chapter 3

Air pollution dispersion modelling

A model is a mathematical formulation for simulating real-world phenomena, a simplified depiction of the reality to describe sets of objects, their attributes, and relationships. Over the last few decades the application of mathematical models to simulate natural phenomena has grown. Nowadays, almost every research field makes use of some kind of numerical model to predict or explain all manner of real-life events. This is not surprising when considering the rash development of computing capacities, which has allowed the simulation of quite complex phenomena using a reasonable amount of resources.

An air dispersion model attempts to describe how compounds of any nature disperse in the ambient atmosphere. They are widely used for a manifold of purposes, especially in the framework of environmental impact assessments. However, incomplete understanding of the physical and chemical processes involved in pollutant dispersion is a major difficulty when trying to describe these processes through mathematical algorithms. These algorithms are – to a lesser or a larger degree – simplifications of the reality and as a consequence they cannot accurately predict the behaviour of essential parameters like wind conditions, temperature, topography, and surrounding morphology. Furthermore, some of these parameters also behave dynamically over space and time, making an accurate description of the fate and transport of the particles in their journey through the air a complex task.

This chapter describes the development of a hybrid dispersion model, which integrates a suite of models into a functional system for predicting air quality, focusing on vehicle-related pollutants in urban areas and street canyons. It begins with a literature review on current dispersion modelling techniques, discussing their advantages and limitations relative to estimating pollutant concentrations for different spatial scales. The chapter goes on presenting the concept behind the hybrid dispersion model and describing each component in detail. Finally, the model is used to assess the ambient air quality in Germany in the year 2005 and the results are presented in this chapter as well.

3.1. State of the art

A literature review was undertaken to collate information on the different techniques and methodologies to simulate the dispersion of air pollutants. The main purpose was to identify those models that, under consideration of their performance, data requirements and treatment of vehicle-related pollutant concentrations, could be implemented for this research. It would be an impossible task to include all existing models in this attempt and, for this reason, this review focused on identifying those models that could be suitable for predicting multi-scale pollutant concentrations, covering from regional to urban areas. Special emphasis was also laid on their capability for depicting pollutant concentrations generated by road traffic.

A standard classification of air pollutant dispersion models is not possible since they can be classified according to a number of schemes and in terms of several describing parameters. For instance, considering their spatial scale one can distinguish between micro-, local-, regional-, continental- and global-scale models. The source types that the models are intended to simulate (point, line, area, or volume sources) provide another criterion for model categorization. Models can even be classified according to the policy issue they address (e.g., urban air quality, nuclear accidents, acidification or climate change).

Nevertheless, two general approaches for estimating air pollution concentrations can be distinguished, namely statistical and deterministic models (Moussiopoulos et al., 1996; Zannetti, 1993). Although deterministic models are more widely implemented for air quality management purposes, statistical approaches, which include spatial interpolation and stochastic methods, have gained considerable interest over the last two decades (P. Ryan & LeMasters, 2007). In the following section, a brief description and some of the strengths and weakness of different modelling approaches are presented.

3.1.1 Deterministic models

Deterministic models are based on the description of cause-effect relationships of physical processes, giving an estimation of a value that is as close as possible to the actual value, based on certain quality or goodness criteria. These models can be classified addressing their mathematical structure into semi-empirical, Gaussian, three-dimensional Lagrange and Euler models, along with computational fluid dynamics (CFD) models.

Semi-empirical models build on simplified deterministic mathematical approaches, which are preferred to physical modelling approaches. Whilst they deal with general case solutions, their performance can be evaluated as satisfactory (e.g., Coppalle & Abart, 2001), and sometimes even better than more complex models (e.g., Gualtieri & Tartaglia, 2004). Yet this may not be surprising as generally such models are calibrated using site-related conditions and assumptions, which may or may not apply to different conditions. Box models belong to this category as they are based on the assumption that air mass is well mixed and concentrations are entirely uniform within a specific volume of air called a box. More sophisticated box models may include detailed chemical reaction schemes (PBM Model, Shere & Demerjian, 1986) and aerosol dynamics (UHMA Model, Sihto et al., 2007).

Gaussian models are widely used in atmospheric dispersion modelling due to their simple applicability for estimates on a local scale. They are based on a closed solution of the advection-diffusion equation in a collinear wind field. The horizontally and vertically time averaged pollutant concentrations generated by a point source are described by Gaussian distributions of the plume under steady state conditions. The plume spread sigma parameters are generally expressed in terms of Pasquill atmospheric stability classes (Gifford, 1976; Pasquill, 1961) or Monin-Obukhov similarity theory parameters.

These models are not best suited for small-scale dispersion within the urban canopy as they do not resolve well in areas with buildings or complex topography. Moreover, due to its simplified treatment of turbulence and meteorology they do not resolve episodic-like phenomena well and may be more suitable for estimating long-term concentrations. Classical examples of Gaussian models are CALINE-4 (California Line Source dispersion model, Benson, 1984), ISC3 (Industrial Source Complex dispersion model, U.S. EPA, 1995) and UK-ADMS (Carruthers et al., 1994; CERC, 1998). Following the same trend as semi-empirical models, some Gaussian models have been further developed integrating vehicle-induced and ambient turbulence, surface roughness parameterization for treating obstacles within complex environments or parameterised chemical reaction schemes, such as CAR-FMI (Contaminants in the Air from a Road - Finnish Meteorological Institute, Härkönen et al., 1996) and AEROPOL (AERO - POLlution, Kaasik & Kimmel, 2003) Additionally, more advanced models can include additional modules to resolve physical processes, fast chemical reactions and aerosol dynamics.

The central principle of Lagrangian models is the tracking of a multitude of virtual particles representing trace species on their path through the atmosphere. The particles move along the mean flow within a three-dimensional wind field. Each particle is then subjected to the influence of turbulence as its mean velocity is modified by an additional random factor, which is a function of the turbulence intensity and is normally derived from a Markov process. As a consequence, particle motion can be simulated using deterministic velocities or Monte Carlo techniques (see for instance Roberti, Souto, de Campos Velho, Degrazia, & Anfossi, 2004). Lagrangian models are similar to box models in that both define volumes of air as boxes comprising an initial pollutant concentration. The concentration distribution is then computed by counting the particles within the defined sampling volumes as mean values over the volume elements and time intervals. The Lagrangian approach allows for depicting, to a large degree, the natural processes involved in turbulent diffusion through the generation of semi-random numbers, avoiding in this way the problems of numerical diffusion.

Altogether, these models represent a good alternative for dealing with heterogeneous environments since it can be applied to any source geometry and it is possible to include buildings and complex terrain in the modelling scheme (Du, 2001; Raza, Avila, & Cervantes, 2001). However, these models also have some disadvantages. For instance, for a given finite number of fictitious particles, any calculated mean concentration value depends on the shape and size of the volume in which the mean value is calculated. Hence, uncertainties in the results arise from the number of particles used in the analysis and several thousand particles have to be included continuously in the analysis for obtaining statistically reliable results. Difficulties may arise in the parameterisation of these models and since the trajectory computation for each particle is computationally intensive, the use of Lagrange models for air quality issues is, to some degree, limited by available resources. LASAT (Lagrange Simulation of Aerosol Transport, Janicke, 1983; Janicke & Janicke, 2003) and SPRAY (Tinarelli, Anfossi, Bider, Ferrero, & Trini Castelli, 1998; Tinarelli et al., 1994) are some examples of Lagrange models.

In contrast to the Lagrangian approach, Euler models solve numerically the atmospheric advection-diffusion equation – the equation of conservation of mass of the pollutant – with respect to a fixed geo-plane table to characterise the transport of gaseous or aerosols materials. These models are more complex in structure and implementation than Lagrange models, mainly associated with modelling the advection term in the diffusion equation. In fact, depending on the method used for resolving advection, mass deficits or negative mass densities may occur, hampering the performance of the model. Nevertheless, they are more flexible in adapting to spatial and temporal flow and turbulence inhomogeneties, making it possible to describe the flow and the concentration fields near built-up areas, e.g., underground parking garages or street canyons (Lohmeyer, Eichhorn, Flassak, & Kunz, 2002). More advanced Eulerian models include refined sub-models for the description of turbulence (e.g., second-order closure models and large-eddy simulation models). MISKAM (Microscale Model, Eichhorn, 1989; Eichhorn, Schrodin, & Zdunkowski, 1988) and MIMO (Ehrhard et al., 2000) are some examples of models using an Eulerian scheme.

It is interesting to note that due to their similarities, the performance of Lagrange and Euler approaches has been analysed in several studies, the results of which suggest that Lagrange models resolve better for small-scale features within building-influenced areas (Nielinger, Röckle, Höfl, & Kost, 2004). Additionally, some models use both approaches allowing the user to choose the most suitable dispersion model for a specific application, for instance the model TAPM (The Air Pollution Model, Hurley, 2008; Hurley, Edwards, Physick, & Luhar, 2003) and the model ARIA in its regional version (ARIA technologies, 2000).

Computational Fluid Dynamic (CFD) codes can also be considered to use a deterministic approach. These models are commonly used for simulating the flow and the corresponding dispersion field around 3D complex structures, taking into account turbulence effects with the application of various turbulence models, particularly the standard κ-ε two-equation model. Furthermore, microscale processes such as solar heating with shadowing and infrared cooling, vegetation and turbulent energy exchanges can be taken into account. CFD models have been used to model dispersion within urban environments (e.g., Hanna, Hansen, Ichard, & Strimaitis, 2009) and street canyons (e.g., Murena, Favale, Vardoulakis, & Solazzo, 2009). The application scope of CFD models can be further extended by coupling them with other models with better performance at a larger scale (e.g., Tripathi, 2004). However, extensive use of CFD models is limited due to their intrinsic complexity and large computational cost, making their use for operational applications rather difficult. Examples of CFD models are the model ARIA in its local version (Moon, Albergel, Jasmin, & Thibaut, 1997) and the more widely used FLUENT code (e.g., Hamlyn & Britter, 2005; Solazzo, Cai, & Vardoulakis, 2008).

Another widely used modelling technique is model nesting. Basically, this approach consists of embedding high-resolution models within the domain of models with coarser resolution (e.g., Y. Tang, 2002). Nesting techniques are used to describe the inflow of emissions into the most inner modelling domain in a one- or two-way direction. This approach is particularly useful for assessing air quality in areas with mixed emission sources structures and complex terrain or when high-resolution data for a specific area, such as a city, are available and the analysis scope can be limited to such area. An example of nesting modelling is the CARLOS system (Chemistry and Atmospheric transport in Regional and LOcal Scale, Brücher et al., 2000; Kessler et al., 2001). However, the applicability of this approach is limited given that the requirements for input data and computational resources increase strongly with increasing domain size. Therefore, it is not feasible to employ this technique for assessing pollutant concentrations in a whole country.

In contrast to the dispersion models presented above, whose performance relies on the use of high-quality emission and meteorological data, receptor-oriented modelling starts with a detailed analysis of the pollutants collected at measure points and statistically apportions the measured concentrations among possible sources (Gordon et al., 1984). The basic assumption underlying these models is the conservation of mass in the form of the Chemical Mass Balance (CMB) solution, although multivariate receptor methods using Principal Components Analysis (Guo et al., 2009; Liu, 2009) or factor analytic models (Okamoto, Hayashi, Nakajima, Kainuma, & Shiozawa, 1990; Salvador, Artiñano, Alonso, Querol, & Alastuey, 2004) can be implemented as well. On the other hand, both concepts have also been integrated in the hybrid model COPREM (Constrained Physical receptor Model), providing good results in several air pollution studies (Wåhlin, 2003). It is worthy to note that, as this approach is based on observations, it provides an interesting alternative for evaluating predictions made by conventional models or for testing the accuracy of emission inventories (e.g., Kenski, Wadden, Scheff, & Lonneman, 1995).

3.1.2 Statistical models

The models presented in the last section are of deterministic nature since they are mainly based on the description of physical processes and the understanding of their interactions and dynamics over spatial and temporal scales. They give an estimation of a value that is as close as possible to the actual value, based on certain quality or goodness criteria. Statistical methods, on the other hand, do not deal with the mechanism of atmospheric diffusion but they rather rely on the evaluation of monitored data for calculating concentrations. Thus, they do not give information about effect-cause relationships but uses restrictive assumptions about the relationship between the independent variables and dependent variable (s).

Parametric statistical models provide functions to calculate pollutant concentrations which are derived from the analysis of long-term air quality indicators. These models can deliver quick results with satisfactory accuracy, though they tend to work best for long-term averages of concentrations. Because the functions rely on site-specific measurements, their applicability may be narrowed to sites where similar conditions prevail and a detailed evaluation of the phenomena with high temporal resolution proves to be a difficult task. Nevertheless, they are widely used as screening tools before more complex models are implemented, representing the best option to solve concrete questions when data availability is a relevant constraint. The method developed by the Design Manual for Roads and Bridges (Department of the Environment Transport and the Regions, 2007) from the British Highway Agency, and the MLuS model (Lohmeyer, Bächelin, & Ketzel, 2000) make use of this kind of simple statistical functions.

Over the last decade, the quick development of spatial data management in the framework of Geographic Information Systems (GIS) has enhanced the applicability of spatial interpolation techniques within environmental modelling. For instance, Land-Use Regression (LUR) models combine measured air pollution data at several locations within the study area and GIS to identify predictor variables (P. H. Ryan et al., 2008). LUR models have been successfully used for assessing intra-urban air pollutant variability and in epidemiological studies (Brauer et al., 2003; Briggs et al., 1997; Madsen et al., 2007). Kriging methods have also found a broad spectrum of applications and although a stand-alone application of this technique does not provide sound results due mostly to the large distances between measure points, this technique has been successfully implemented as a complement to other more complex models (e.g., Ferreira, Tente, Torres, Cardoso, & Palma-Oliveira, 2000; Hjellbrekke & Tarrascon, 2001).

Given that traditional statistical approaches do not account for randomness in the development of future states of the system, they produce the same output for a given starting condition. However, the growing need of a reliable depiction of air quality and other environmental issues under consideration of uncertainty have encouraged the development of dispersion models going beyond traditional statistical methods. Thus, most recent techniques involving the application of stochastic methods have found wide application in environmental assessment issues.

Neural networks simulate mathematically the neurophysical structure and decision-making process of the human brain. From a statistical perspective, they are closely related to linear models but they differ in that they use a feed forwards and back propagation estimation procedure, resulting in nonlinearity (West, Brockett, & Golden, 1997). Neural modelling has been applied to calculate spatial distribution of pollutants (e.g., Pfeiffer, 2006).

In contrast to traditional statistical methods, stochastic approaches do not neglect the influence of random processes and include them in the analysis, allowing assessment of the uncertainty in the response. These models describe processes whose behaviour is non-deterministic, e.g., a state does not fully determine its next state. They are also characterized by conjecture and randomness, describing phenomena that change in time and space in a more or less random way. Thus, stochastic techniques can be viewed as a confident way of dealing with phenomena where many factors are not known. Among the stochastic approaches, Monte Carlo methods are currently widely used for addressing environmental issues.

In a Monte Carlo approach, probability distributions are used as a replacement for parameters that are difficult to measure accurately or are inherently variable. Thus, the Monte Carlo method relies on random draws from the known probability distribution functions to perform the simulations. Using an ensemble Kalman filter, Monte Carlo techniques have been used for assessing dispersion of reactive pollutants within street canyons (e.g., Garmory, Kim, Britter, & Mastorakos, 2008) and the consequences of nuclear accidents (Zheng, Leung, & Lee, 2009). However, model misspecification regarding a selected input probability distribution function and underestimated errors can lead to false precision estimates (Rochet & Rice, 2009; Small & Fischbeck, 1999).

3.1.3 Conclusion

In the last section, numerous deterministic and statistical approaches for modelling the atmospheric dispersion of pollutants were reviewed, outlining their main characteristics and identifying differences among model approaches. Not surprisingly, this review shows that there is a broad range of modelling solutions, each of which has strengths and shortcomings related to the problem to be addressed.

In Table 3.1, an overview of the modelling approaches is depicted, focusing on relevant characteristics in relation to the scope and objectives of this work. The first two factors indicate whether the model approach is suitable for describing long-range transport and urban scale phenomena. The third parameter relates to the ability of the model to simulate multi-scale problems, covering from regional to urban and near road areas simultaneously. Lastly, the fourth factor evaluates the feasibility of the application of the modelling approach for a whole country, taking into account requirements for input data and computational resources. Because the main criterion for including a model approach in this review was its ability to estimate vehicle-related pollutant concentrations, all models comply with this requirement and, therefore, this characteristic is not included in the overview.

From Table 3.1, it is evident that none of the modelling approaches meets all requirements defined by the objectives pursued in this work. Whereas it is true that some modelling approaches are able to simulate pollutant concentrations on a regional and urban scale, a multi-scale analysis is most likely not feasible due to the large amount of input data and computational resources needed. Furthermore, maintaining consistency between dispersion processes at a local scale and larger-scale features influencing the dispersion is also a major issue to be address. In this sense, only the nesting approach may be able to handle multi-scales problems covering from regional to local areas and simulate specific areas with a higher spatial resolution. However, the applicability of this approach is limited as requirements for input data and computational resources increase strongly with increasing domain size. For this reason, an application of nesting modelling for assessing vehicle-related pollutant concentrations in the whole of Germany is not feasible.

Table 3.1 Overview of dispersion modelling approaches reviewed.

Modelling Approach		Long-range Transport	Urban Scale	Multi-scale	Countrywide Application	Application Example
Deterministic	Semi-empirical	no	no	no	no	PMB WHMA
	Gaussian	no	no	no	no	CALINE4 ISC3 UK-ADMS CAR-FMI AEROPOL
	Lagrangian	yes	yes	no	yes	LASAT SPRAY
	Euler	yes	yes	no	yes	MISKAM ABC MIMO
	CFD	no	no	no	no	ARIA FLUENT
	Nesting	yes	yes	yes	no	CARLOS
	Receptor-oriented	yes	yes	no	yes	COPREM
Statistical	Parametric	no	no	no	no	DMRB MLuS
	Land Use Regression	yes	yes	no	yes	Briggs et al., 1997 Brauer et al., 2003 Madsen et al., 2007
	Neural networks	yes	yes	no	yes	Pfeiffer, 2006
	Monte Carlo	yes	yes	no	yes	Garmory et al., 2008

It is therefore reasonable to argue that one single modelling approach is not sufficient to simulate both pollutant concentrations at street level and, at the same time, the long-range pollutant transportation over a large domain. This argument is supported by the fact that current dispersion modelling trends point towards developing combined approaches in order to take advantage of specific model strengths, i.e., deterministic with statistical components (e.g., Gokhale & Khare, 2005), Gaussian models with street canyon (e.g., C. Mensink & Cosemans, 2008) and CFD (e.g., Sahlodin, Sotudeh-Gharebagh, & Zhu, 2007) models. The integration of individual models into a tool to reproduce the spatial variability of pollutant concentrations is another approach to tackle multi-scale problems (e.g., De Leeuw, van Zantvoort, Sluyter, & van Pul, 2002; Stein, Isakov, Godowitch, & Draxler, 2007). In this way, the advantages of each approach can be combined to increase the model's predictive performance.

Thus, bearing in mind that one of the main objectives pursued in this work is to develop a modelling system for simulating vehicle-related pollutant concentration gradients over different spatial scales, a novel approach for addressing this challenge is presented and discussed in the next section.

3.2. A hybrid dispersion modelling approach – Concept and structure

Arguments speaking for the integration of several models into a modelling tool as the best alternative to resolve fine-scale variations of vehicle-related pollutant concentrations were presented in the literature review. Following this reasoning, a hybrid dispersion modelling approach was developed in this work for predicting air quality across different spatial scales: from regional to urban and kerbside scale. Partially making use of existing methodologies and under consideration of their respective strengths at resolving dispersion phenomena for a specific scale, a suite of models was integrated into a functional system for predicting air quality focusing on vehicle-related pollutants concentrations in urban areas and street canyons. In addition, this modelling approach may provide valuable insight into the actual exposure levels experienced by the urban population and, due to its flexibility in simulating different emission scenarios, this approach can be readily applied to the analysis of external costs – a topic discussed in Chapters 5 of this work. In the next sections, the model's conceptual idea along with its assumptions and structure are outlined, followed by a comprehensive description of each model element.

3.2.1 Conceptual idea and assumptions

Certainly one of the main sources of information for assessing air quality is provided by measurements from monitoring networks. In order to provide reliable environmental information, a European Air Quality Monitoring Network (EUROAIRNET) have been developed and maintained by the European Topic Centre on Air Quality (ETC-AQ). This monitoring network comprises a selection of monitoring stations from networks that are in operation in each European country (Larssen, Sluyter, & Helmis, 1999). The ETC-AQ also manages and improves the European Air Quality database (AirBase) which contains air quality monitoring data and information submitted by the participating countries (Airbase, 2008). While there are different monitoring station types according to the EUROAIRNET criteria, three types are particularly relevant for the objectives pursued in this work: rural background, urban background and urban traffic stations. Rural background stations monitor air pollution levels resulting from long-range transport of air pollutants and from emissions in the region in which the station is located. Urban background stations measure the average air quality in urban areas, which results from the regional concentration and from emissions generated within the city. Finally, traffic urban stations are located near major streets within urban areas and measure pollution levels directly attributed to such streets.

In order to gain insight into air quality trends in Germany, observational data for the three monitoring stations types mentioned above were retrieved from the European Air Quality database Airbase (Airbase, 2008). In Figure 3.1 and Figure 3.2 the PM_{10} and NO_2 average annual concentrations for rural and urban background, along with traffic urban monitoring station types in Germany are depicted.

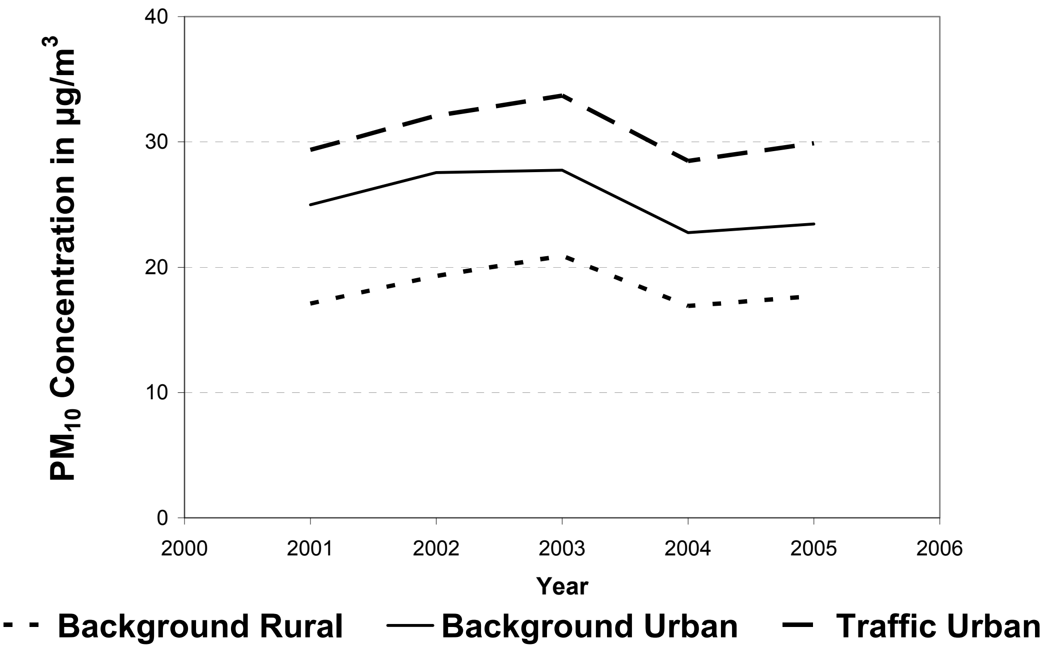

Figure 3.1 Changes in PM_{10} air quality in Germany based on annual mean concentrations over the period 2001-2005. Source: AirBase, 2008.

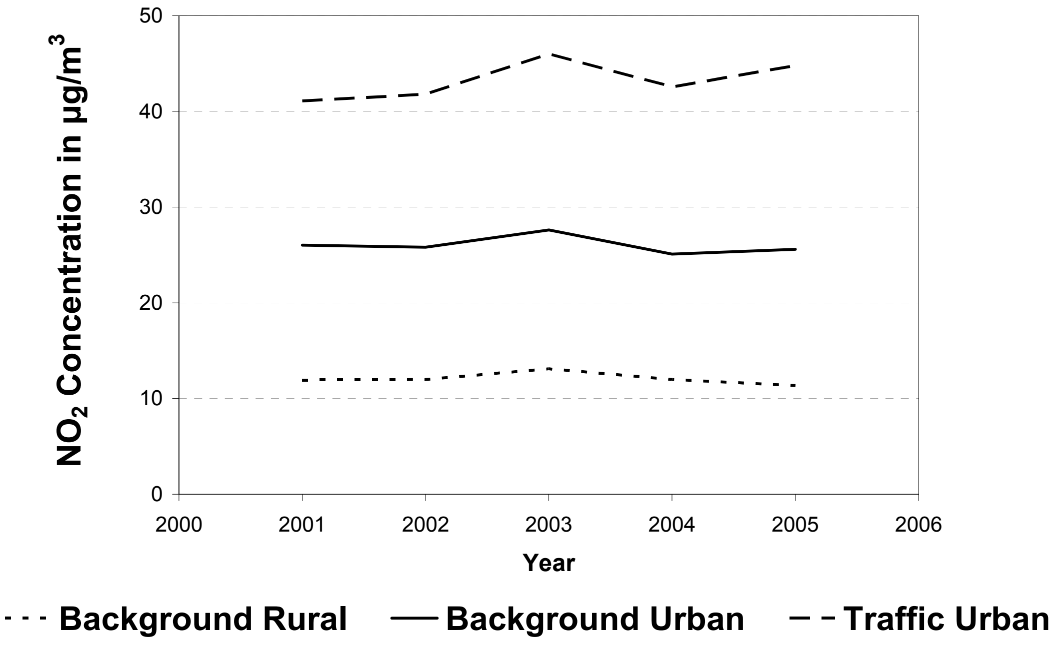

Figure 3.2 Changes in NO_2 air quality in Germany[2] based on annual mean concentrations over the period 2001-2005. Source: AirBase, 2008.

[2] For the years prior to 2005, there is no data available for NO_X expressed as NO_2 equivalent. However, analysis of NO_X data for the years 2005 and 2006 shows the same trend as NO_2

Looking at both figures, it seems evident that pollutant concentrations significantly increase as one moves from regional into urban to traffic-influenced areas. Indeed, it should be evident that pollution concentrations are generally higher with increasing proximity to the corresponding emission sources, in this case PM_{10} and NO_2. It is worth noting here that the same trends for both pollutants can be observed across Europe (Mol, Van Hooydonk, & De Leeuw, 2008).

Concerning $PM_{2.5}$ concentrations, changes for the period 2003-2006 are shown in Figure 3.3. Here, the differences across monitoring station types are not as clearly defined as for PM_{10} and NO_X, displaying instead rather fluctuating values. This behaviour can be partly explained by the very limited number of valid data available as this pollutant has been measured routinely only until recently, as shown in Table 3.2. Nevertheless, considering that road transport exhaust emissions are an important source of $PM_{2.5}$, it is likely that $PM_{2.5}$ concentrations are higher within urban areas than outside as well. This issue is discussed further in Section 3.4.4.

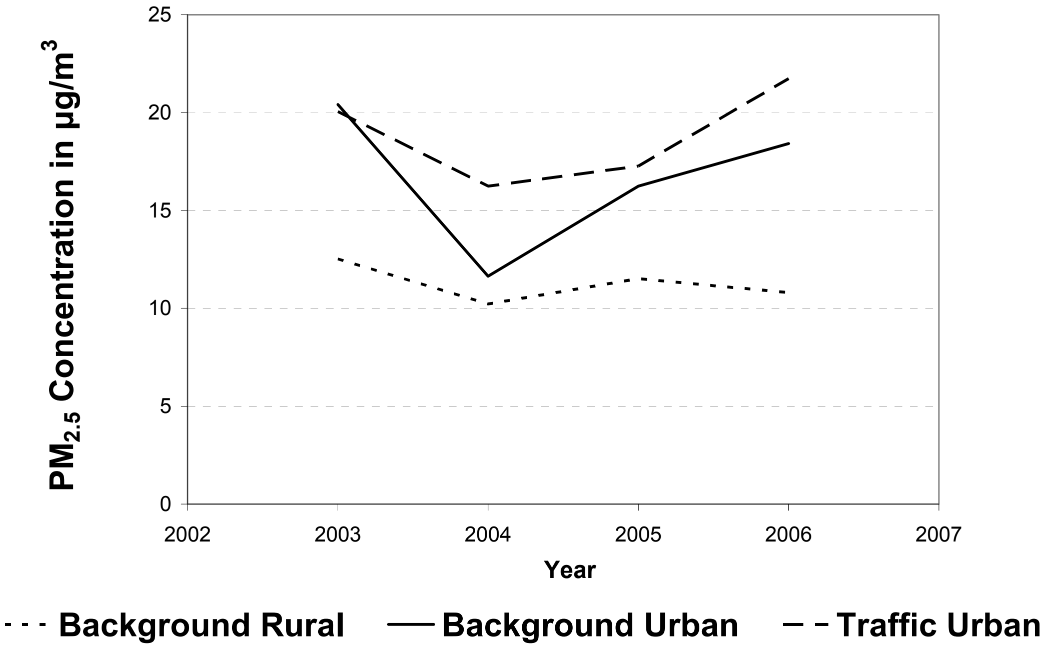

Figure 3.3 Changes in $PM_{2.5}$ air quality in Germany based on annual mean concentrations over the period 2003-2006. Source: AirBase, 2008.

Table 3.2 Data availability by pollutant and measure station type.

	2001			2002			2003			2004			2005		
	RB	UB	TU	RB	UB	TU	RB	UB	TU	RB	UB	TU	RB	UB	TU
PM_{10}	50	78	82	51	73	74	60	66	65	65	81	83	64	90	112
$PM_{2.5}$		n.r			n.r.		1	2	2	2	1	4	2	3	5
NO_2	89	112	117	87	116	125	92	111	124	88	103	127	78	103	140
O_3	101	98	48	99	102	46	99	95	38	96	90	34	86	89	34

RB = Rural Background; UB = Urban Background; TU = Traffic Urban; n.r. = not reported

Source: AirBase, 2008.

Thus, considering how pollutant concentrations vary across monitoring stations, it is reasonable to argue that the total pollutant concentration measured at traffic sites can be thought of as being composed by three distinct concentration layers: the regional layer comprising the rural background concentration; the urban layer depicting the concentration increment normally found within cities; and the traffic layer accounting for the additional load directly attributed to vehicle-related emissions. It can be furthermore suggested that each of the layers can be estimated individually, using the better approach for the corresponding scale and building on the subjacent layer. This concept is the basic idea behind the hybrid dispersion modelling approach developed in this work.

It is important to remark that not all pollutants behave in the same way as PM_{10} or NO_2. In fact, when calculating the same averages for ozone it is clear that the trend is even reversed, as shown in Figure 3.4. An important factor influencing these trends can be the fact that road transport even contributes to its depletion near roads through the so-called titration process. This process consists of the removal of ozone through reaction with nitric oxide at night time and in the immediate vicinity of large NO_X emission sources. Furthermore, ozone is a highly reactive oxidant that interacts with a number of other compounds, the rates of which also depend on location variables, such as temperature and meteorological conditions.

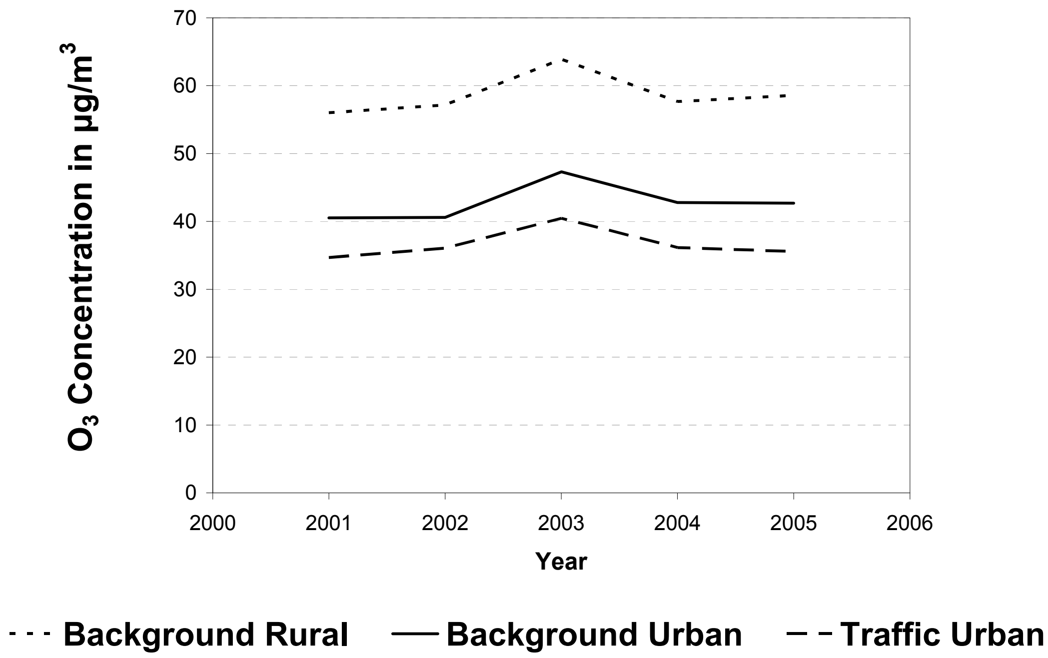

Figure 3.4 Changes in O_3 air quality in Germany based on annual mean concentrations over the period 2001-2005. Source: AirBase, 2008.

It can be concluded that due to the complex behaviour of ozone in the troposphere, the simplified treatment of the urban and near roads concentration layers presented here might be not robust enough to resolve adequately the behaviour of ozone on the urban and hotspot scale. Nevertheless, considering that particulate matter and nitrogen dioxide are currently the main concerns in the European environmental agenda, the model presented in this research focuses on these pollutants.

3.2.2 Model structure

Considering the objectives pursued in this work and on the basis of the concept presented in the last section, a hybrid dispersion modelling approach for assessing air quality from regional to urban and near-road areas was developed. Depending on whether the area under study is an urban or non-urban area, a two-tier or a three-tier analysis is performed. The first tier is common for all areas and it comprises a modelling using a regional pollutant transport and chemical model. The second tier comprises a multiple regression model and it is implemented only for urban areas to resolve the additional load in background concentration commonly found in cities. Finally, localized effects of vehicle pollution are captured in a third tier using empiric dispersion functions along with a Monte Carlo approach. Figure 3.5 shows a scheme of models and their application domain.

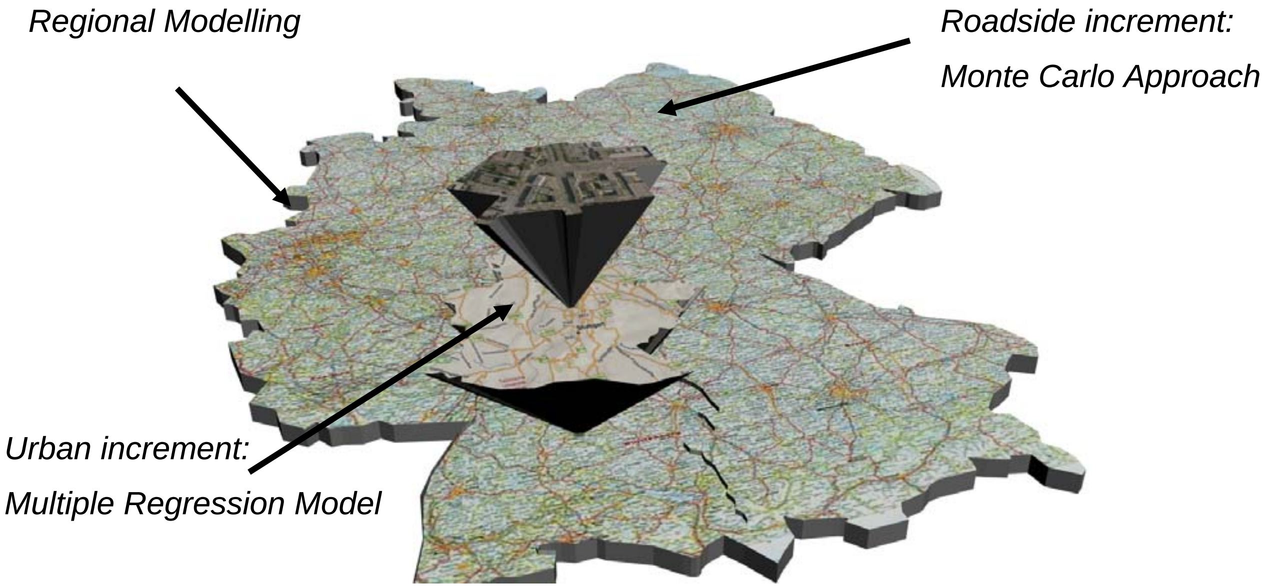

Figure 3.5 Modelling concept.

In this way, the total pollutant concentration ($C_{i\ total}$) due to vehicle-related pollutants can be estimated using:

$$C_{i\ total} = C_{i\ regional} + C_{i\ urban} + C_{i\ roadside} \qquad \text{Equation 3.1}$$

where the subscript i refers to one specific pollutant, and the subscripts regional, urban and roadside refer to the corresponding tier, each of which is described in detail in the subsequent sections.

3.3. Regional air pollution dispersion modelling

The first tier of the analysis certainly comprises the most complex part of the whole system. Not only because of the large spatial domain being analysed but also because of the complex processes involved in the atmospheric transport, chemical transformations, and aerosol dynamics for a myriad of compounds.

Regional concentrations result from the overlapping of emissions from different sources such as energy plants, industry activities, domestic use, and traffic. At the same time, interacting atmospheric processes occurring at several scales influence fluxes and transport of pollutants, making an adequate treatment of meteorological conditions essential for computing pollutant concentrations for this scale. The outcome of regional models provide valuable information about background concentrations on a European scale allowing for considering important regional and continental atmospheric chemical effects along with transboundary pollutant transport. The first tier of the hybrid modelling approach can be delivered by any regional air dispersion model and its results can be integrated with the models developed in this work (i.e., urban and roadside concentrations models).

In spite of the valuable information provided by regional models, the spatial resolution gained with them is rather coarse reflecting only part of the true pollutant concentrations in ambient air. This drawback is more evident in cities where the most severe damaging effects directly attributed to vehicle-related emissions can be found. It is within cities where traffic density is largest and pollutant concentration levels are higher than in rural areas for most pollutants. Moreover, the complexity and uncertainty of pollutant dispersion within urban environments do not allow regional models to capture a number of relevant phenomena, such as pollutant accumulation within street canyons.

There have been many attempts to integrate urban features into regional models for an accurate estimation of pollutant concentration gradients. For instance, Dupont et al. (2004) developed a detailed urban and rural canopy parameterization to resolve the meteorological fields within and above the urban and rural canopies. This parameterization simulates quite well important features observed in the urban and rural areas, as noted by Taha (2008). The value of using high-resolution urban data in meteorological and air quality simulations has been also demonstrated by means of sensitivity studies based on mesoscale modelling systems that incorporate urban canopy parameters (Chen, Tewari, Kusaka, & Warner, 2006; Ching, Dupont, Gilliam, Burian, & Tang, 2004). Another widely used approach to tackle this problem is nesting modelling for addressing different spatial.

However, as already mentioned earlier in this work, a drawback of such detailed models is their high input data requirements in the form of multiple surface topography, detailed emission dataset and surface cover digital datasets including land use, street network, and others. Thus, these models do not represent a feasible option for assessing a large number of cities.

The second tier of the hybrid modelling approach addresses this challenge, providing a model for estimating ambient air pollution levels in urban areas. In the following section, the second tier model is described in detail.

3.4. Urban increment concentration

Over 75% of the European population is living in urban areas; by 2020 it should be 80%, and for some countries will be even 90% (EEA, 2006b). As a consequence, the number of people affected by elevated pollutant concentrations is notably higher in urban areas than in rural environments. Trying to shed light on the mechanisms accountable for the typical urban pollution increment for most pollutants, the topic has become the subject of a number of studies over the last few decades (Charron, Harrison, & Quincey, 2006; De Leeuw et al., 2002; Stedman & Derwent, 2007; Yin et al., 2005). Thus, the second tier of the hybrid dispersion modelling approach focuses on urban areas.

In terms of environmental issues, one of the most observable evidence of anthropogenic climate modification within cities is the urban heat island process, which has been studied for several decades (e.g., Auer, 1978; Gallo, Tarpleya, McNabb, & Karlb, 1995; Narumi, Kondo, & Shimoda, 2009; Roth, Oke, & Emery, 1989). Observational data have shown that the temperature of urban air is about 2 to 10 °C warmer than in the surrounding rural area. The reason comes down to differences between energy gains and losses of each region, with absorption and storage of solar energy by the urban environment and the heat released into the air from industrial and human activities being the main factors driving this process (Li, Zhang, Liu, & Huang, 2004). Additionally, some authors suggest that city morphology (i.e., form or structure) may have significant influence over urban air quality. For instance, Borrego et al. (2006) estimated the air quality for three imaginary cities with diverse urban structures and found that, considering the same emission totals and overall meteorological conditions, a compact city with mixed land use may provide better urban air quality than one with a disperse structure. These results are similar to those obtained by other authors (e.g., Marquez & Smith, 1999; U.S. EPA, 2001). It is only a step further, then, to suggest that cities may be viewed as 'urban pollution islands' with a distinguishable pollutant increment in relation to levels measured outside urban areas. Thus, considering cities as the unit of analysis, a multiple regression model to estimate urban background increment for several pollutants was developed.

Before proceeding with a detailed description of the model development process and parameters values, it is necessary to elaborate on the treatment of pollutants at a local scale. For this purpose, a brief discussion is presented in the following.

3.4.1 Treatment of pollutants at a local scale

Particulate matter and nitrogen oxides can be transported over large distances, experiencing diverse transformations over time due to chemical and physical processes. Then again, for very short distances between receptor and sources, only the fastest chemical reactions may have a significant influence on the chemical transformation processes at street level. For instance, Wexler et al. (1994) found that some chemical reactions (oxidation of SO_2 to sulphuric acid and reaction of N_2O_5 with particulate matter) in or on aerosol particles are insignificant for typical urban conditions as long as relative humidity is under 100%. Moreover, the authors suggest that dilution is the most important process influencing particulate matter mass distributions. For instance, coagulation – another aerosol dynamical process – has a time scale that is too long to play an important role in particle mass distribution. This also holds true for particle number distribution as has been noted by Vignati (1999) and Zhang and Wexler (2002).

Thus, it seems plausible to treat particulate matter and NO_X (i.e., the sum of NO and NO_2) emissions as inert traces (i.e. non-reactive), given that the photochemical decay rate is small compared to their residence time over the urban area and that their concentration is only altered by dilution for typical urban conditions. De Leeuw et al. (2001) suggest that for cities with a diameter of 20 km or less the residence time would not exceed two hours with a representative velocity of 3 m/s. The situation is however different for more reactive pollutants, such as ozone whose transformation rate is driven by complex non-linear photochemistry. It is important to note that assuming non-reactive pollutants is no longer valid when considering a larger transport scale and, therefore, chemical and physical processes have to be taken into account in regional modelling.

Concerning NO_2, it has to be remembered that this compound reacts almost instantaneously with existent ambient pollutants and, hence, the simplified approach applied for total NO_X and PM cannot be used for estimating NO_2 concentrations near streets. Instead, a simple model is applied to derive NO_2 concentrations from modelled NO_X concentration values, namely the Romberg model (Bächlin, Bösinger, Brandt, & Schultz, 2006; Romberg, Bösinger, Lohmeyer, Ruhnke, & Röth, 1996) which is based on a regression analysis of NO_2 and NO_X measurements from the German monitoring network. According to this model, annual average NO_2 concentrations at roadside are computed from annual average NO_X concentrations as follows:

$$NO_2 = \frac{A \cdot [NO_X]}{([NO_X] + B)} + C[NO_X] \qquad \text{Equation 3.2}$$

where NO_2 and NO_X are the annual average concentrations of those pollutants; A, B, and C are the correlation factors with values 103, 130, and 0.005, respectively.

Here it is important to note that these coefficients are based on measurements made between 1987 and 1993 and, ever since, an increasing trend in the NO_2/NO_X emissions ratio from road traffic exhaust emissions has been observed (e.g., Scholz & Rabl, 2006). Therefore, it is likely that the correlation factors presented above are not suited to describe current NO_2 concentrations at roadside. In order to take into account this development, Bächlin et al. (2006) updated the Romberg function using measured data for the years 2000 to 2003. From this revision, the values for the correlation factors A, B and C from Equation 3.2 were updated to 43, 53, and 0.129, respectively.

Due to its easy application and flexibility, this method has been used in several studies. For instance, Puxbaum et al. (2003) measured NO and NO_2 concentrations in the vicinity of a tunnel portal for almost a year. Satisfactory predictions of NO_2 using the Romberg Method suggest that its use may be regarded as a satisfactory alternative to more complex models. Empirically derived functions to determine the proportion of NO_X as NO_2 have been used in several studies. Derwent and Middleton (1996) developed an empirical function for the ratio of NO_2 to NO_X derived from monitored data at an urban road site in London. Owen et al. (2000) used this function along with a full chemical model for predicting NO_2 concentrations in a large urban area. The results showed that the empirical function provided better agreement with measurements than the complex model.

Thus, as the arguments presented above suggest, it seems reasonable to assume that the parameterised function to derive annual average NO_2 concentrations from modelled annual average NO_X concentration values is an acceptable alternative for more complex full chemical and dispersion models.

3.4.2 Conceptual approach

In an effort to provide robust air quality information with less demanding atmospheric dispersion modelling, several attempts have been made for estimating the urban increment for large cities in a generalized way Europe-wide, for instance De Leeuw et al. (2001) and, more recently, the CityDelta project[3]. One of the objectives pursued by the CityDelta project was to provide concentrations of $PM_{2.5}$ concentration in urban areas to be implemented for Europe-wide integrated assessment of cost-effectiveness of emission control strategies (Cuvelier et al., 2007; Thunis et al., 2007). CityDelta results strongly suggest that the urban increment can be explained as a function of emissions emitted within the city, city size and average meteorological conditions. According to Amann et al. (2007), the urban increment can be expressed as follows:

$$\Delta c = \alpha \left(\frac{D}{U} \right)^{1/2} Q + \beta \left(\frac{D}{U} \right)^{1/2} Q \cdot \frac{d}{365} \qquad \text{Equation 3.3}$$

where

Δc = Urban increment

Q = Emission rate in ton/year.

D = City diameter in km.

U = Yearly mean wind speed in m/s.

d = Number of low wind speed days in winter.

α and β = Constants.

Even though the CityDelta project provides an important contribution to the understanding of the mechanism involved in the urban increment, some issues remain to be addressed. For instance, the characterisation of the city areas is mostly defined by its administrative boundaries or its diameter. Yet, these parameters do not provide information concerning the actual extent of the urban sprawl. This distinction is vital for addressing the difference between pollution levels within urban areas with respect to rural levels and this fact may have influence on the estimation of the corresponding urban emissions. Furthermore, land use changes over time may not be adequately captured if the only parameter to characterize the size of a city is its diameter. Another issue to consider is that the variability in the urban increment across all countries within Europe can be expected to be large due to the heterogeneity in meteorological, topographical and emission release conditions. This suggests that a unique functional relationship for all European countries may not be able to capture such differences across countries.

Addressing the issues pointed above, a similar approach as that of the CityDelta project was followed in this work to estimating the urban increment for German urban areas. Thus, a model based on multiple regression analysis was developed in this work for estimating the urban pollution increment. The urban increment is explained in terms of the following variables: the emissions released within the city; the urban morphology; and the average wind speed[4]. In the following section, each variable is described and discussed.

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[3] It is interesting to note that both methodologies mentioned here do not attempt to assess the additional pollutant concentrations for places under direct influence of emission sources, such as major streets or urban canyons

[4] Due to scarce data availability, the number of low wind speed days could not be included in the model developed in this work. Nevertheless, considering that this factor accounted for roughly only 10% of the urban increment for $PM_{2.5}$ calculated within the CityDelta project, it is likely that the omission of this parameter may not largely affect the final results.

3.4.2.1 Urban pollution increment

Within the framework of the CityDelta project, the urban increment was computed using results from an ensemble of three complex atmospheric dispersion models for seven European cities (Amann et al., 2007). However, high-resolution dispersion modelling for individual cities is highly data-demanding, mainly regarding meteorological conditions and urban morphology. Due to the lack of comprehensive datasets and computational resources, it was not feasible to carry out such simulations in this work. Alternatively, a pragmatic approach was followed: observational data from paired rural and urban background measuring stations were used for obtaining the urban increment. For this purpose, observational data for urban and rural background stations for PM_{10} and NO_X were retrieved from the European Air Quality database (AirBase). Concerning $PM_{2.5}$, the limited availability of measurements hampered developing the estimation of the urban increment for this pollutant. Later in this work, an alternative approach for addressing this issue is presented.

According to the EuroAirnet criteria, rural background stations are used to monitor air pollution levels resulting from long-range transport of air pollutants and from emissions in the region in which the station is located. These stations are commonly located between 10 and 50 km from large pollution sources, such as cities, power plants and major roads. On the other hand, urban background stations measure the average air quality in urban areas, which results from the regional concentration and from emissions generated within the city, taking care of not being directly influenced by large emission sources like industry plants or busy streets (Larssen et al., 1999). Annual mean concentrations based on hourly values for urban and rural air quality stations with over 80% valid measurements were included in this analysis. Using spatial analysis, urban and sub-urban background stations located within urban entities were identified and are presented in Figure 3.6. The urban entities were defined in Section 2.4.1 and depict urban areas with more than 50 000 inhabitants[5].

[5] It is interesting to note that no measure stations classified as rural were found within an urban entity, further reinforcing the notion that the CORINE dataset provides a reliable picture of the urban sprawl extent.

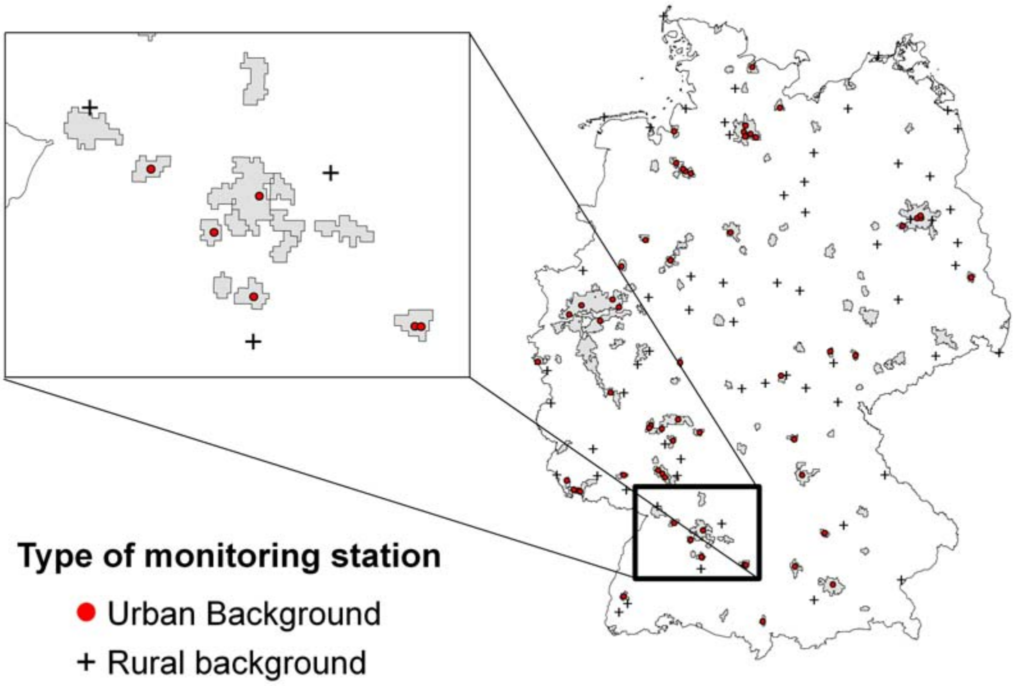

Figure 3.6 Rural and urban background stations within urban entities.

From Figure 3.6 it is evident that sometimes several urban background stations can be found within the same urban entity. For these cases, an average urban background concentration for each urban entity was estimated. The main reason for this simplification lies in the fact that, as the urban entity is viewed as the unit of analysis, only one urban increment for each urban entity was considered to be enough for characterizing such unity. Further disaggregation within the urban entity was in fact tested but the gains in accuracy did not outdo the larger uncertainties resulting from using coarse wind fields and the lack of specific urban morphology data. Additionally, local effects within cities are assessed in the third tier of the hybrid modelling approach and, therefore, it seems reasonable to neglect small differences at a neighbourhood level.

Each urban background station was associated with the nearest rural background station and, restricting the distance between them to 50 km, station pairs for PM_{10} and NO_X were built. Ideally, a rural background station should be chosen in such a way that it is located upwind with respect to the urban background station in order to avoid a significant influence of urban emissions on the measurements at the rural station. However, wind direction varies on a daily and seasonal basis due to a number of factors, such as local topographical features, land use and anthropogenic structures near the monitoring stations. Furthermore, it is possible that for a given location there is more than one dominant wind direction or a wide range of dominant winds, requiring the use of several rural stations for estimating the difference between urban and rural pollution levels (e.g., Jones, Yin, & Harrison, 2008). Given that such detailed analysis goes beyond the scope of this work, this aspect was not investigated. Nevertheless, it is important to note that, by definition, rural stations are located within a distance of 10 to 50 kilometres from built up areas and other major sources. Despite this distance, measurements from rural stations may be partially influenced by regional traffic activity, larger power plants, and industrial complexes in the area at a distance of 100-500 km. Therefore, a certain influence of urban emissions on pollution levels measured at rural stations is likely unavoidable.

A detailed analysis was carried out for detecting station misclassification (e.g., rural background station instead of sub-urban industrial or remote station) and for ensuring that medium or larger cities were not influencing the observations at the rural background station. Finally, a total of 24 stations pairs for PM_{10} and 26 stations pairs for NO_X were identified and the urban increment were then computed as the difference between the corresponding urban/rural stations. Half of the stations pairs were used for model development and the other half was used for model evaluation, which is discussed in Chapter 4.

The urban increment values used for model development are summarised in Figure 3.7 and Figure 3.8. These values constitute the dependent variable to be used in the multiple regression analysis presented later in this chapter.

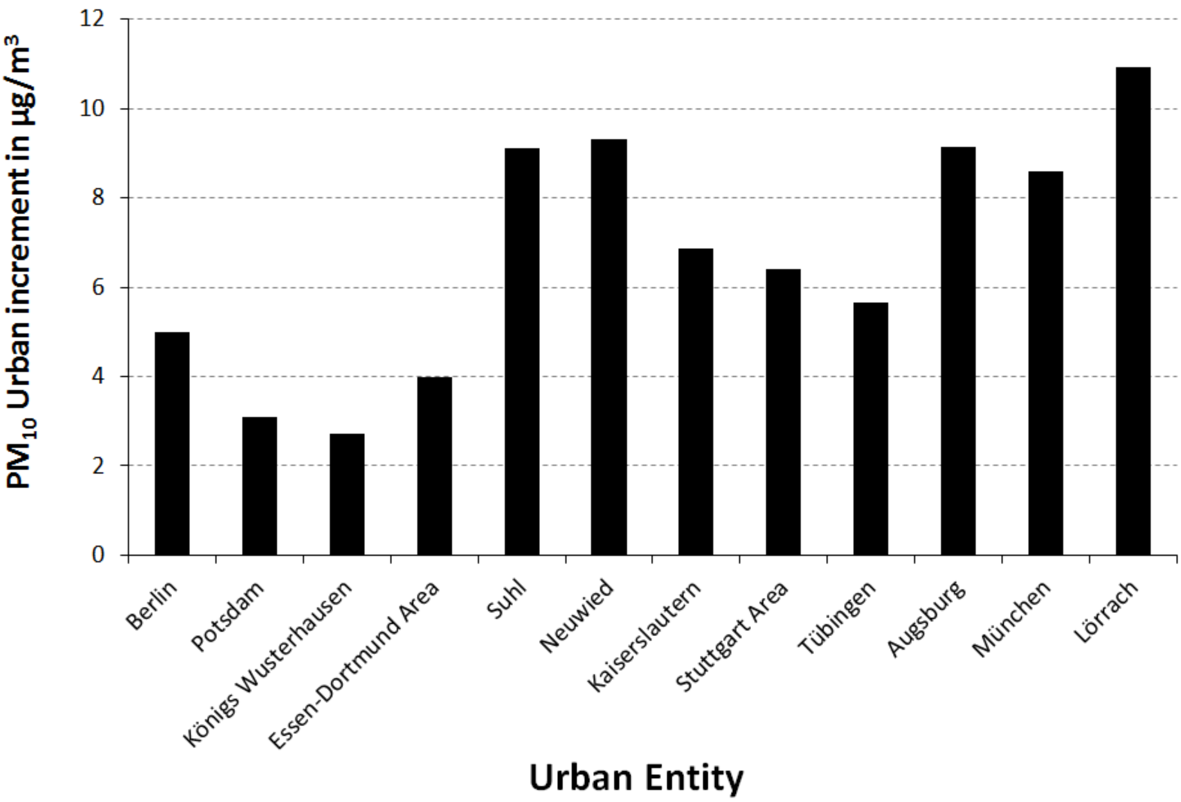

Figure 3.7 PM_{10} urban increment for several urban entities.

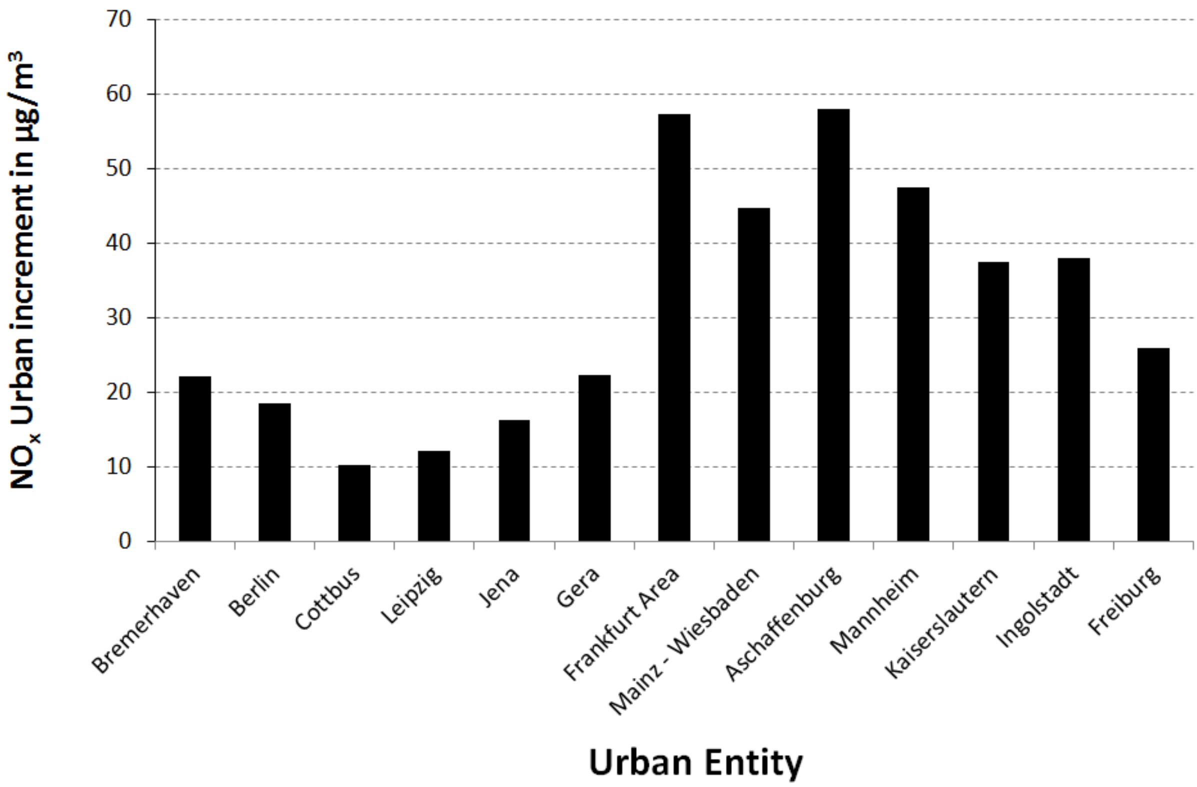

Figure 3.8 NO_X urban increment for several urban entities.

3.4.2.2 Urban emissions

One of the most important factors influencing urban pollution levels is certainly the emissions emitted within the urban boundaries. For this reason, a reliable and accurate emission inventory is crucial for any urban air quality analysis. The highly disaggregated emissions dataset provided by the IER was used to estimate urban emissions for the urban entities identified in Germany. The methodology, and assumptions used in the emissions spatial allocation were described thoroughly in section 2.3.2. Furthermore, it is also assumed that only primary emissions released from low sources increase concentrations within the cities (Amann et al., 2007) and the emissions were split into low- and high-level sources following Pregger and Friedrich (2009).

3.4.2.3 Urban morphology

A critical issue encountered when analysing urban areas, namely their spatial boundaries, has been already overcome by defining the urban entities (see section 2.4.1.). According to the results of the CityDelta project, city diameter is an important factor influencing the urban increment (Equation 3.3). However, determining city diameter proved to be a difficult task since urban sprawl normally does not follow specific geometric patterns, as is shown in Figure 3.9. For this reason, other parameters related to urban morphology were tested, such as urban entity area and fractal geometry. The latter parameter has been used extensively to estimate urban sprawl complexity as a function of shape, allowing to distinguish different types of urban patterns (Batty & Longley, 1994; Frankhauser, 2004). Moreover, several studies have analysed the relationship between the fractal measurement of road systems and the urban area it serves (e.g., Lu & Tang, 2004; J. Tang, 2003). These studies suggest that fractal geometry provides an effective way to describe complex geographical features. Drawing on this argument, it was hypothesized that this factor could describe the influence of urban sprawl and road network on urban air quality. For testing this assumption, fractal indices for the corresponding urban entity were estimated following Thomas et al. (2008). However, the results revealed that, contrary to the hypothesis, only the urban entity area is statistically significant for estimating the urban increment. Therefore, only urban entity area was included in the model to take into account urban morphology.

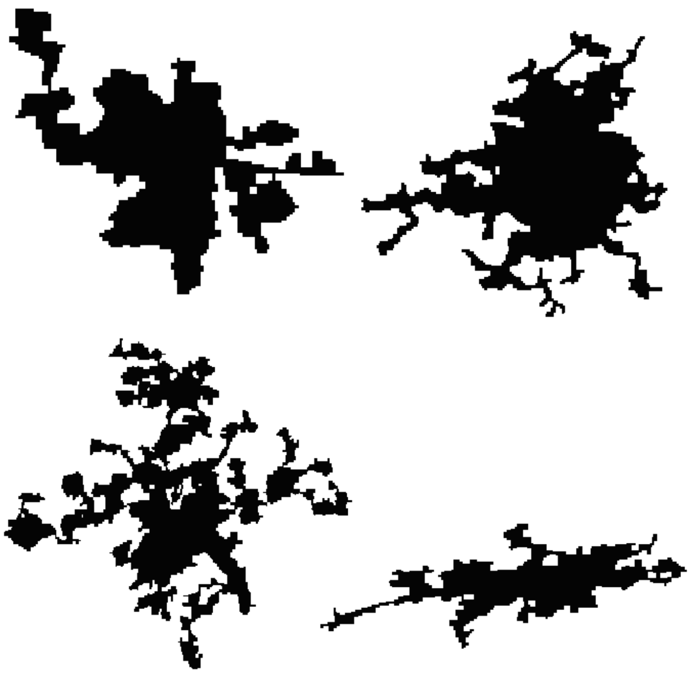

Figure 3.9 Urban contours of Aachen, Chemnitz, Stuttgart and Kaiserslautern (from top left to right, without scale).

3.4.2.4 Wind speed

A wind-speed dataset modelled within the EU project NATAIR (Vautard, 2006) was integrated into this analysis. Profiting from a four-year dataset (1997, 2000, 2001 and 2003) and a spatial resolution of 25 by 25 kilometres, the average 10-metres-over-the-surface wind-speed was estimated for Germany. This dataset was generated using the prognostic meteorological model MM5 (PSU/NCAR Mesoscale Model) developed by the Pennsylvania State University (PSU) in cooperation with the University Corporation for Atmospheric Research (UCAR). The results are presented in Figure 3.10.

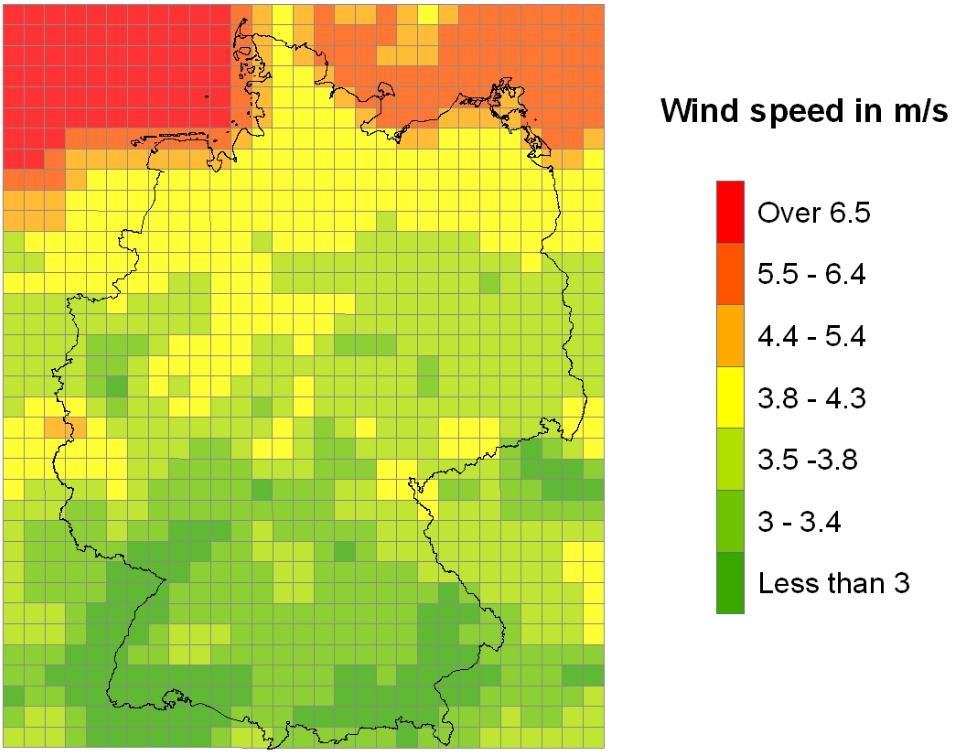

Figure 3.10 Four-year average wind speed at 10 metres over the surface.

3.4.3 Multiple regression analysis

To obtain the relationship between the dependent variable – in this case the measured urban increment – and predictor variables (i.e., urban emissions, urban area, and wind speed), a multiple regression analysis was carried out.

An important assumption underlying the urban increment formulation is that urban increment is positively correlated to emission density (i.e., amount of emissions per km^2). Looking at the scatterplots of measured urban increments against emission density in Figure 3.11 and Figure 3.12, it is evident that this conjecture holds true for NO_X and for almost all cases for PM_{10} but a contradictory behaviour can be observed in one case: low urban PM_{10} increment is related to high emission density. One possible explanation for this effect may be that the monitoring stations for that urban entity are located in an area with many closely located cities (Essen-Dortmund Area). In this case, measurements from the rural stations may be strongly influenced by urban emissions and the urban background concentration for this urban entity does not clearly stands out against the rural background concentration levels. It can be then suggested that the measured rural background is inversely correlated to the urban increment. Thus, according to these findings, the rural background concentration was included as a parameter into the PM_{10} urban increment function. As Figure 3.12 shows, a similar behaviour could not be found for NO_X.

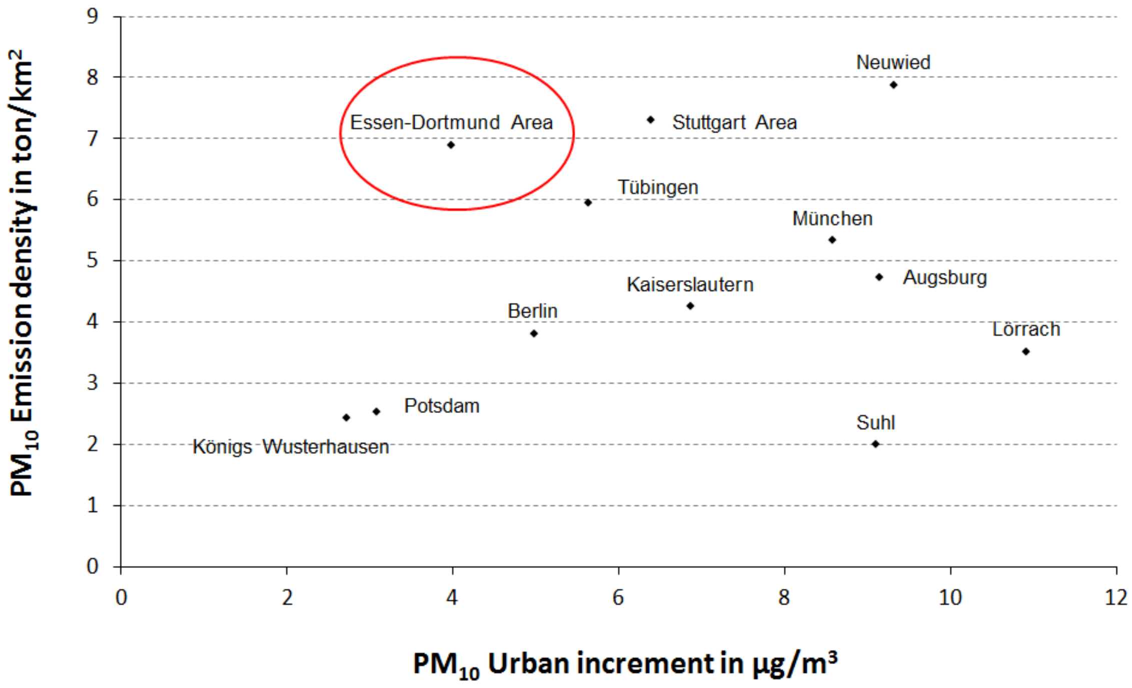

Figure 3.11 PM_{10} urban increment and emission density.

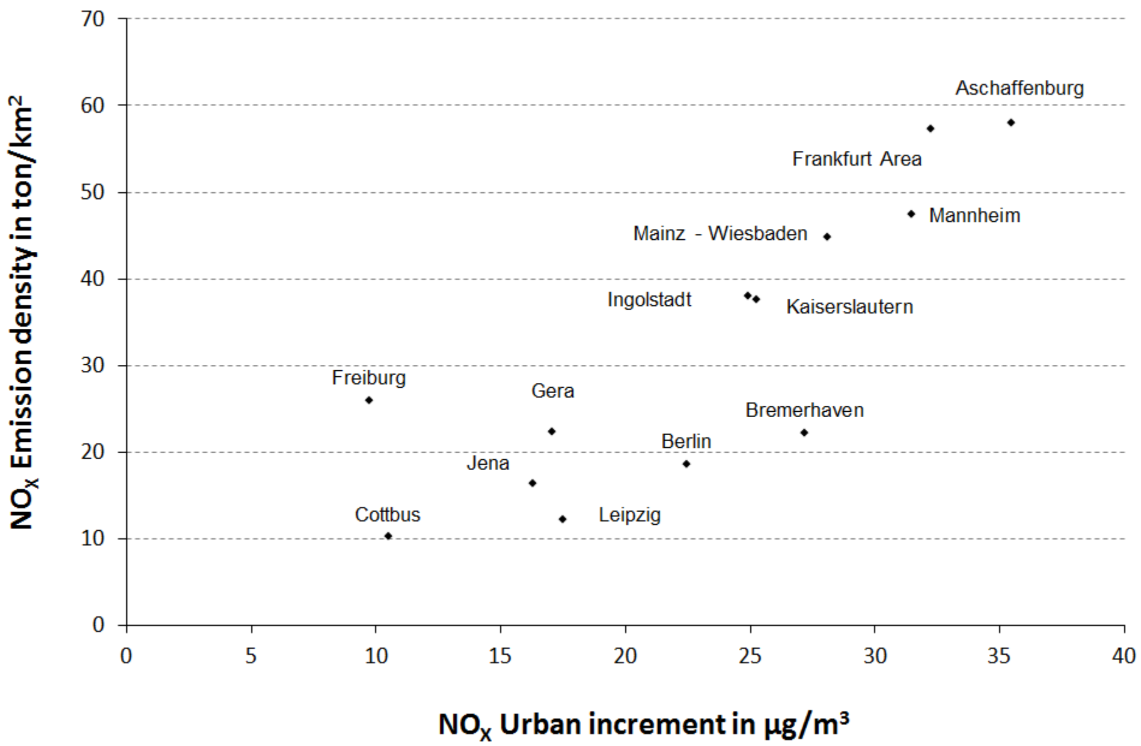

Figure 3.12 NO_X urban increment and emission density.

After all parameters, namely emission density, average wind speed, and rural background concentration were tested for statistical significance, a multiple-regression analysis was conducted to predict urban increment from the predictor variables discussed in this section.

Thus, the urban increment was estimated using the following formulation:

$$C_{i\ urban} = \varpi_i + \phi_i \frac{E_{iUE}}{A_{UE} \cdot u_{avg}} + \gamma\, C_{i\ rural}$$ Equation 3.4

where

$C_{i\ urban}$ = Urban increment of pollutant i.

E_{iUE} = Total emission of pollutant i within the UE in tons.

A_{UE} = Urban entity area in km^2.

u_{avg} = Urban entity average wind speed in m/s.

$C_{i\ rural}$ = Rural background concentration of pollutant i in $\mu g/m^3$ (only for PM_{10}).

ω_i, ϕ_i, and γ_i = Multiple-regression parameters for pollutant i.

To ensure that the parameters represent independent disturbances, they were tested for multicollinearity by means of verifying the condition number which takes into account the magnitude of the eigenvalues of the correlation matrix of the regressors (Berry & Feldman, 1990). It was found that multicollinearity was not an issue for the predictor variables in the regression analyses. Moreover, the data were also tested for outliers using the standardized residuals or studentized residuals. The multiple-regression analysis yielded the results presented in Table 3.3 , Figure 3.13 and Figure 3.14.

Table 3.3 Multiple-regression parameters and coefficients of determination.

Parameters	**PM_{10}**	**NO_X**
ω	15.27	-6.95
Φ	0.24	5.64
γ	-0.53	n.s.
R^2	**0.80**	**0.83**
Adjusted R^2	**0.75**	**0.82**

n.s. not significant

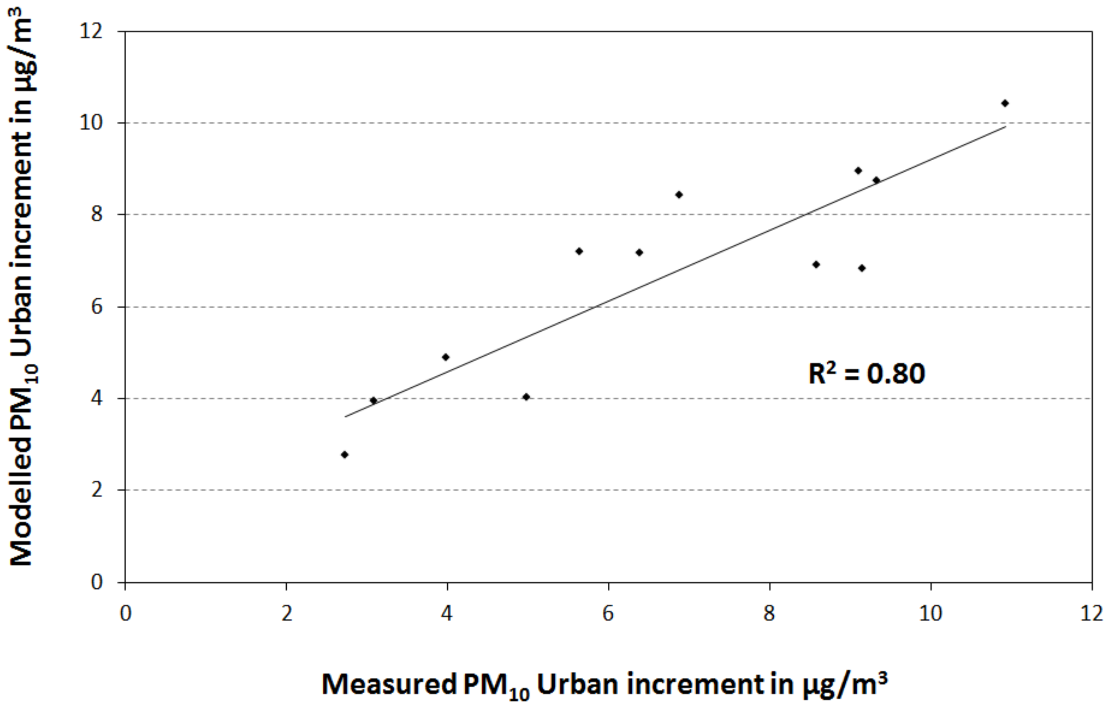

Figure 3.13 Modelled and measured PM_{10} urban increment.

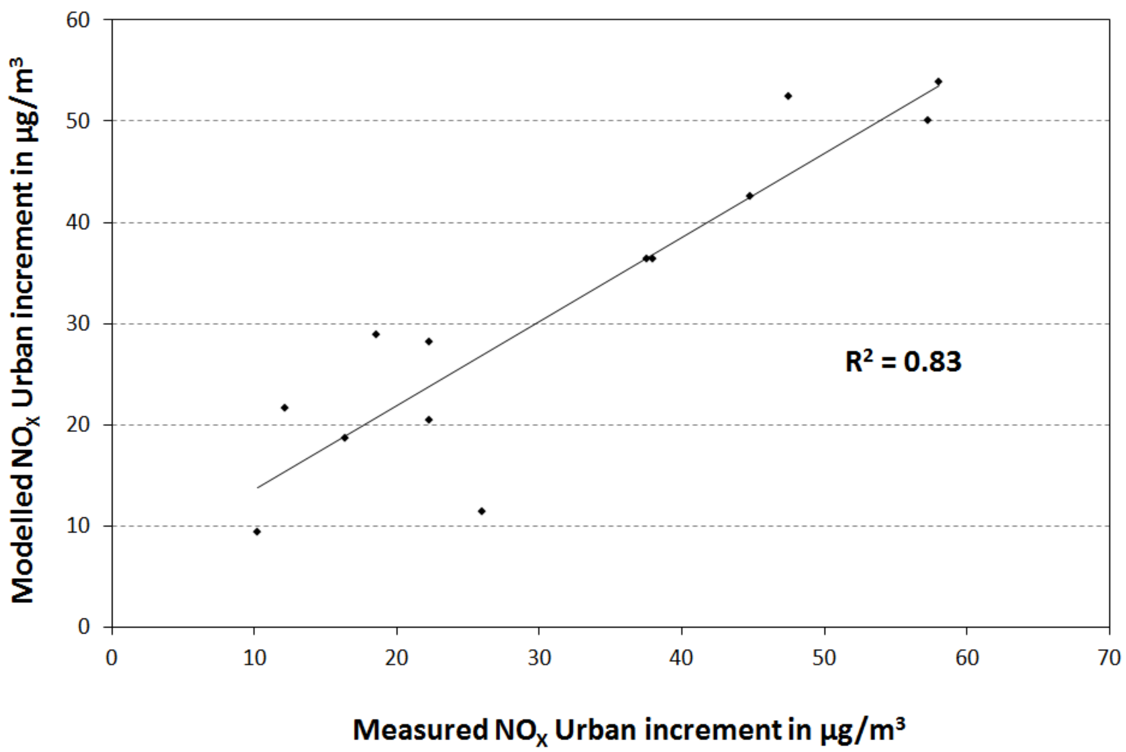

Figure 3.14 Modelled and measured NO_X urban increment.

It is important to note that the PM_{10} urban increment was estimated using measured rural background concentration data obtained from Airbase (see Equation 3.4). Furthermore, since the measured data for both pollutants presented here were used for the development of the model, these results must not be viewed as a complete validation of the model. For evaluation purposes, a comparison with the other half of the stations pairs described in Section 3.4.2.1 is presented in Chapter 4.

3.4.4 Urban increment for $PM_{2.5}$

As it has been mentioned earlier in this work, an urban increment model for $PM_{2.5}$ could not be estimated directly due to the limited availability of valid measurements for this pollutant. However, considering that ambient concentration levels of this pollutant are relevant to assessing human health, an alternative approach was used for making a rough estimation of $PM_{2.5}$ urban increment, namely the $PM_{2.5}/PM_{10}$ concentration ratio. A number of studies have been conducted to shed light on the ratio $PM_{2.5}/PM_{10}$. For instance, Gehrig and Buchmann (2003) analysed long-term data from several urban monitoring stations in Switzerland noting that the mean $PM_{2.5}/PM_{10}$ ratios of daily values were 0.75 with a standard deviation of 0.11. They also found out that the ratio remained rather constant at the different stations and through a period of four years. Van Dingenen et al. (2004) carried out a comprehensive analysis of the physical characteristics of particulate matter using data from 31 monitoring stations across Europe. They report that the $PM_{2.5}/PM_{10}$ ratio vary between 0.57 and 0.85, depending strongly on the type of monitoring station. In the case of urban background stations, the ratio ranged between 0.66 and 0.80. Moreover, combining measurements and detailed dispersion modelling, Graff et al. (2006) evaluated the $PM_{2.5}/PM_{10}$ ratio for seven large regions in Germany, finding that the proportion of $PM_{2.5}$ in PM_{10} urban background ranged from 0.70 to 0.75. Thus, although it is recognized that the ratio of $PM_{2.5}$ to PM_{10} depends on factors which vary both spatially and temporally, a value of 0.75 for the $PM_{2.5}/PM_{10}$ urban background ratio is considered to be a reasonable assumption.

3.4.5 Results – Urban increment for German urban entities

The PM_{10}, $PM_{2.5}$ and NO_X urban increment for all German urban entities was estimated using Equation 3.4 and the parameters described in Table 3.3. It should be noted that Equation 3.4 requires PM_{10} rural background concentration as input for estimating the urban increment. Considering that measured PM_{10} rural background concentration values are available only for a limited number of urban entities, an alternative approach was used to estimate the values at locations were no data were available. An interpolation of all PM_{10} regional background concentration values available for Germany was considered the best solution for the given conditions. The interpolation method used was the Inverse Distance Weighting (IDW). In this interpolation method, values of a variable are estimated based on the distance from the nearest neighbour of a known point (Davis, 2002). The interpolation method can be written as:

$$z_0 = \frac{\sum_{j=1}^{m} k_j z_j}{\sum_{j=1}^{m} k_j} \qquad \text{Equation 3.5}$$

where the z_j are from the "m" closest position and the weights k_j are chosen larger for data values near to where the estimate z_0 is to be made. The essential assumption in this technique is that nearby locations are more likely to have more similar values than when the locations are far apart. In this way, an interpolated geo-referenced grid was generated using the spatial analysis tool included in the software ArcMap.

Once PM_{10} rural background values for all large urban entities were estimated, PM_{10} urban increments were estimated and the modelled average PM_{10} urban increments for several urban entities are depicted as a horizontal line in Figure 3.15. The vertical bars depict the minimum and maximum urban increment for those urban entities with several rural background concentration values. As stated in Section 3.4.4, urban increments for $PM_{2.5}$ were estimated as a fraction of the PM_{10} increment and, therefore, the values estimated depict a trend similar to PM_{10} and are shown in Figure 3.16. Figure 3.17 shows the NO_X urban increments for several urban entities. Keeping in mind that NO_X rural background concentration is not a parameter to estimate the urban increment, only one value was estimated for each urban entity. Urban increments for PM_{10} show values ranging from 2 to almost 10 µg/m^3. These values are within the range of measured increments used for developing the model. Furthermore, they are also similar to those reported by Graff (2006).

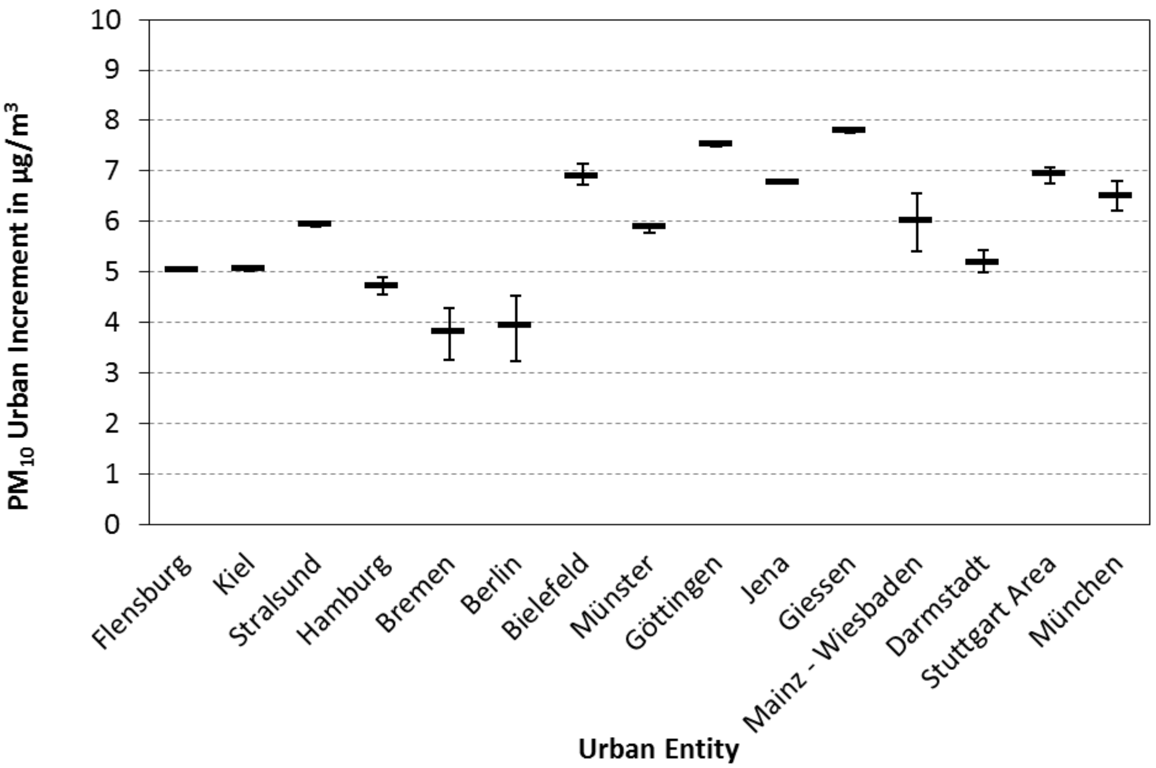

Figure 3.15 PM_{10} urban increment estimated for several large German urban entities.

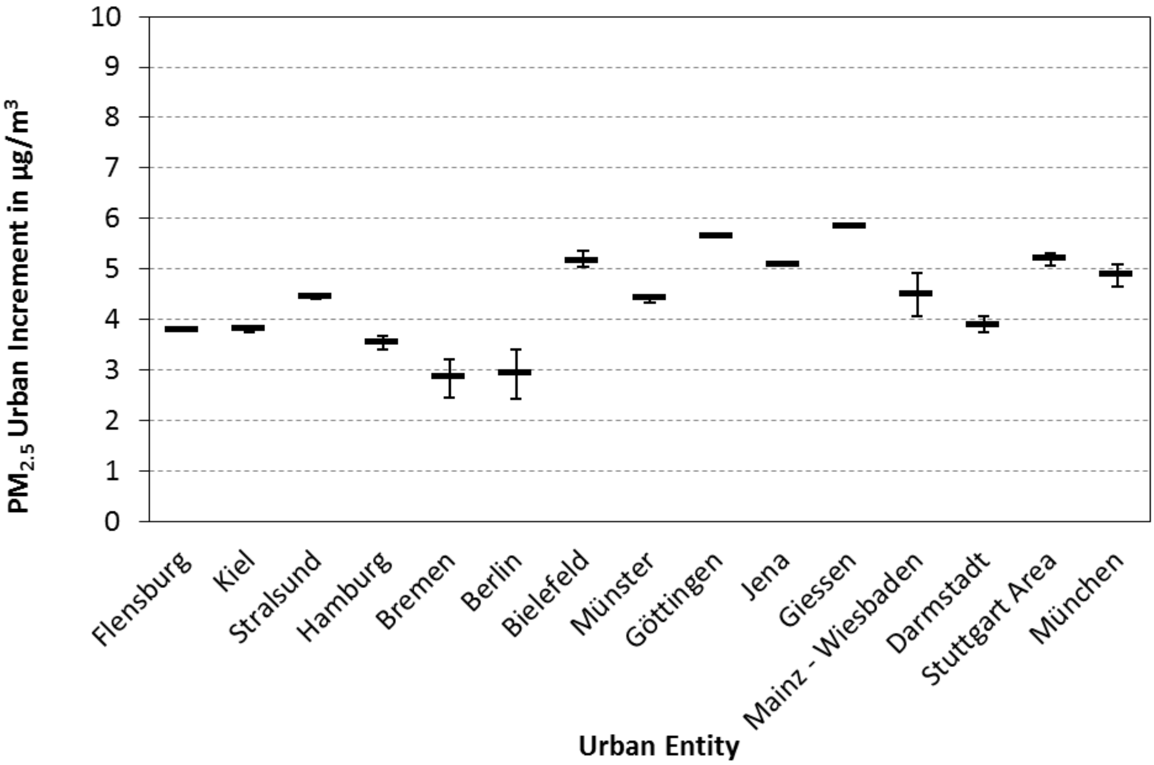

Figure 3.16 $PM_{2.5}$ urban increment estimated for several large German urban entities.

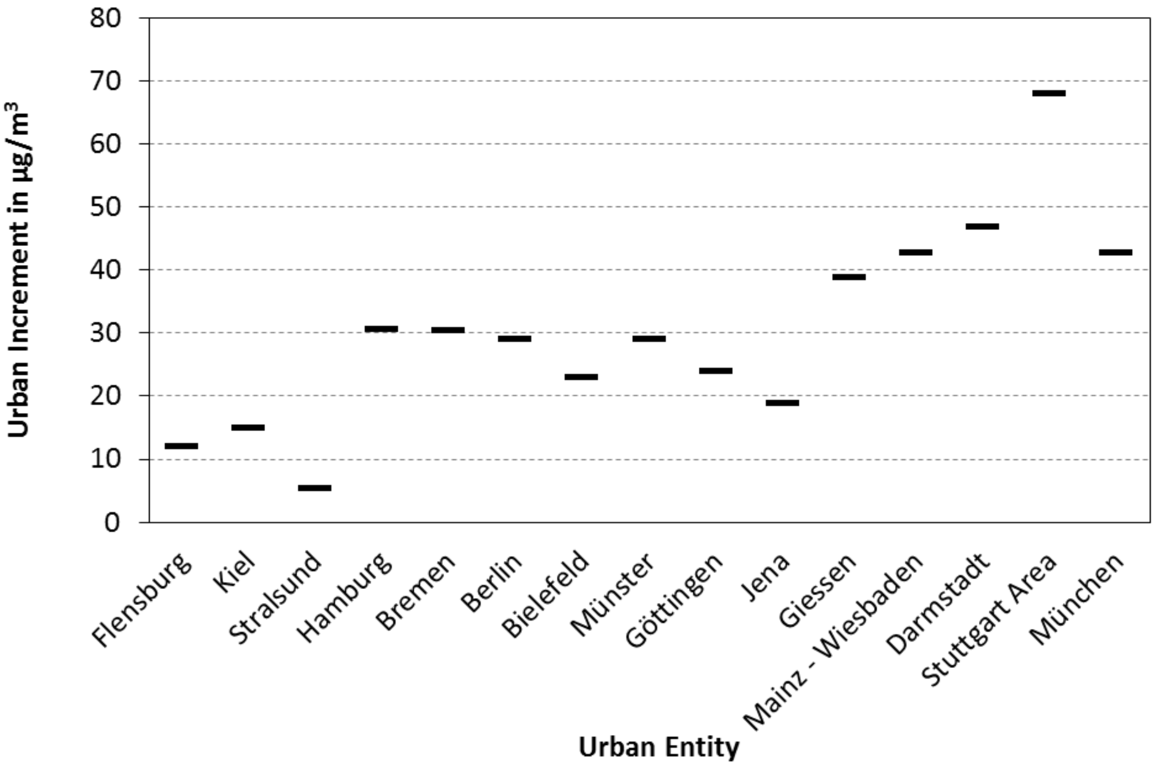

Figure 3.17 NO_X Urban increment estimated for several large German urban entities.

Concerning NO_X urban increments, it is pertinent to note that two values over 70 µg/m^3 were obtained. Although differences between urban and rural background concentrations accounting for over 70 µg/m^3 can be found for cities like Milan, Trento and London, such high values are commonly not found in Germany. Moreover, the NO_X model was built using measurements accounting for urban increments from 10 to 58 µg/m^3 and, therefore, urban increments over 70 µg/m^3 are likely to be overestimated. Finally, it is important to remember that measurements of nitrogen oxides are defined as the sum of nitric oxide and nitrogen dioxide added as a part of per billion and expressed as nitrogen dioxide in µg/m^3 (Mol, 2007). Therefore, despite a detailed spatial disaggregation of NO_X emissions, important chemical processes at the urban scale are difficult to take into account using the simplified approach presented here.

Nevertheless, despite minor discrepancies the results presented here support the notion that NO_X concentrations are a significant tracer of the NO_2-equivalent concentrations. Furthermore, the estimates provide valuable insight into spatial variability of pollutant concentrations across large cities. A comprehensive validation of the computed results by comparison with physical measurements is presented in Chapter 4.

3.5. Road increment concentration – Main road network

In the last section, a model to estimate urban concentration increments for several pollutants was described and results were presented. This model allows a more accurate assessment of air quality within urban areas and, due to its simplicity and rather low input data requirements, can be used for other purposes (e.g., assessment of emission reduction scenarios, external costs, among others). However, growing scientific evidence suggests that people living near major roads are at higher risk of developing or experiencing worsening health problems and, on account of this, there is a compelling incentive to draw the road increment concentrations in the health effects assessment. In order to address this challenge, the third tier of the hybrid dispersion modelling was developed.

It should be evident that dispersion conditions are quite different for roads outside urban areas and those within them. The characteristic urban morphology outlined by buildings near the roads, street canyons and the lower speed limits can be mentioned as some of the most evident differences between both sites. Additionally, data availability is also a relevant factor considering that, on the one hand, a highly spatially disaggregated emission dataset is available for the main German road network, and, on the other hand, such comprehensive information is not available for all urban areas analysed in this work. Accounting for these differences, the third tier of the hybrid dispersion modelling addresses each road type separately according to the following typology:

- Roads belonging to the main network and outside urban areas
- Roads belonging to the main network and inside urban areas[6]
- Urban streets.

[6] Roads are commonly named streets when they diverge through a built environment. However, roads belonging to the main German road network normally maintain their classification name, i.e., motorways and federal roads. Thus, in this work the terms urban and non-urban roads are used for these roads and streets for roads within urban areas that do not belong to the main road network.

In this section, road increment concentrations for the main road network outside and inside urban areas are analysed and, later in this work, a model for estimating pollutant concentrations within urban streets is presented.

3.5.1 Main road network - Outside urban areas

While it is true that people are more frequently exposed to pollution burden resulting from urban roads than from roads outside cities, emissions generated by road transport outside urban areas may also largely contribute to air quality decay in nearby areas. Hence, taking advantage of the highly spatially disaggregated road emissions for the main German road network, a model for estimating the increment of pollution concentrations near roads outside urban areas was developed. Drawing on findings from the literature review, the regression functions embedded in the MLuS dispersion model were identified as the best suited for the goals pursued in this work. A short description of the model is provided in the following section.

3.5.1.1 The MLuS dispersion function

The technical leaflet on air pollution along roads (MLuS from its initials in German: Merkblatt über Luftverunreinigungen an Straßen) was developed by the German Research Association for Roads and Traffic engineering (FGSV, 2005). The static regression model aims to analyse the concentration change due to road traffic emissions. It is based on concentration measurements at different distances from streets, including seven-year time series from monitoring points at both sides from a motorway. The model estimates additional annual concentration averages for classical pollutants near roadways with built-up areas at road side limited to less than 50%. The model is also restricted to roads with an Annual Average Daily Traffic (AADT) larger than 5000 vehicles and velocities greater than 50 km/hr. As for lorries, their volume share is limited to 50% and their speed to 80 km/hr. Furthermore, concentrations can be estimated for observation points as far as 200 metres. For roads complying with these criteria, pollutant concentrations can be estimated as:

$$C_i(s) = c_n \cdot e_i \cdot g(s) \cdot f_u \qquad \text{Equation 3.6}$$

where

C_i (s) = concentration of pollutant i at a distance s (mg/m^3),

e_i = length-specific street emission (mg/m · h),

c_n = near-ground concentration standardised with respect to e_i (h/m^2) with a value of 0.067.

g(s) = dispersion function (dimensionless) ; It is estimated using:

$$g(s) = 1- 1.166 \ln(1+s)$$

where s is the distance between road shoulder and an observation point,

fu = function to consider wind speed (dimensionless); It is evaluates as follows:

$$f_u = \frac{2.3}{u_{avg}}$$

where u_{avg} is the annual average wind speed in m/s measured at 10 metres over the surface.

Although the MLuS model includes a module to estimate emissions as well, it is important to note that only the pollutant dispersion component of the model was implemented in this work.

Using the equation described above, additional concentrations near roads outside urban areas were estimated. For this purpose, length-specific emissions were retrieved from the IER dataset and wind speed data were drawn from the same dataset used for estimating urban increments (see Section 3.4.2.4). Results obtained for the main German road network are presented in section 3.5.3.

3.5.2 Main road network - Within urban areas

The model presented in the last section is not best suited to calculate additional pollutant concentrations for roads passing through urban environments because it does not account for the influence of buildings along the roads on the dispersion processes. Therefore, another model had to be used for this purpose. Drawing on findings from the literature review, the CAR International dispersion functions were identified as best suited for estimating the additional pollutant concentration at roadside. In the following section, the aforementioned model is briefly described.

3.5.2.1 The CAR International Model

The CAR International (den Boeft, Eerens, den Tonkelaar, & Zandveld, 1996) model is a semi-empirical screening model that makes a first appraisal of pollutant concentrations caused by road traffic. It is based on investigations in wind tunnels, theoretical considerations and measurements of dispersion and it estimates the annual average pollutant concentration and percentiles for five different road types, which are considered typical within cities.

Car International (in the following abbreviated CI) draws on the Car model (Eerens, Sliggers, & Van den Hout, 1993) which was developed mainly to provide a simpler tool for evaluating air quality within urban street canyons in the Netherlands. The model has undergone evaluation using measurements as reported by Heida et al. (1989), and ever since the model has been calibrated annually against measurements to ensure its reliable application. Therefore, parameters like average wind speed, emissions factors and, foremost, background concentration values are revised and updated in order to provide results better suited to the Dutch condition (Teewisse, 2006).

The international version allows user-defined emission factors and local meteorological conditions to be implemented, making possible its use for other regions and traffic profiles as well. With traffic density, type of roadway and yearly average wind speed as main inputs, the model predict concentrations for inert gases at distances up to 30 metres from the axis road. Furthermore, the model also includes an empirical expression to estimate NO_2 concentration, providing that the fraction of NO_X directly emitted as NO_2 and the rural background ozone levels are known. For a detailed model description, the reader is referred to Van den Hout et al. (1989), Eerens et al. (1993), and den Boeft et al. (1996). The model formulation can be written as follows:

$$C_{roadside} = E\,\theta\,w\,f \qquad \text{Equation 3.7}$$

where $C_{roadside}$ is the additional pollutant concentration due to the vehicles that travel on a specific street, E are the emissions generated by said vehicles; finally, *w* and *f* are wind and tree factors, respectively. The effect of urban building geometry is included in an empirical way, using a modification component in the form of the dilution factor θ, which is determined by the geometry of roads and surrounding buildings. The dilution factor θ is calculated as follows:

$$\theta = aS^2 + bS + c \qquad \text{Equation 3.8}$$

where a, b, and c are dilution parameters and S is the distance from the road axis to the receptor location in metres. As already mentioned, the model distinguishes between five different road types, which determine the values of the dilution parameters, as described in Table 3.4 and Table 3.5. These definitions are valid only if the street has the same configuration over at least 100 metres. More recently, additional dilution parameters have been obtained for road-type 1 (Teewisse, 2006). Given that it is evident that roads of type 1 are rarely found within urban areas, this type was not included in this study. Moreover, as detailed data describing building geometry for whole cites were not available[7], for this research it was assumed that within a city buildings are found at both sides of the street and, thus, road-type 4 was not considered as well[8].

Table 3.4 Road types description.

Road Type	Description
1	Road through open terrain, sporadically there are buildings or trees within 100 metres from the road axis
2	Roads other than roads represented by type 3a, 3b and 4
3a	Road with buildings at both sides; distance road axis-façade between 1.5 and 3 times the height of buildings
3b	Road with buildings at both sides; distance road axis-façade smaller than 1.5 times the height of buildings
4	Road with buildings at one side, but about continuously built; distance road axis-façade smaller than 3 times the height of buildings

Source: den Boeft et al., 1996.

[7] Although nowadays city-specific digital and geographical information remain too expensive to consider their use for research purposes, within the next five to ten years these data may be more accessible as three-dimensional city models are becoming more popular, being used for a wide range of purposes, such as advertising, urban planning, and tourism services (e.g., Brenner & Haala, 2000; Kettemann, 2004).

[8] It should be noted here that street intersections represent an especial case within the urban morphology where complex flow patterns can occur. Given that those effects cannot be assessed with the CI model, street intersection are beyond the scope of this research.

Table 3.5 Dilution parameters.

Road Type	Dilution parameters		
	a	b	c
1	0.000075	-0.007	0.17
2	0.00031	-0.0182	0.33
3a	0.000325	-0.0205	0.39
3b	0.000488	-0.0308	0.59
4	0.0005	-0.0316	0.57

Source: den Boeft et al., 1996.

Even though the model provides only mean yearly concentrations and does not allow detailed analysis in terms of spatial or temporal resolution, the aforementioned values are better suited for the type of problems addressed in this work. Due to its flexibility and easiness to implement, the model has been used in a number of studies dealing with air pollution generated by vehicle-related emissions in urban areas (see for instance Huijbregts, Meijer, Hertwich, & Reijnders, 2006; Meijer, 2004). Here it is important to note that, although the CI model includes a module to estimate emissions, only the dispersion element of the model was implemented in this study. In order to test the applicability of the dispersion functions for German conditions, their performance was evaluated individually using two detailed datasets, the results of which are presented in the following section.

3.5.2.2 Comparison against the two TRAPOS datasets

The lack of detailed data regarding vehicle flow and fleet composition, local meteorological conditions, and site geometry represents a serious burden for evaluating the performance of dispersion models. In the frame of the network Optimization of Modelling Methods for Traffic Pollution in Streets (TRAPOS), important deficiencies in the modelling tools used for prediction of traffic pollution in urban streets were addressed (Berkowicz, Britter, & Di Sabatino, 2004) and, along with several technical and methodological improvements, one of the outcomes of this project was the production of several comprehensive datasets for testing and developing street pollution models. Data available include street geometry, traffic volume and composition, local meteorology, and pollutant measurements not only from stations located directly at the roadside but also from urban background stations, allowing in this way to identify the additional pollutant concentration associated to one specific street. Thus, the datasets have been used a number of times for validating street pollution models (e.g., Aquilina & Micallef, 2003; Ketzel, Berkowicz, & Lohmeyer, 2000; Le Bihan, Wåhlin, Ketzel, Palmgren, & Berkowicz, 2002; Sahm, Louka, Ketzel, Guilloteau, & Sini, 2002).

The CI model performance was applied for estimating the additional concentrations of carbon monoxide and nitrogen oxides for two field datasets from the TRAPOS project[9]. The datasets used in this research are briefly described below.

[9] Particulate matter measurements were not available because at the time the measurement campaigns were carried out, this pollutant was not routinely measured.

Göttinger Street

Göttinger Street in Hanover, Germany is a busy four-lane street canyon with a total traffic load of about 30 000 vehicles/day and a large percentage of heavy-duty vehicles (about 16%). The width of the street canyon is 25 m and buildings on both sides of the street are around 20 m high. Street orientation is 163 degrees with respect to north and the average wind speed is 3.9 m/s. Concentrations were measured at a height of 1.5 metres above the pavement (Berkowicz et al., 2004; NLÖ, 1994, 1995).

Jagtvej Street

Jagtvej Street in Copenhagen, Denmark has two traffic lanes but often with two rows of cars in each of the lanes. The width of the street canyon is 25 m and the buildings on both sides of the street are about 18 m high. The total traffic load is roughly 22 000 vehicles per day including about 3.5% heavy-duty vehicles. The street is oriented at a 30-degree angle with respect to north. Concentrations were measured at a height of 3.5 metres[10] above the pavement (Berkowicz et al., 2004; Kemp, Palmgren, & Manscher, 1996).

The corresponding site geometry and yearly average wind speed were used as input for the CI model. To account for differences in measurement height, the Jagtvej-results were corrected following Eerens et al. (1993). Concerning emission, available data were used as input for the emission model embedded in the CI model. Since the pollutants are modelled as inert pollutants, the modelled concentration is directly proportional to the emission rate and any errors in the emission rate translate directly into errors in the concentration estimates. It can then be argued that since the field sites have significant differences in their vehicle fleets and, most likely, have different emission factors, using the same average emission factors may not be the best way for testing the model performance. However, given that reverse dispersion modelling to estimate emission rates was not possible because data needed for such analysis were not available, using average emission factors as a first approximation allows insight to be gained into the model performance under clearly different conditions. The results of this comparison are presented in Table 3.6.

It is reasonable to argue that these differences may be largely explained by the use of average emission factors, which do not reflect the characteristics of the actual vehicle-fleet composition. Hence, in order to test this argument, the CI model was again tested using site-specific emission factors for Göttinger Street found in Schatzmann et al. (1999). In this study, three different emission factor sets were calculated using detailed vehicle-fleet data: one set was estimated according to the methodology in Schädler et al. (1996) and reports of the German Environmental Agency, assuming an urban street with average speed of 46 km/hr, 30 percent of cold-start trips and 10% congestion time (in the following called Method I); and two were computed with the emission model MOBILEV version 1.3 assuming a similar drive cycle as for Method I but one set included explicitly two hours of stop and go for each working day (in the following called Method II) and the other set calculated internally stop and go time (in the following called Method III). Details regarding formulation and assumptions for estimating these factors can be found in Schatzmann et al. (1999) and references therein.

[10] The calculations were corrected to account for differences in measure height according to Eerens et al. (1993).

Table 3.6 Comparison CAR International model against measured values from the TRAPOS project.

	Additional concentration in µg/m³	
	CO	NO_X
Göttinger Street (Hanover, Germany)		
Measured	1353	254
Car International	1471	478
Difference	+9%	+88%
Jagtvej Street (Copenhagen, Denmark)		
Measured	1113	67
Car International	706	92
Difference	-36%	+37%

From Figure 3.18 can be concluded that the CI model presents significant improvement using site-specific emission factors, which is more evident for NO_X. The best results are obtained with Method II, which underestimates CO by a factor of roughly 1.2 and NO_X only slightly.

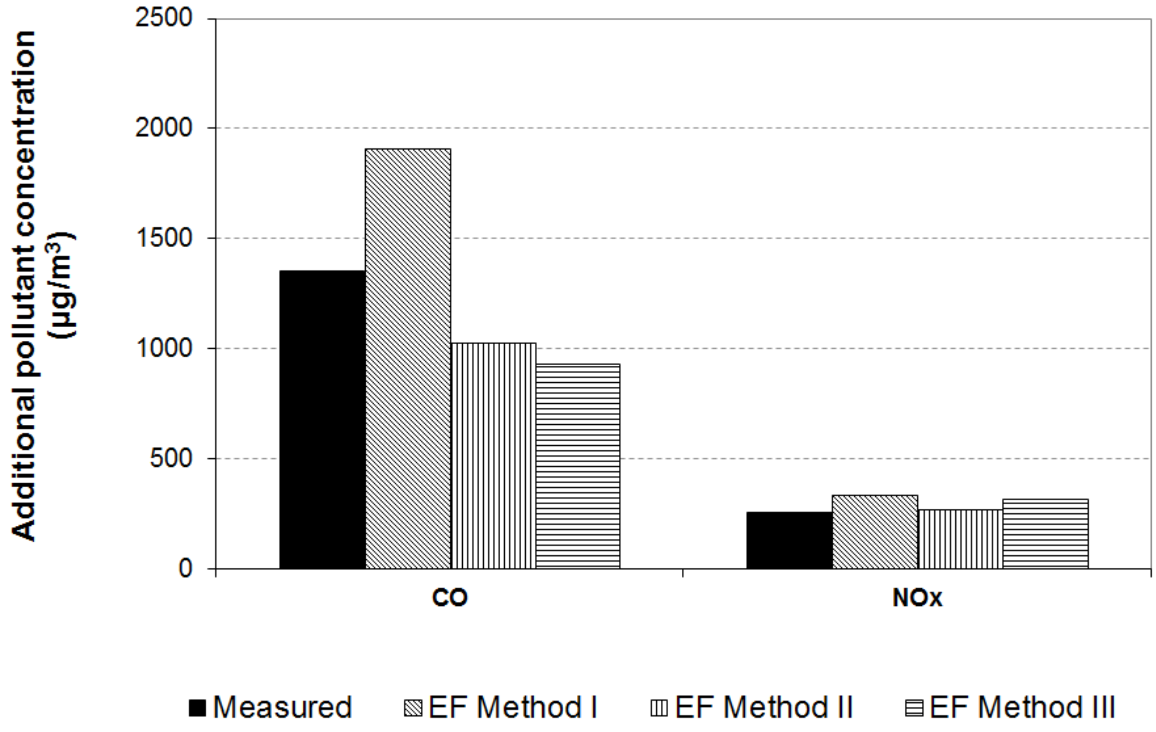

Figure 3.18 Additional pollutant concentrations measured at Göttinger Street against CI estimations using three different methods for calculating the emission factors.

Because in the aforementioned study a systematic wind-tunnel study and the MISKAM model (Microscale Model, Eichhorn, 1989; Eichhorn et al., 1988) were compared against the field data, an intercomparison between the three approaches – using the same emission factors – was possible (Figure 3.19). An overall good performance of the CI model can be drawn from these results, most notably so when considering that the more complex dispersion models provide similar results but requiring a significant larger and more detailed amount of data.

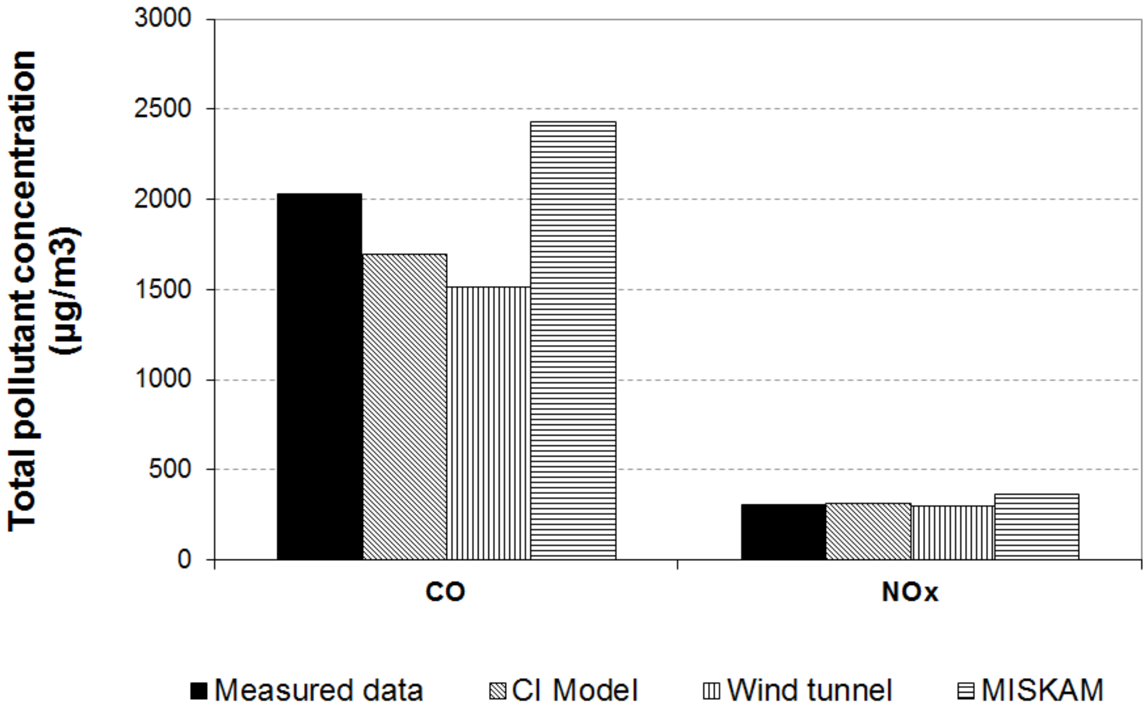

Figure 3.19 Total pollutant concentrations measured at Göttinger Street against CI model, a wind-tunnel study and MISKAM

It may be argued that the intercomparison was carried out against models using a now ten-year-old dispersion modelling technology and that they may have undergone significant improvements since the study was conducted. However, it should be noted that the intercomparison exercise was not intended to assess the performance of those models but rather to emphasise the advantages of using a simpler model, as the validation using transport-specific datasets demonstrated. Thus, it can be concluded that the CI model yields satisfactory estimates of inert pollutant concentrations near streets.

3.5.3 Results – Road increment for main road network

Using the models presented in the last sections, it is possible to estimate pollutant concentrations for a given road segment. As one of the models is better suited for roads passing through urban areas (CI model) and the other for roads located outside urban areas (MLuS model), the spatial location of the roads was obtained using a georeferenced framework. A simple algorithm was also implemented to choose the appropriate model based on whether the road segment was located outside or inside urban areas.

Looking at Equation 3.6 and Equation 3.7, it is evident that pollutant concentrations can be estimated at any distance from the road, which raises the question: at what distance should the concentrations be estimated? The answer to this question is simple and complicated at the same time. Basically, when addressing air quality issues, pollutant concentrations should be estimated at the receptors location. Earlier in this work, results depicting urban increment concentrations for urban areas where presented and, in this case, it is reasonable to suggest that all inhabitants of such urban areas are likely to be equally affected by the additional burden. However, when addressing the additional burden associated to specific roads, more detailed data on receptors location and time use are needed to accurately describe their exposure to vehicle-related pollutants. Given that such comprehensive analysis is beyond the scope of this work, concentrations are estimated at a specific distance from the roads, which depends on whether the road is located outside or within urban areas. Regarding roads outside urban areas, it is not attempted to assume that people spend time alongside motorways or federal roads since this is rather uncommon. Therefore, considering that several studies suggest that concentrations of ultrafine particles and black carbon decline to background levels within 150 – 500 metres of major roads (Hitchins, Morawska, Wolff, & Gilbert, 2000; Zhu, Hinds, Kim, Shen, & Sioutas, 2002), a distance of 100 metres from the road was set to estimate the concentration increments. Although these values serve only to illustrate the application of the MLuS model, it sets the framework for future modelling development and applications, e.g., human exposure assessment.

Similar to non-urban roads, the distance from the road axis to the receptor location cannot be readily defined for roads passing through urban areas because neither street width nor receptor location data are available country-wide. However and in contrast to non-urban roads, it can safely be assumed that receptors are likely located alongside a carriageway, i.e., on the pavement[11]. Therefore, receptor location was assumed to be around one metre from the kerbside. Taking into consideration that the CI model estimates pollutant concentrations based on the distance from the road axis (see Equation 3.7), the parameter road width has to be accounted for in the calculations. Additionally, this parameter is also relevant to the selection of a dilution function, which is chosen on the basis of the average height of the surrounding buildings and the distance between the road axis and the building façade (see Table 3.4). Therefore, both parameters are analysed in the following lines to determine which dilution function is better suited for the purposes of this work.

3.5.3.1 Road width

Roads are designed on the basis of transport network needs as well as structural, social and economic requirements. Furthermore, road cross-sections are chosen according to the expected vehicle-fleet mix, the projected traffic volume and the selected design speed. In Germany, the Guidelines for Road Construction – Part Cross-Section (RAS-Q from its initials in German) are a technical framework for the construction and design of road sections published by the German Road and Transportation Research Association (FGSV from its initials in German). This directive sets the width dimensions for roads belonging to the main road network on the basis of predefined standard cross-sections and as a function of traffic load (Pietzsch & Wolf, 2000). Thus, three cross-section categories were defined based on the annual average daily traffic (AADT) and they are shown in Table 3.7.

Table 3.7 Cross-section width categories for motorways and federal roads.

[11] Although pedestrians are the focus of this argument, it is recognized that street concentration levels also have influence on indoor and in-vehicle concentrations, and, therefore, on human exposure. However, it is considered that this assumption is adequate for addressing air quality issues.

AADT	Assumed road width [m]
< 30 000	20
30 000 – 60 000	30
> 60 000	36

3.5.3.2 Building height

Urban building geometry varies along a broad spectrum reflecting the unique historical urban development of each city. Unfortunately, detailed data concerning this feature are still scarce due to the large costs required to process high-resolution elevation data gained through laser scanning aerial surveys, which have to be complemented with building outlines and heights for obtaining accurate digital elevation models[12]. Although comprehensive quantitative analyses are rather scarce, there has been some research looking into this topic. Theurer (1999) analysed typical building arrangements along urban roads for three cities in south-western Germany: a small town with 50 000 inhabitants, a medium-sized city with about 160 000 inhabitants and a large city (300 000 inhabitants). In this study, Theurer reports average building heights from 10 to 15 metres (excluding city centres). Thus, taking into account the average values for road width and building height provided in this section and the transition threshold values for choosing dilution functions, Figure 3.20 provides an overview of the area of application of each road type: road type 3b applies for building height/road width combinations above the dotted line; road type 3a should be used for building height/road width combinations below the dotted line.

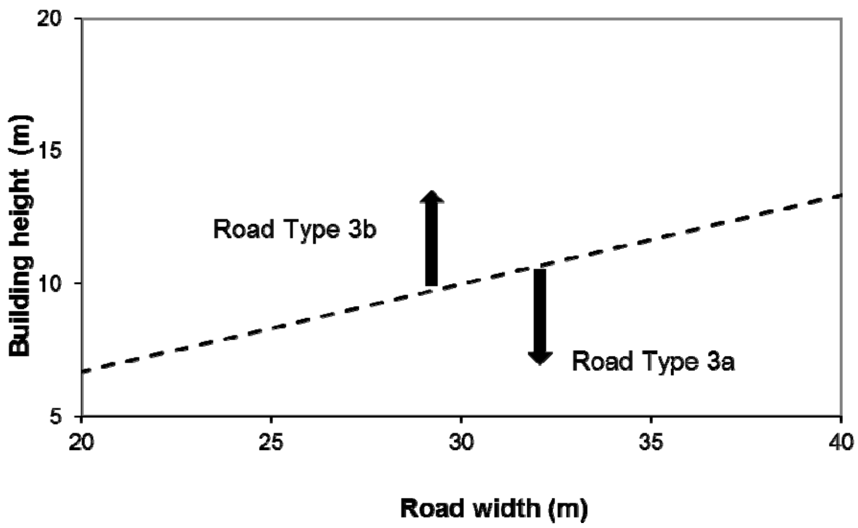

Figure 3.20 Transition threshold for dilution functions.

[12] Whilst the investment may not be feasible for research projects, local authorities and consultants may be able to implement relatively simple methods for extracting detailed building geometry data for small domains (Kettemann, 2004).

From this figure, the road type most likely to be found is 3b, as the larger diagram area above the dotted line suggest. However, considering that this road type represents the worst case scenario for the dilution of pollutants and that its implementation would likely lead to an overestimation in pollutant concentrations, it was decided to use the road type 3a instead. Another reason supporting this argument is that pavement width should also be added to the road width, meaning that the total distance between the road axis and the building façade is larger than the values presented in Table 3.7. Using Equation 3.6, Equation 3.7, and the assumptions presented above, the additional PM_{10} concentrations for the main road network are presented in Figure 3.21.

It may be suggested that, analogue to the procedure carried out for the urban increment model, the concentration estimates computed by the third tier of the model should be corrected to avoid double-counting as well. Yet, because the parameterised model provides only the additional concentration generated by road traffic and it assumes that there is a subjacent urban background concentration, it is concluded that double-counting in this tier can be neglected. Finally, similar as with the first two tiers of the hybrid modelling approach, a comprehensive validation of the computed results by comparison with physical measurements is presented in Chapter 4.

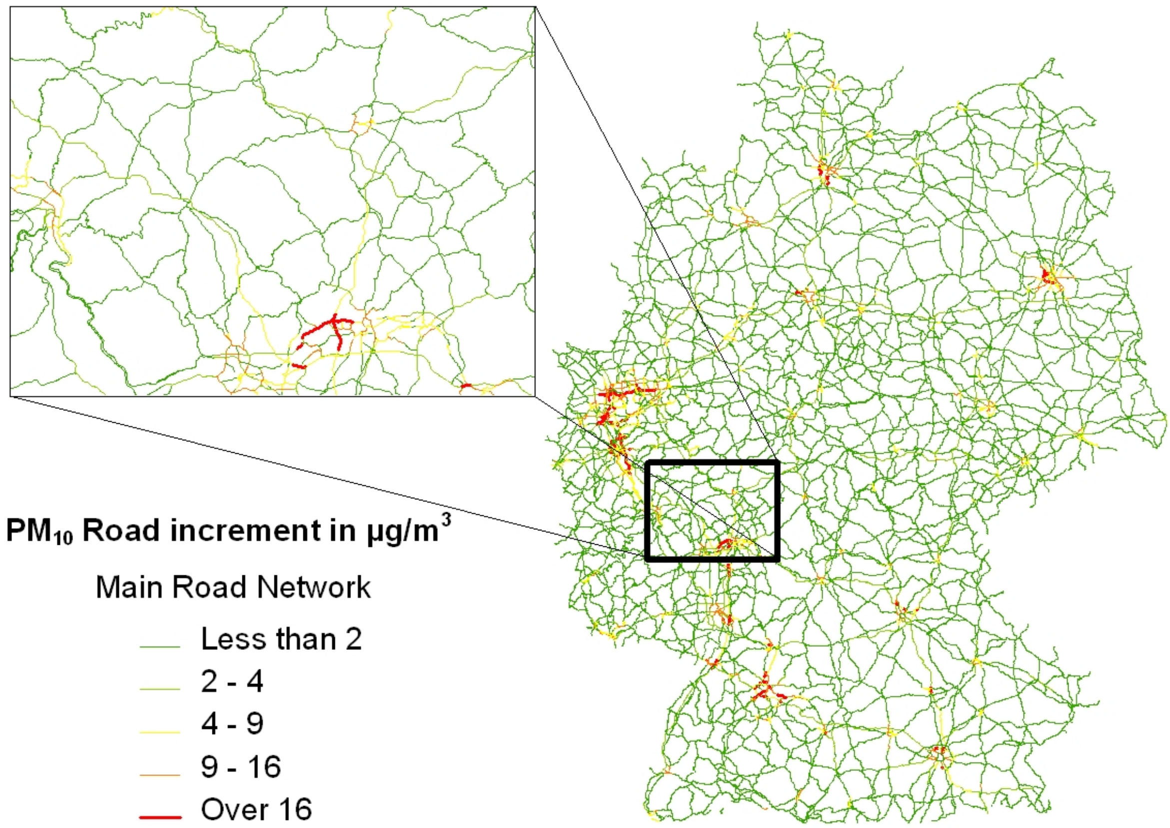

Figure 3.21 Modelled PM_{10} increment near major roads

3.6. Road increment concentration - Urban streets

So far, the third tier of the hybrid dispersion modelling approach has dealt with two roads categories: roads belonging to the main road network inside and outside urban areas. Yet, the remaining road category, i.e., urban streets, represents an even larger challenge as urban morphology is an important factor that influences pollutant dispersion within urban areas. Many studies dealing with dispersion of vehicle emissions in street canyons have been conducted over the last two decades (e.g., Aquilina & Micallef, 2003; Berkowicz & Hertel, 1997; Heida et al., 1989; Karathanasis, Simeonidis, & Ziomas, 2001; F. Mensink, Lefebre, Janssen, & Cornelis, 2006; Taseiko, Mikhailuta, Pitt, Lezhenin, & Zakharov, 2009). However, a rigorous treatment of urban streets in dispersion models requires information not only about vehicle flow and composition but also parameters like street geometry, orientation, building height, presence of trees and pavement condition. The lack of comprehensive vehicle flow data, which has been extensively discussed in section 2.4.2, is a relevant factor hampering detailed dispersion modelling. Furthermore, since pollutant concentration increases in street canyons as the aspect ratio (ratio of building height to street width) increases, urban building morphology is another important factor to consider. Urban building morphology also varies along a broad spectrum and, although detailed data concerning this feature has become more accessible over the last decade due to the increasing popularity of Digital Elevation Models (DEM), their availability for research purposes is still strongly limited.

Thus, it is clear from the arguments presented above that a deterministic approach for modelling each urban street in each large German city is currently not feasible. On the other hand, stochastic modelling approaches represent an alternative when many relevant factors are not entirely known and, therefore, a stochastic approach by means of a Monte Carlo simulation method is applied in this thesis to evaluate the additional pollutant concentration for urban streets.

For this purpose, a simple deterministic model for calculating pollutant concentrations near streets serves as the basis for building a stochastic formulation of the problem. Essentially, the deterministic model is turned into a stochastic model using random values as inputs. A comprehensive description of the Monte Carlo model structure and input data is presented in the following section.

3.6.1 Monte Carlo simulation

Earlier in this work, it was shown that a semi-empiric model can estimate additional concentrations near roads with good results, provided that street morphology, local meteorology, fleet composition, and vehicle flow are known. It was also argued that the collection of such an amount of data for a large number of streets for all major cities in Germany would take too much effort.

In the view of these difficulties, a Monte Carlo (MC) simulation using the aforementioned deterministic model as the underlying basis was used; that is to say, the input parameters of the deterministic model are described by means of probability density functions and a single set of input data is randomly generated following the corresponding distribution. After running the model, one output dataset is obtained and stored, subsequently creating a new set of input data and their corresponding output. These steps are repeated until the probability distribution of the results is not significantly influenced by an additional run. Finally, the entire set of results is analysed and conclusions are derived.

The MC simulation presented in this research analysed 10 000 runs for each urban entity. For these calculations, an infinite sequence of random numbers (with respect to the size of the problem) is needed. Although there is no such a thing as a truly random number, sound algorithms exist for the generation of pseudo-random numbers that satisfy the essential properties of the actual random numbers. In this way, random numbers uniformly distributed between 0 and 1 were used to simulate the parameter distribution. It should also be mentioned here that it would be impossible to infer a probability distribution with only one realization of the phenomenon in space and time. An important assumption is, therefore, that the underlying random probability function remains stationary for the time it is investigated, i.e. it remains stationary and the model assumes that the probability distribution does not change when shifted in time or space.

The CI dispersion model, which was described extensively in section 3.5.2.1, was used as the underlying deterministic model to build the stochastic simulation algorithm. Equation 3.7 can be then rewritten as follows:

$$C_{roadside} = AADT \cdot EF \cdot \theta \cdot w \cdot f \qquad \text{Equation 3.9}$$

where $C_{roadside}$ is the additional pollutant concentration due to the vehicles that travel on a specific street; AADT is the Average Annual Daily Traffic; EF is the emission factor; *w* is a wind factor related to average wind speed; *f* is a tree factor; and θ is a dilution factor, which is computed using Equation 3.8.

It is important to note that earlier in this work two of the parameters in Equation 3.9 have been defined for each urban entity: the wind factor, which was computed using annual average wind speed; and average emission factors, which were determined by dividing the amount of vehicle-related pollutants released within each urban entity by the corresponding vehicle kilometres travelled. As both parameters have been extensively discussed in sections 2.4.2 and 3.4.2.4, the analysis in this section focuses on the remaining three variables: dilution function (θ), Average Annual Daily Traffic (AADT), and tree factor (F).

In order to serve as input for the stochastic model, the three parameters have to be defined by means of Probability Density Functions (PDF)[13]. Given that none of the variables analysed has a known PDF, a crucial task was to find the underlying PDF for each variable. A commonly used procedure to achieve this goal is to fit observed distributions to a theoretical distribution by comparing the frequencies observed in the data and the theoretical distributions. Thus, available random samples of observational data were assumed to come from several theoretical distributions and goodness-of-fit tests were carried out by comparing the frequencies observed in the data to the expected frequencies of the theoretical distribution. Goodness-of-fit tests indicate whether or not it is reasonable to assume that a random sample comes from that particular distribution. In this research, two methods are used to evaluate the goodness-of-fit: a visual evaluation of the hypothetical distribution using probability plots and a more rigorous statistical test for examining the distribution assumptions.

[13] A probability density function for a continuous random variable is a function that describes the relative likelihood for this variable to occur at a given point.

A visual evaluation allows to qualitatively assessing if a given set of data follows some specified distribution. A histogram allows a quick visualisation of the data distribution but a comparison across different distributions can be difficult. Another method used to find out if a given sample of data follows a hypothesised distribution is the probability-probability plot (P-P plot). The P-P plot is constructed mapping two cumulative distribution functions against each other, i.e., the observed data against a theoretical distribution. If both probabilities closely agree, then the points should approximately depict a straight line. Departures from this straight line indicate departures from the specified distribution. In this way, P-P plots can be generated for several distributions to see which provides the best fit.

A formal statistical test was also conducted: the Kolmogorov-Smirnov test (in the following referred as K-S). The K-S is a non-parametric test designed to assess the goodness of fit of a data sample to a hypothesised continuous distribution. It is based on the computation of the maximum distance between the empirical and the theoretical cumulative distribution function, which is called the K-S statistic D value. If the calculated D value is greater than the critical value at a certain level of confidence, the two distributions are significantly different in a statistical sense (Davis, 2002).

In the following sections, observational data for each variable is analysed and hypothesis about their specific distribution are formulated and tested using the methods described above.

3.6.1.1 Dilution functions

Street morphology is defined within the CI model by means of the average height of the surrounding buildings (H) and the distance between the road axis and the building façade (L). According to the definitions provided in Table 3.4, the ratio L/H is used as discriminator for selecting the dilution function. The pragmatic approach would have been to select the street-type 2 for all cases, since detailed street morphology data do not exist. However, considering the CI model results presented in section 4.4.42, this would have lead to a systematic under estimation of pollution levels at the street level. Aiming at finding how often the street types 3a and 3b are expected to occur, distribution functions for street and sidewalk width along with building height were explored using available data.

a) Street and sidewalk width

Earlier in this work, several cross-section width categories for major roads were defined based on the annual average daily traffic (see Section 3.5.3). However, street width varies across a wider range due to heterogeneous requirements related to urban mobility. As a consequence, the street and sidewalk width of about fifty streets (one hundred streets for larger UE) randomly selected from nearly thirty urban entities were estimated using satellite images freely available from Google Earth mapping services. Given that the resolution of most satellite images in Google Earth allows a clear distinction between the individual components of the street, it was possible to measure the streets and sidewalks with acceptable accuracy. Care was taken to evaluate only streets within the urban entities defined in Chapter 2 and, since roads belonging to the main road network were already addressed in 3.5, they were also not included in the sample. The resulting histograms for four urban entities are presented in Figure 3.22.

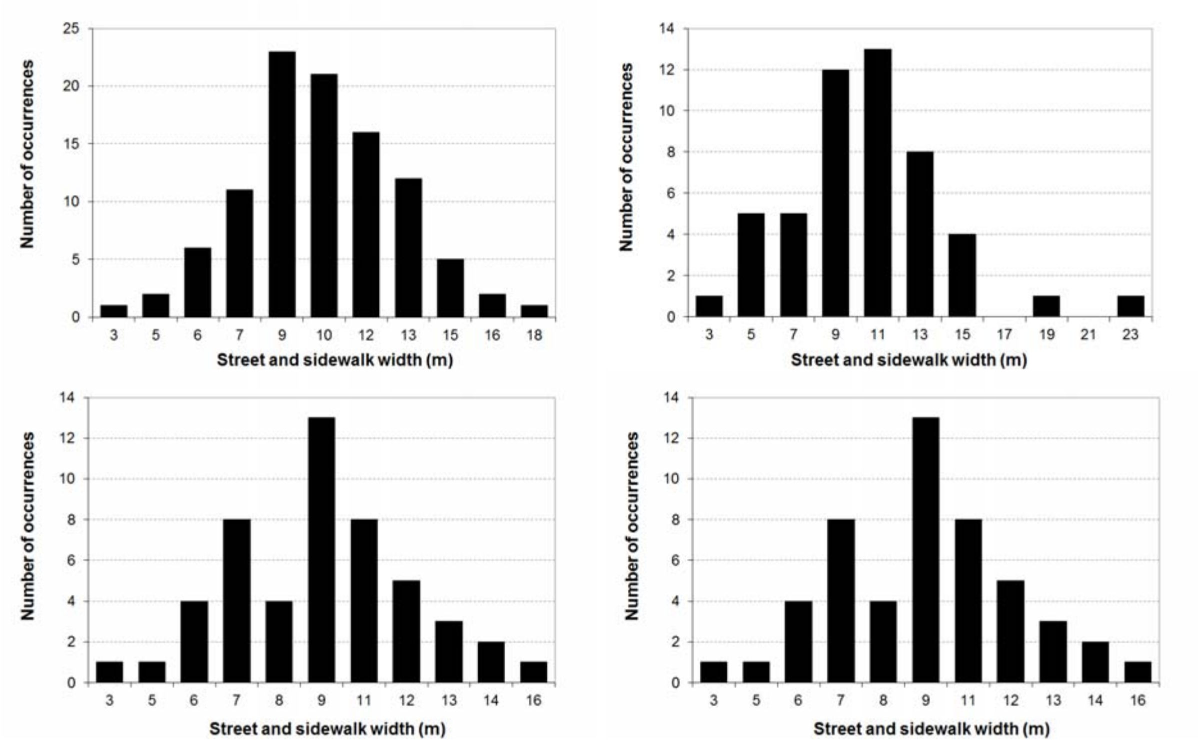

Figure 3.22 Histograms depicting occurrence of street and sidewalk width for four urban entities.

Afterwards, each sample was tested for normality using the K-S test and the results of the analysis are presented in Table 3.8. On the basis of these results, it was found that the normal distribution fits all samples at α = 0.05 significance level. Therefore, the normal distribution was adopted for the street and sidewalk width parameter. Furthermore, the overall mean value was assumed to be 8.7 metres with a standard deviation of 2.7.

Table 3.8 Street and sidewalk width in metres for several UE and goodness-of-fit results.

UE ID	n	Mean	Standard Deviation	K-S test	
				D-value	Critical value α = 0.05
12396	100	9.53	2.68	0.06365	0.13403
13371	50	9.28	3.68	0.09329	0.18841
13469	50	8.80	3.30	0.07964	0.18841
13594	50	8.88	2.60	0.08827	0.18841
14083	60	7.37	2.75	0.0714	0.17321
14384	50	9.11	2.03	0.08215	0.18841
15218	75	8.53	2.22	0.06856	0.15442
16115	100	8.55	2.37	0.09425	0.13403
16601	50	9.15	3.14	0.06488	0.18841
16729	50	7.98	3.35	0.08838	0.18841
16849	50	8.41	2.42	0.0641	0.18841
17151	50	9.81	2.98	0.08707	0.18841
19074	50	9.17	3.04	0.07996	0.18841
19372	100	7.79	2.42	0.10517	0.13403

19596	50	7.97	1.99	0.12365	0.18841
20489	50	8.72	1.96	0.08112	0.18841
22660	50	8.15	3.36	0.09398	0.18841
22770	100	9.79	3.86	0.1176	0.13403
24638	50	8.23	2.55	0.08698	0.18841
24642	100	9.43	2.39	0.1323	0.13403
24767	50	9.53	2.45	0.09542	0.18841
25006	50	8.56	1.99	0.07882	0.18841
25736	50	8.36	2.56	0.08601	0.18841
25868	100	8.29	2.26	0.06521	0.13403
25914	50	9.32	2.19	0.08477	0.18841
26759	50	7.61	1.98	0.06549	0.18841
26920	100	8.28	3.16	0.06491	0.13403
32700	50	10.21	3.31	0.06664	0.18841
Average		**8.7**	**2.68**		

b) Building height

As building height plays an important role in the definition of dilution functions, an average value of deterministic nature was estimated for this parameter in section 3.5.3. However, an average value is not sufficient to characterise the variable building height. Ideally, a representative sample of this parameter should be analysed to fit a probability distribution to the observed data. Given that a suitable representative dataset was not available for this work, an alternative approach was used in which a uniform distribution for this parameter was assumed. The rationale behind this decision lies in the lack of representative data and, on the other hand, the feasibility to determine the upper and lower bounds for said distribution using values found in the literature. It is recognized that this decision adds uncertainty to the model, yet it is important to remark that building height is needed only to choose the dilution function and it has no further influence on the estimation of the receptor location, which depends solely on street and sidewalk width. Moreover, it is evident from Figure 3.20 that the dilution function is more sensitive to changes in road width than to changes in building height. In view of these arguments, a uniform distribution was chosen for the parameter building height.

Concerning the lower bound, a value of 3 metres was assumed, which corresponds to the height of a typical one-story building. As for the upper bound, Theurer (1999) analysed typical building arrangements along urban roads for three cities in south-western Germany: a small town with 50 000 inhabitants, a medium-sized city with about 160 000 inhabitants and a large city (300 000 inhabitants). Despite differences in city size, Theurer found that the average building height in the city centres (18 - 21 metres) did not vary significantly between the cities under study. This correlates fairly well with results provided by other authors regarding German cities. For instance, Ratti et al. (2006) calculated the average building height of 18.6 metres for a city centre area in Berlin making use of digital elevation models; Lachat et. al. (1997) analysed a large building height dataset for Munich, Germany and they report a value of about 17 metres. Furthermore, Valcarce et al. (2007) measured an average building height of 20 metres for a central area in the German city of Saarbrucken. Moreover, based on a number of studies, these values may not change significantly within Europe, e.g., Ratti et al. (2006) reported a value of 15.3 metres for Toulouse and Long et al. (2003) report an average building height of 15 metres in Marseille city centre and 10 metres in the peripheries. However, higher values may be found outside Europe, as Burian et al. (2002) and Ratti et al. (2002) noted.

Yet, the building height estimates presented above refer for the most part to city centres where, as noted by Theurer (1999), the highest buildings are commonly located. This development can be explained by what economists call rent gradient, which indicates the rate at which the value of urban land declines with distance from the city centre (Moses & Williamson, 1967). Due to higher land prices in areas closer to city centres, these areas tend to be used more intensively in the centre than at the peripheries. For this reason, most large cities display a building height profile that is similar to their rent profile, being highest in the city centre and tending to decline when moving away from it (Lipsey & Chrystal, 2007). Taking this observation into account, it is evident that the average building height of city centres cannot be considered as representative of whole cities. Nevertheless, the values presented above provide insight into the upper bound of this parameter.

3.6.1.2 Average annual daily traffic

The second variable to be analysed is the Average Annual Daily Traffic (AADT). AADT is a fundamental traffic statistic for planning, designing and maintaining roads. Since this parameter is considered in the road design phase, one can only expect that when the road is in operation, a close relationship between geometry and AADT persists. Indeed, one can find that when a road exceeds the projected AADT, the road has to be improved or users have to be provided with alternatives in order to maintain the desired level of service and security standards. This procedure also holds true for urban roads where the alternatives range from speed limitations to vehicle access restrictions to certain areas.

As already mentioned elsewhere in this work, freely available, comprehensive urban AADT datasets are rather scarce, posing a serious limitation for the analysis of this parameter. Nevertheless, it was possible to analyse three AADT datasets for the German cities of Berlin, Stuttgart and Münster. The datasets containing the AADT by road segment were sampled to analyse the frequency with which a certain AADT-value occurs. The resulting histograms for the three cities are presented in Figure 3.23.

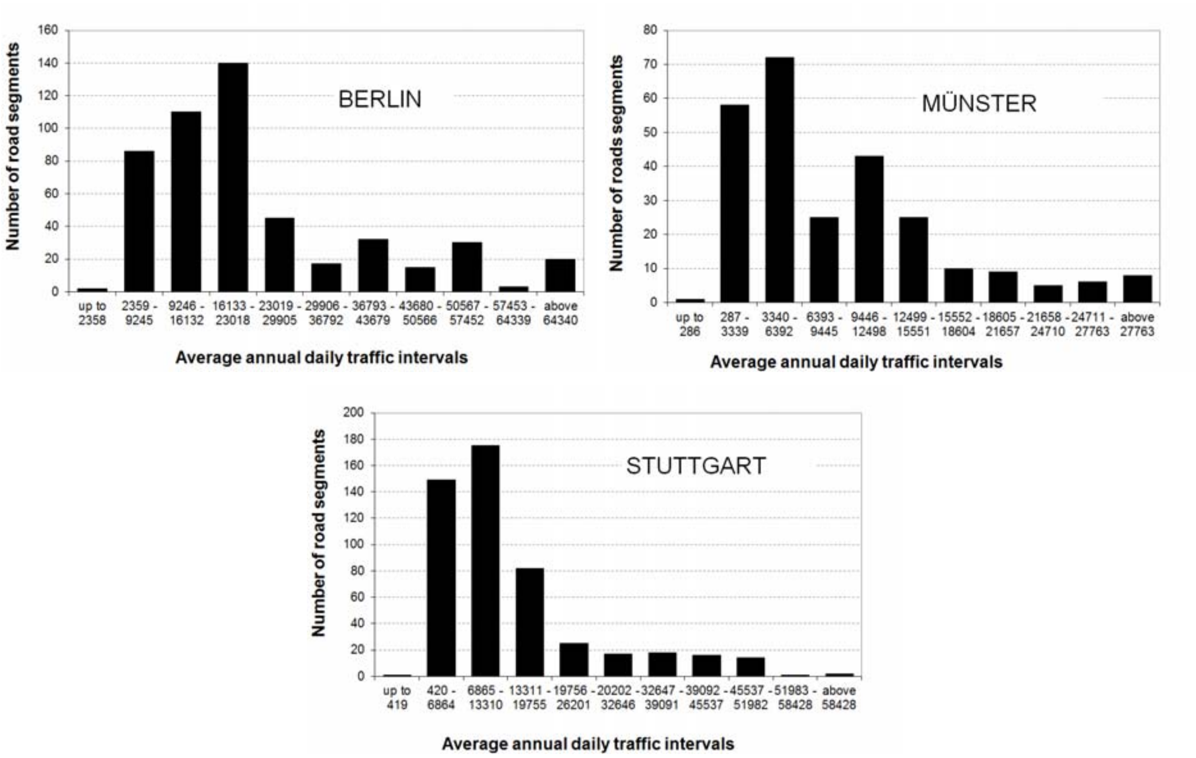

Figure 3.23 Histograms depicting the number of road segments (occurrence) with a certain average annual daily traffic intervals for Berlin, Münster and Stuttgart.

From this figure, it is interesting to see that the AADT variable does not follow a normal distribution. Moreover, the first histogram bin depicts a small number of occurrences for low AADT. The reason for this lies in the fact that information about vehicle volume is frequently concentrated on streets with a high volume of traffic. This is reasonable as those streets are relevant not only for addressing environmental issues but for many transportation planning, design, operation, and maintenance activities as well. Therefore, it is likely that the number of occurrences for low AADT is underestimated in the three datasets. Given that the Berlin dataset provided the more comprehensive information from the three dataset, this dataset was chosen for defining the probability distribution and the results were tested afterwards using the other two datasets. The Berlin dataset, which was retrieved from the website of the Senate Department for Urban Development Berlin (2008), comprises detailed information related to AADT, concentrations and other parameters relevant for addressing air quality issues. Several hypothetical distribution functions were tested for fitting the distribution of a random subsample of the AADT dataset. It is important to note that because concentrations near major roads were already estimated (see Section 3.5), motorways and federal roads were not considered in the subsample. Figure 3.24 depict the P-P plots for some of the tested distributions.

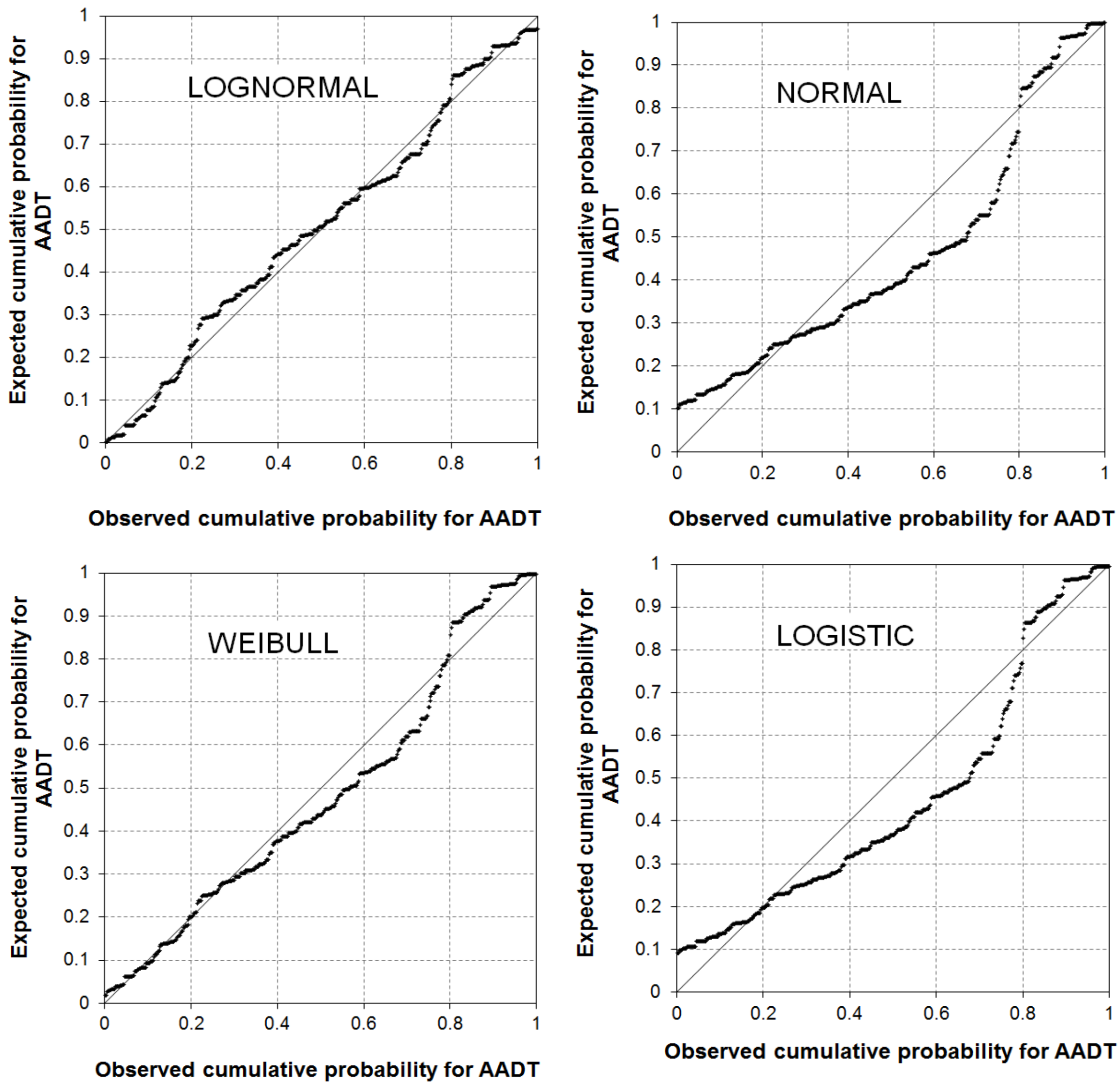

Figure 3.24 P-P plots of the average annual daily traffic (AADT) in Berlin for different probability density functions.

Figure 3.24 shows that while the lognormal P-P plot is approximately linear, large differences can be seen for the Normal, Weibull and Logistic functions. In order to further test the hypothesis that the variable AADT is better described by a lognormal distribution, a formal statistical K-G test was carried out. The results are depicted in Table 3.9 and they support the hypothesis suggested, albeit at $\alpha = 0.02$ significance level, which is lower than the significance obtained for street width.

This assumption was tested using a sample of the other two datasets: Münster (Schneider, Niederau, Fafflok, & Nacken, 2007) and Stuttgart (Ohlau, 2009). The P-P plots of the samples against the lognormal distribution are shown in Figure 3.25. Both plots show deviations from the straight line larger than those observed in the Berlin dataset. A reason for this development might be that both datasets are not as detailed as the Berlin dataset and thus, a certain bias towards urban streets with high traffic volume can be expected.

Table 3.9 Goodness-of-fit results for AADT Berlin (n= 500).

Distribution	K-S test D-value	Critical value at α = 0.05	Critical value at α = 0.02
Lognormal	0.06594	0.06073	0.06789
Normal	0.1825	0.06073	0.06789
Weibull	0.14443	0.06073	0.06789
Logistic	0.18339	0.06073	0.06789

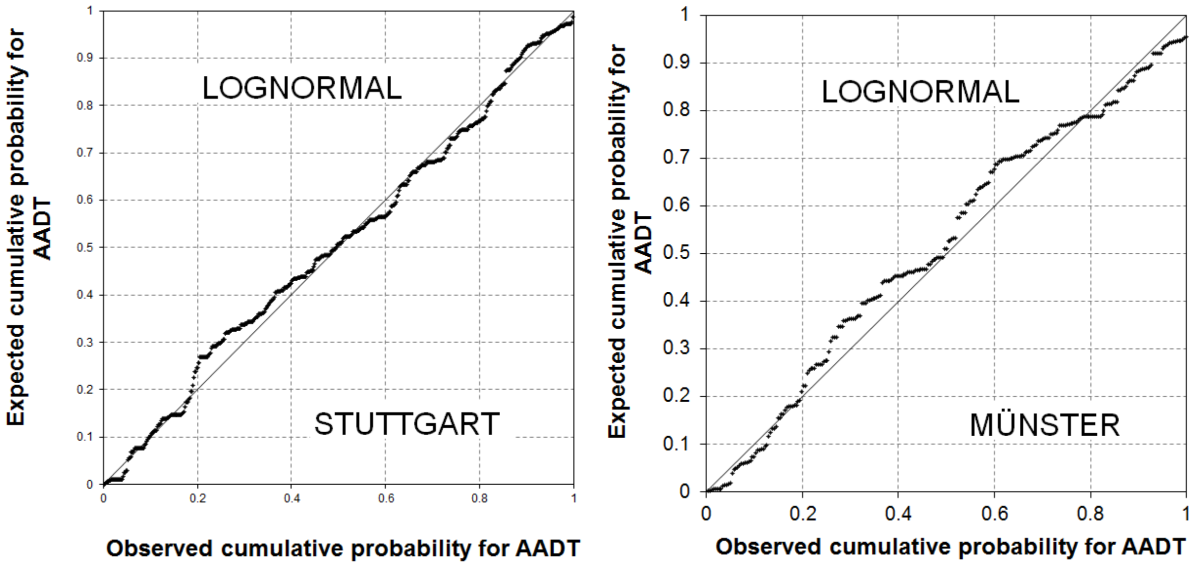

Figure 3.25 Lognormal distribution P-P plots for the cities of Stuttgart and Münster.

A formal statistical Kolmogorov-Smirnov test was also carried out to both samples and the results are presented in Table 3.10.

Table 3.10 Goodness-of-fit results for Stuttgart (n=500) and Münster (n=262).

Distribution	K-S test D-value	
	Stuttgart [b]	Münster [c]
Lognormal	0.06403	0.08684
Normal	0.18376	0.14941
Weibull	0.09899	0.06561
Logistic	0.19312	0.16794

[b] Critical value at α = 0.05 is 0.06073 and at α = 0.02 is 0.06789
[c] Critical value at α = 0.05 is 0.0839 and at α = 0.02 is 0.09378

Looking at the results presented in this section, the Weibull distribution actually passes the K-G test for Münster but fails to provide the same results for Stuttgart and Berlin. On the other hand, the lognormal distribution hypothesis was accepted in the three cases at α = 0.02 significance level. In view of the results presented in this section, it seems feasible to assume that the average annual daily traffic better described by a lognormal distribution. Thus, this distribution is used in the Equation 3.9.

3.6.1.3 Tree factor

The third and final variable to analyse in order to find a suitable probability distribution is the tree factor. Emissions released by plants represent a vital part of life on Earth, interacting with the environment and helping in a myriad of replenishing processes in the atmosphere. Hence, trees in urban areas play a significant role in improving urban life, not only by reducing energy use, runoff and removing air pollutants by dry deposition (Nowak, Crane, & Stevens, 2006; Xiao & McPherson, 2002) but also by enhancing human health and emotional well-being (Kaplan, 2007; Smardon, 1988). Regarding CO_2, trees act as a sink for this pollutant by fixing carbon during photosynthesis and storing excess carbon as biomass (Nowak & Crane, 2002).

Nevertheless, trees also affect wind speed at street level and, therefore, the CI dilution functions account for this effect by introducing a tree factor (den Boeft et al., 1996). Values for this parameter are given in Table 3.11.

Table 3.11 Tree factor definition.

Tree factor	Definition
1	Some trees or not at all
1.25	One or more rows of trees with a separation between trees smaller than 15 meter and gaps between the tree crowns
1.5	The tree crowns touch each other and cover at least one third of the road width

Source: Teewisse, 2006.

An accurate definition of the distribution function of this factor was not possible due to data availability. Nevertheless, given that the highest tree factor represents a large increment on the concentrations (50%) and that the uncertainty regarding the actual tree coverage is large, a pragmatic approach was taken. So as to avoid overestimation due to highly uncertain assumptions, the tree factor is described by means of a uniform function, using 1 and 1.5 as lower and upper boundaries, respectively.

3.6.2 Results – Road increment for urban streets

In the last sections, the variables needed for the Monte Carlo simulation were discussed and appropriate probability density functions for each of them were estimated. A summary of the results is presented in Table 3.12.

Table 3.12 Summary input data for the Monte Carlo Simulation.

Variable name	Condition	Distribution shape
AADT	Probabilistic	Lognormal
Emission factor	Deterministic	*Not required*
Wind factor	Deterministic	*Not required*
Dilution function	Probabilistic	Street width – normal Building height - uniform
Tree factor	Probabilistic	Uniform

Using the variables depicted in the aforementioned table and Equation 3.9, a Monte Carlo simulation was carried out for estimating the additional concentration at roadside within urban entities. In order to perform the thousands of MC simulations required for each urban entity in a more efficient way, a VBA (Visual Basic for Applications) program was developed in this thesis. It is important to keep in mind that the Monte Carlo simulation generates a large number of possible scenarios using all valid combinations of possible inputs to simulate all possible outcomes, resulting in a distribution of possible outcomes. In this sense, the probabilistic approach provides robust estimates which account for uncertainty in the input parameters. To illustrate this concept, consider the cumulative probability plot for Berlin presented in Figure 3.26. The cumulative probability provides the range of possible additional concentrations that could occur at any street roadside within Berlin (excepting major roads) and the likelihood of any concentration to occur. As an example, it is estimated that there is a 95% probability that the additional PM_{10} concentration at roadside in Berlin will be lower than 8.5 µg/m^3.

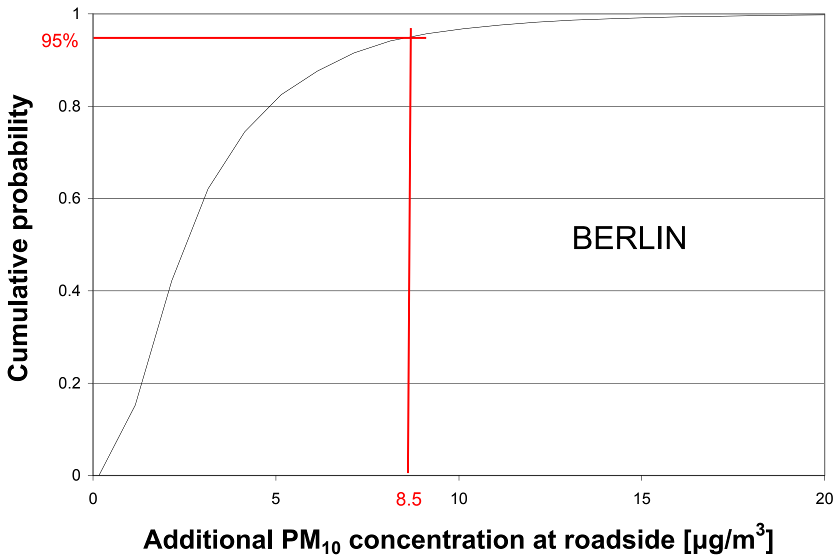

Figure 3.26 Cumulative distribution function of the additional PM_{10} concentration at roadside for Berlin.

An analogous analysis was carried on the MC simulation results for each urban entity and the mean of these values for the three most relevant vehicle-related pollutants, i.e., PM10, PM2.5, NOX, and NO2 are presented in Figure 3.27 and Figure 3.28.

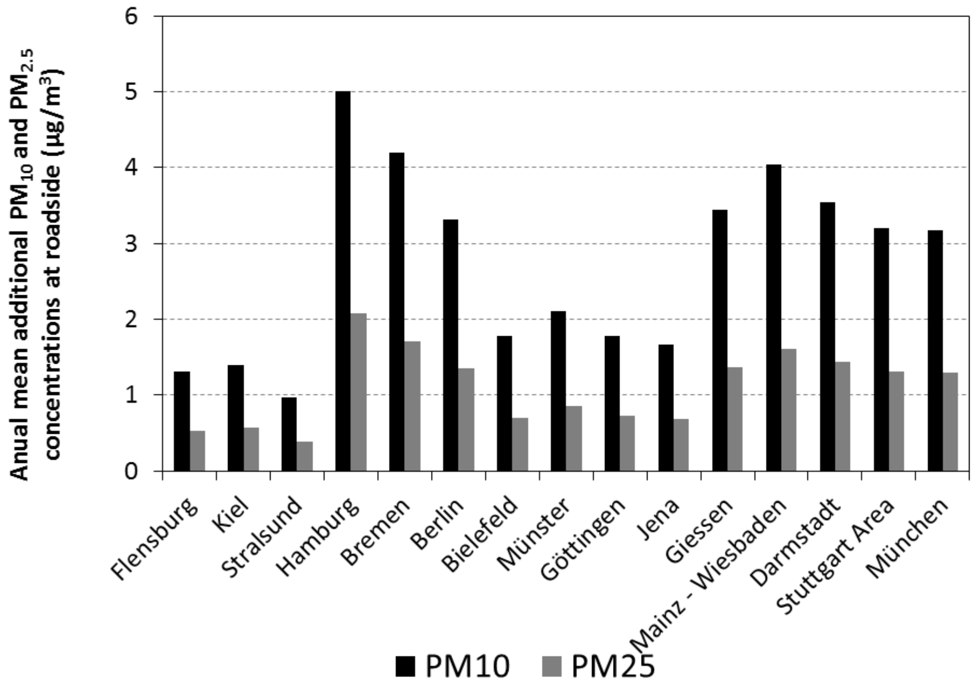

Figure 3.27 Annual mean additional PM_{10} and $PM_{2.5}$ concentrations at roadside for several urban entities.

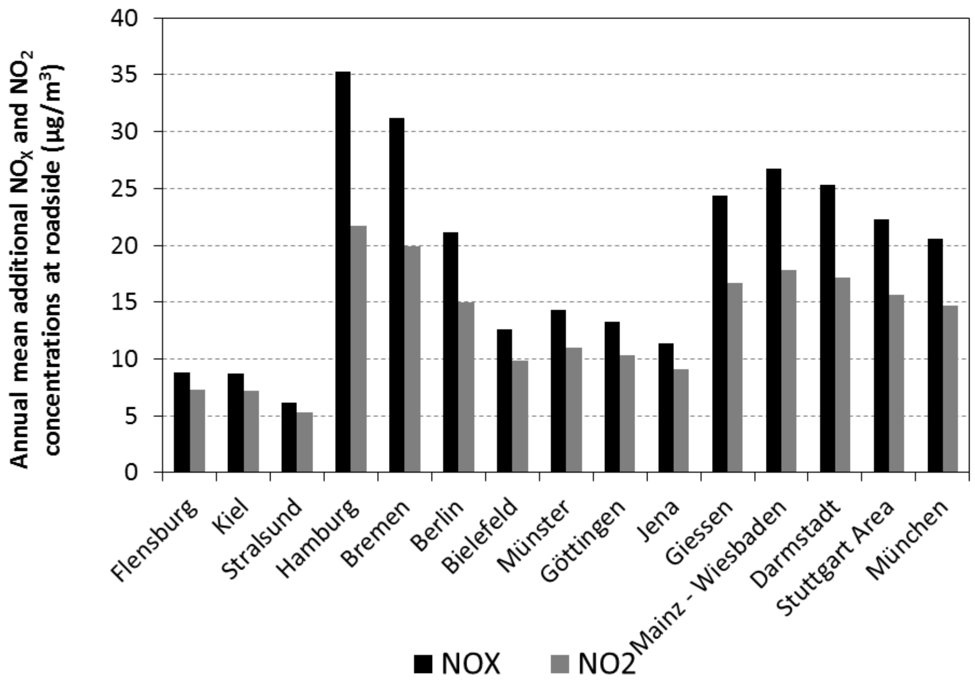

Figure 3.28 Annual mean additional NO_X and NO_2 concentrations at roadside for several urban entities.

There are several advantages of using a stochastic approach for assessing the additional burden related to vehicle activity within urban areas and, when facing the challenge of analysing a large number of areas, one of the most important virtues is certainly the relatively low data requirements. It is also noted that, whereas this approach does not allow for assessing specific streets within the city, it provides information about the probability that a specific pollutant concentration value occurs within the urban entity. In this way, not only it is possible to assess air quality but also the probability of having values greater than a certain threshold, which is relevant for evaluating air quality regulations. Furthermore, changes due to implementation of emission reduction measures, i.e. emission scenarios, can be readily analysed.

It may be suggested that the concentration estimates computed by the third tier of the model should be corrected to avoid double-counting. However, as it was already discussed earlier in this work, the CI dilution functions provide only the additional concentration generated by road traffic assuming that there is a subjacent urban background concentration. Thus, it seems reasonable to conclude that there is no double-counting in this tier of the analysis. Finally, a comprehensive validation of the results by comparison with physical measurements is presented in Chapter four of this work.

3.7. Application of the model – Urban air quality in Germany in the year 2005

The relevance of assessing urban air quality along with the myriad of challenges that a detailed analysis entails have been discussed throughout this thesis. In an effort to address this complex task, a hybrid dispersion modelling approach was developed in this work for predicting air quality across different spatial scales: from regional to urban and near-roads scale. So far, a comprehensive description of the modelling approach structure, input parameters, and assumptions has been presented. In this section, the partial results for each tier of the modelling are brought together in order to give insight into the urban air quality levels within large urban areas in Germany in the year 2005.

Annual concentrations of PM_{10} and NO_2 for the year 2005 are provided in Figure 3.29 and Figure 3.30, respectively. In order to improve the readability of the graphs, the results presented here are restricted to ten urban entities and the results for the remaining urban entities are provided as in Annex B in this work.

All figures are constructed following the same structure: the lower bar segment depicts rural background concentration estimates; the second bar segment represent the urban concentration increment; the mean additional concentration for urban streets is represented by the left third bar segment, including the 95% confidence interval obtained through the Monte Carlo simulation; finally, the right third bar segment represent the mean additional concentration estimated for the main road network (motorways and federal roads) including the 95% confidence interval.

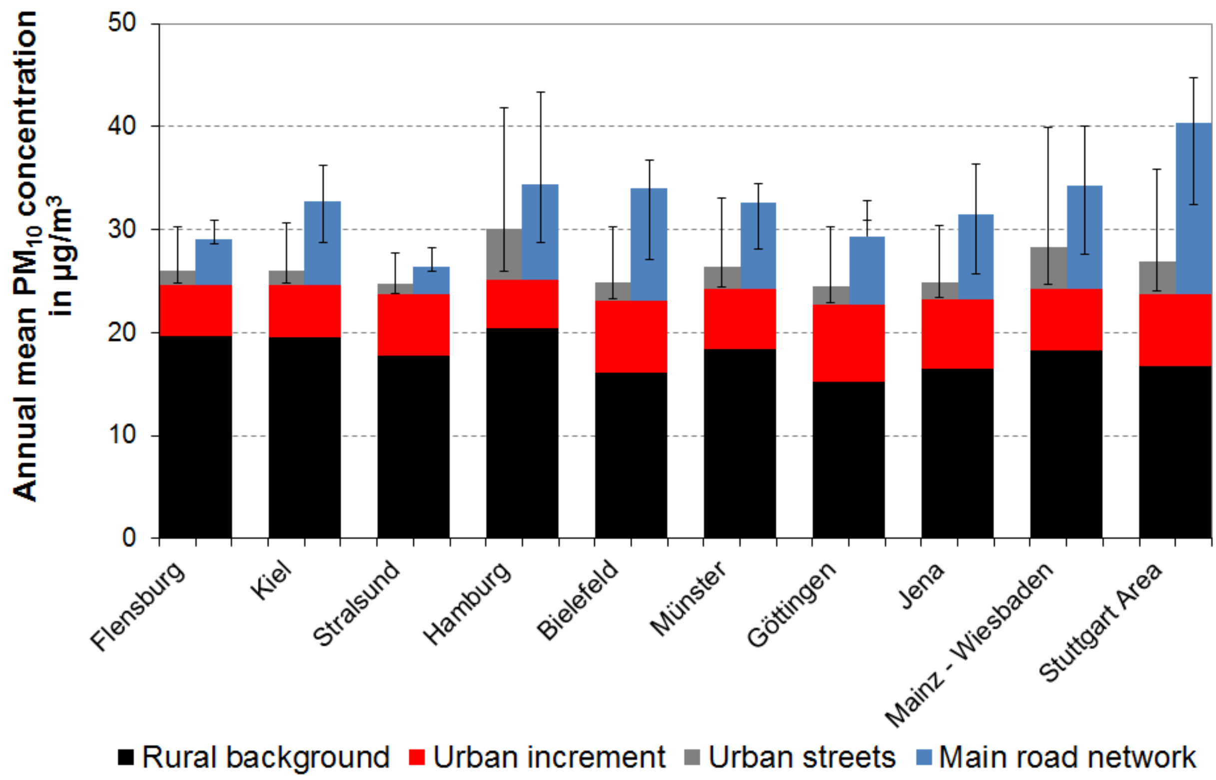

Figure 3.29 Annual mean PM_{10} concentration in ten large German urban entities.

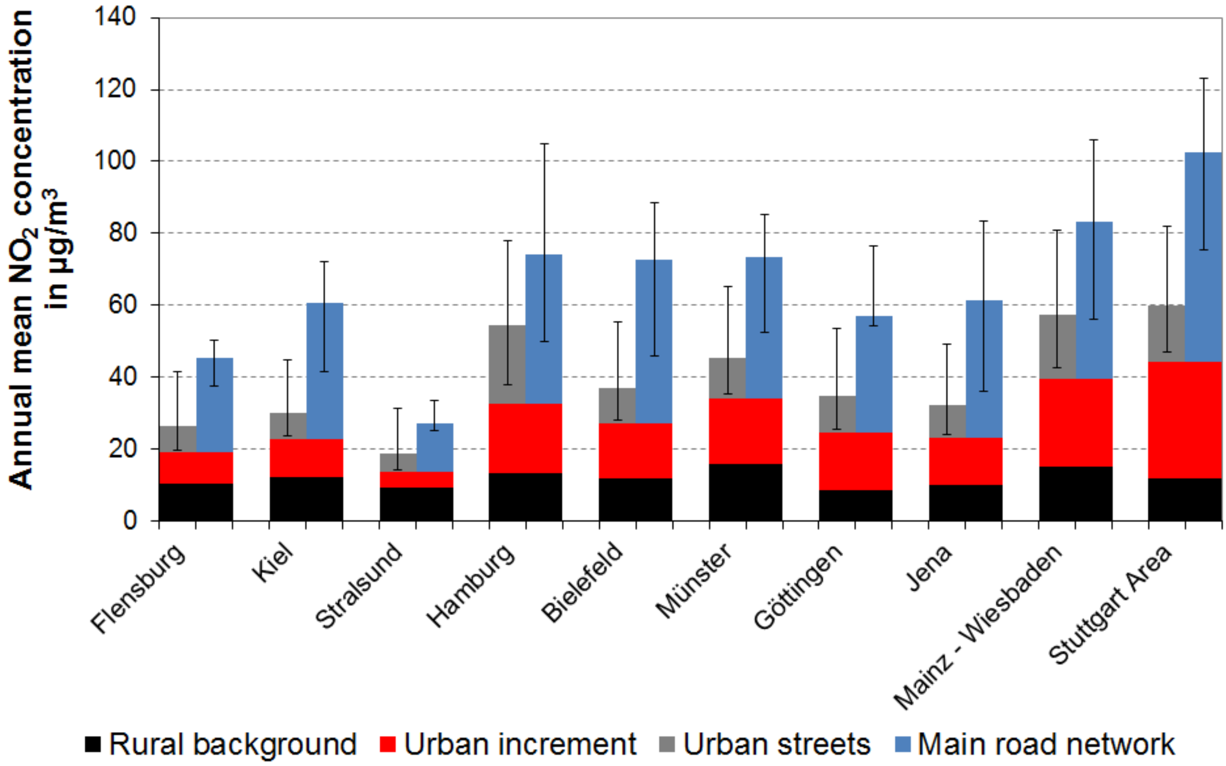

Figure 3.30 Annual mean NO_2 concentration in ten large German urban entities.

Although a detailed validation of these results by means of a comparison against measured data is presented in the next chapter, some general comments can be made upon them at this time. For this purpose, a summary of measured average annual concentrations retrieved from the European Air Quality database is presented in Table 3.13.

Table 3.13 Average annual concentrations according to the monitoring station type for the year 2005 in μg/m^3.

Pollutant	**Monitoring Station Type**		
	Rural Background	Urban Background	Traffic Urban
PM_{10}	17.7	23.4	29.9
NO_2	11.4	25.1	44.8

Source: Airbase, 2008.

Comparing the results presented in this section and the average values of Table 3.13, it can be said that, overall, the regional estimates for PM_{10} and NO_2 seem to fit quite well the average concentrations measured at the monitoring stations. As for urban background concentrations, a good agreement of the results against PM_{10} measurements is obtained, whereas NO_2 concentrations are slightly overestimated. Here it is important to keep in mind that the NO_2 urban increment was estimated using the NO_X urban increment model along with the NO_2/NO_X conversion values suggested by the Romberg model (see Section 3.4.1). Thus, given that limited data were available for developing the NO_X urban increment model, it is possible that this fact introduced a certain positive bias. Furthermore, the NO_2/NO_X conversion values also entail uncertainties which are reflected in the slight overestimation of NO_2 concentrations in urban areas.

Until now, the comparison of modelled against measured values has been carried out in a straightforward manner facilitated by the deterministic nature of both values. For assessing the concentration levels at urban streets, the mean additional concentration is used for this first comparison. As it can be expected, the trend in the modelled concentrations follows the trend set out by the urban increment. Indeed, a good agreement of the results against PM_{10} measurements is noted, whereas NO_2 concentrations are also slightly overestimated when compared with measured values at traffic urban monitoring stations. A more comprehensive comparison of the results is presented in Chapter 4.

3.7.1 Exceedances of the daily limit value of PM_{10} concentrations

The results presented in the last section give insight into the air quality levels in urban areas with a high spatial resolution, providing relevant information for assessing the compliance with air quality standards regulations. However, not all air quality directives are expressed in terms of annual values, such as the 24-hour limit value of 50 μg/m^3 of PM_{10} which is not to be exceeded more than 35 times a calendar year. In order to address this air quality standard with the modelling approach developed in this thesis, it was hypothesised that there is a relationship between the annual mean PM_{10} concentration and the number of days exceeding the daily limit value of 50 μg/m^3 of PM_{10}. In order to test this hypothesis, measured data from German traffic urban monitoring stations for both indicators were retrieved from Airbase (Airbase, 2008) and a scatter plot of the data is presented in Figure 3.31.

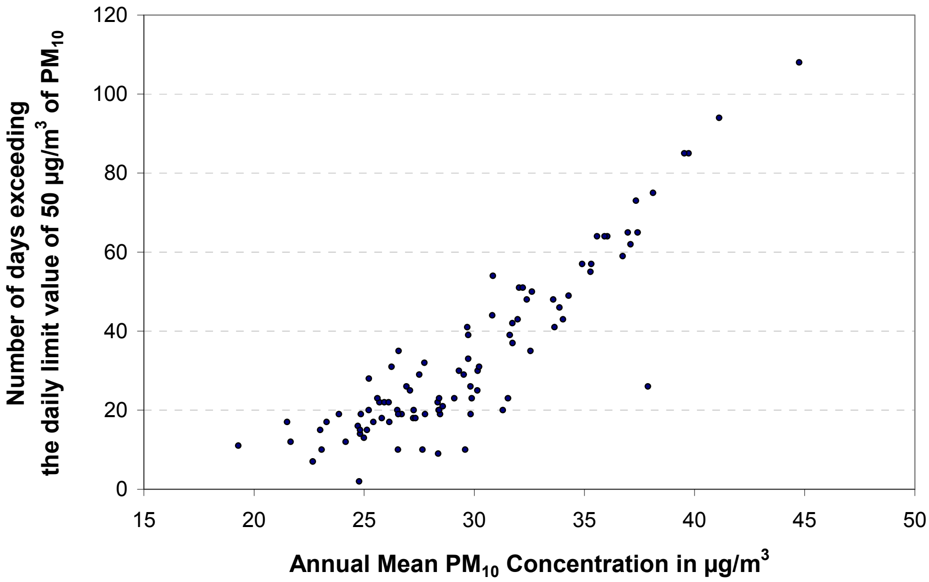

Figure 3.31 Scatter plot of the annual mean PM_{10} against the number of day exceeding the daily limit of 50 µg/m^3 of PM_{10}.

The scatter plot presented above shows that there is a strong positive correlation pattern between both indicators, which was further examined using regression analysis. For this purpose, the data were first tested for outliers using the standardized residuals or studentized residuals. From a total of 95 stations with over 80% valid values for the year 2005, only one station was identified as an outlier: a station located in the German city of Düsseldorf, which reported an annual mean of 38 µg/m^3 and 26 days of exceedances (European station code DENW082). Considering that it is not the purpose of this analysis to explain the occurrence of such unusual values but rather to provide an empiric regression function valid for average cases, the outlier was eliminated of the data. The data were then fitted to a second order polynomial curve, which gave the highest adjusted explained variance (adjusted R^2). The resulting regression function is shown in Figure 3.32.

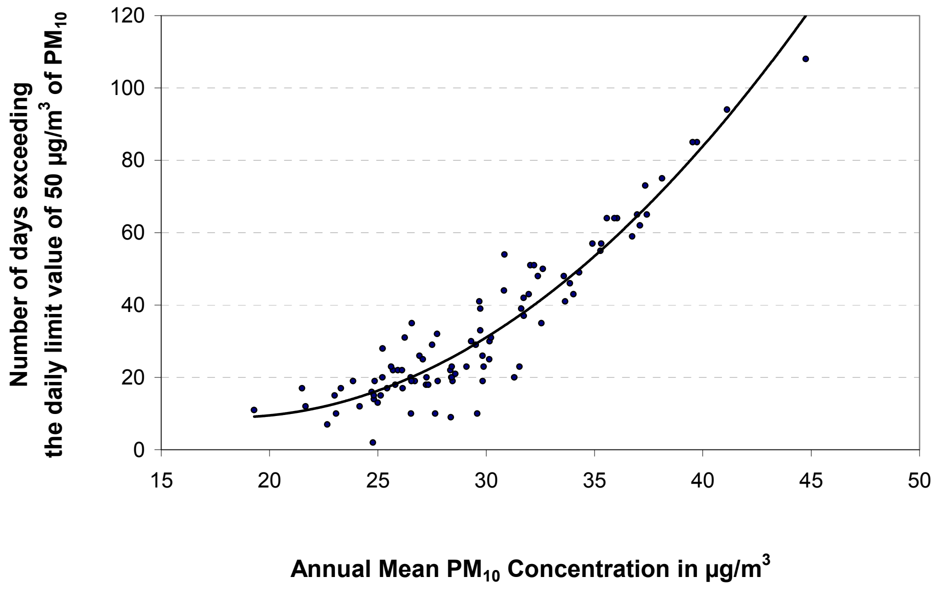

Figure 3.32 Regression function to estimate the number of days exceeding the daily limit value of 50 µg/m^3 of PM_{10} based on annual mean PM_{10} concentration.

The regression function can be written as follows:

$$\Omega = \mathrm{A}\lambda^2 + \mathrm{B}\lambda + C \qquad \text{Equation 3.10}$$

where

Ω = the number of days exceeding the daily limit value of 50 µg/m^3 of PM_{10}.

λ = the annual mean PM_{10} concentration at traffic stations.

A, B, and C = the regression parameters provided in Table 3.14.

In order to investigate whether the strong correlation between the aforementioned indicators is also valid for other years, a similar statistical analysis was carried out with measured data for the years 2003, 2004, and 2006 and the results are also presented in Table 3.14.

From this analysis can be concluded that the strong correlation between both indicators is also valid for other years and that it has remained stable over the period of time analysed. Solving Equation 3.10 for λ, the annual mean PM_{10} concentration over which the number of days exceeding the daily limit values is over 35 was also estimated for each year. According to the regression function developed in this section, an annual mean PM_{10} concentration above 31 µg/m^3 may lead into not meeting the standard related to the number of days exceeding the daily limit value of 50 µg/m^3 of the same pollutant, which can only be exceeded 35 times.

Table 3.14 Parameters of the regression function to estimate the number of days exceeding the daily limit value of 50 µg/m^3 of PM_{10} based on annual mean PM_{10} concentrations.

Year	Parameters of the regression function			Adjusted R^2	Annual mean PM_{10} over which the number of days exceeding the daily limit value is over 35
	A	B	C		
2003	0.088	-1.62	5.41	0.90	29.7
2004	0.130	-4.11	37.19	0.93	31.0
2005	0.157	-5.68	60.44	0.89	31.0
2006	0.115	-3.86	45.18	0.90	30.7

This information can be used to assess the compliance with the PM_{10} daily limit value in the ten large German urban entities presented in Figure 3.29. As can be seen in Figure 3.33, the threshold value for annual mean PM_{10} is likely to be exceeded in seven urban entities, although the likeliness of this occurrence varies across urban entities. Furthermore, the average PM_{10} concentration estimated for the main road network is in all cases but two above the value of 31 µg/m^3, which is the threshold over which the number of day exceeding the daily limit value is over 35. These findings support the notion that people living or staying near roads are more likely to be subjected to higher pollutant concentrations. Although this analysis is restricted to ten cities, it is important to keep in mind that air quality estimates were calculated for all German urban entities and are provided in Annex B.

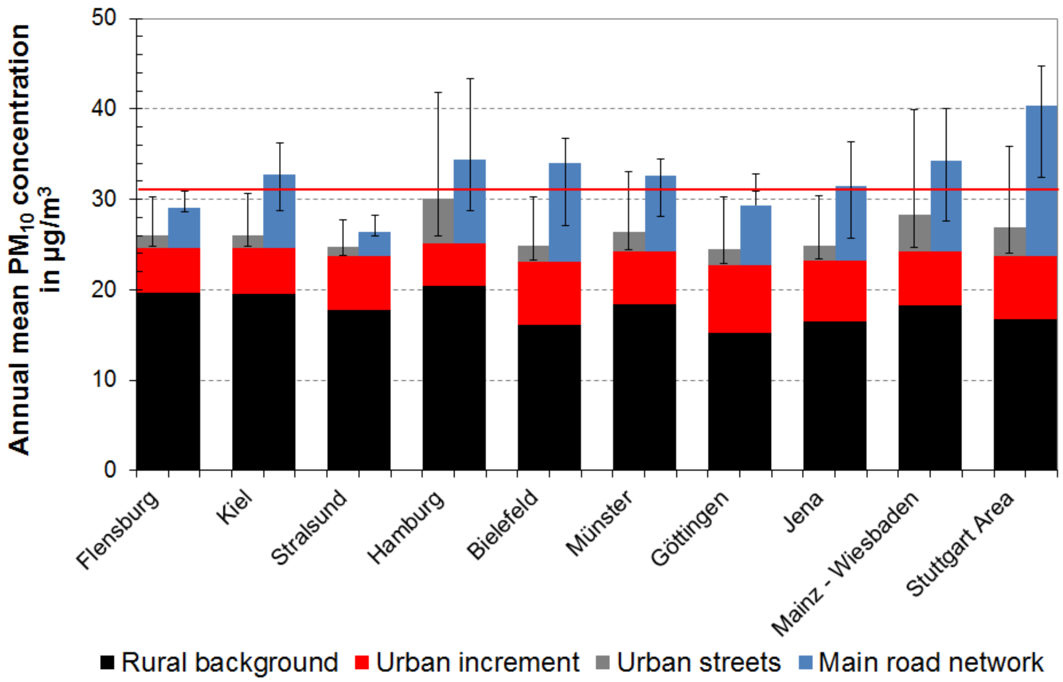

Figure 3.33 Annual PM_{10} concentration in fifteen large German urban entities and the value over which the number of days exceeding the daily limit value is over 35.

Taking advantage of the high spatial resolution in the air quality results described throughout this Chapter, it is possible to analyse the compliance with the 24-hour limit value of 50 µg/m^3 of PM_{10} in the main road network. The results are presented in Figure 3.34, which shows that this directive is not complied in around half of the almost 6 000 kilometres of main road network passing through urban areas (as defined in Section 3.5). It was also estimated that a reduction of 6 µg/m^3 in the annual PM_{10} concentration would result in the compliance in 80% of the length of the main road network and that the compliance in over 95% of the length of the main road network would require a reduction of 10 µg/m^3 in the annual PM_{10} concentrations.

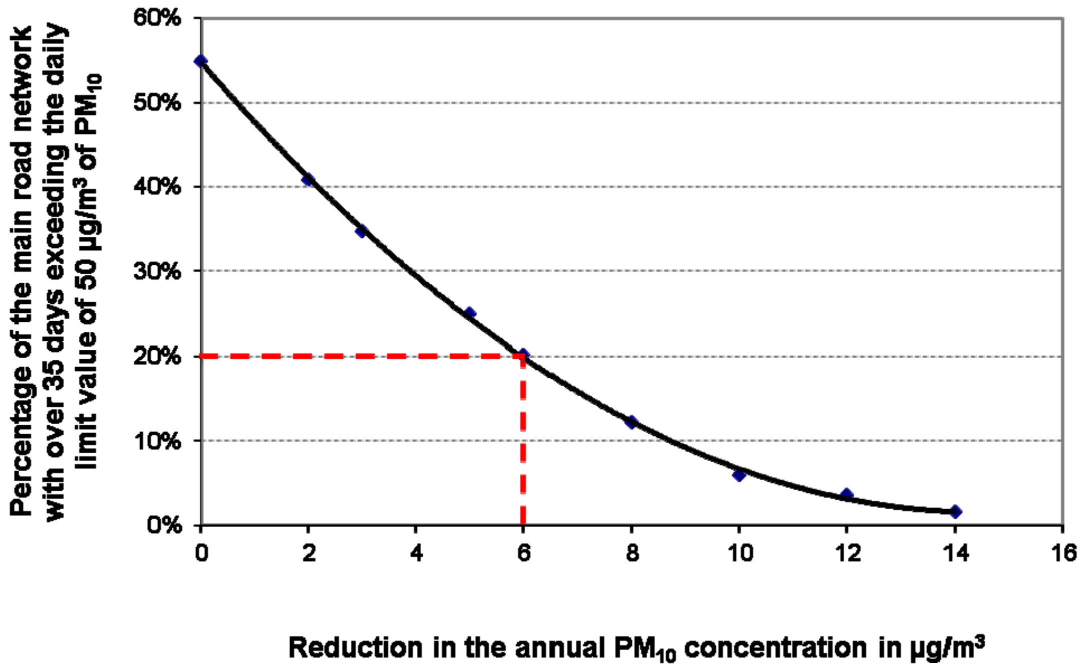

Figure 3.34 Percentage of the main road network length with over 35 days exceeding the daily limit value of 50 µg/m^3 of PM_{10} in function of reductions in annual PM_{10} concentrations.

Although it is recognized that the findings presented above may be not new, it is important to note that the added value of this approach is the large spatial domain covered by the model, the high spatial resolution, and its inherent flexibility to address other environmental issues, such as the analysis of emission reduction scenarios, the human exposure to certain vehicle-related pollutants, and the estimation of the health impacts associated to road transport. Due to its relevance for policy making, the latter issue was also assessed in this work and a comprehensive description of the methodology followed for this purpose is described in detail in Chapter 5 of this work.

In order to assess the accuracy of the results presented in this section, the next chapter of this thesis is devoted to a comprehensive evaluation of the hybrid dispersion modelling approach, including the comparison of results against measured data for each tier of the analysis, and a discussion on the sensitivity of the model to input parameters and the uncertainty in the variables considered.

Chapter 4

Modelling approach evaluation – comparison against measured values, sensitivity and uncertainty analysis

Even the most sophisticated mathematical models can only provide a simplified representation of the reality. Accordingly, air dispersion models cannot fully describe how compounds of any nature disperse in the atmosphere due to an incomplete understanding of the physical and chemical processes involved in pollutant dispersion. Furthermore, lack of certainty is present at every step of the modelling approach developed in this work and absolute certainty cannot be achieved as incomplete knowledge data in addition to the simplified models used for describing the phenomena cannot be avoided, the ubiquitous nature of uncertainty has to be recognised and dealt with. Thus, a model can be evaluated using three approaches: comparison against measured values, sensitivity, and uncertainty analysis. A comparison against measured values is essential to evaluate whether a model or set of models and their results, despite their uncertainties, are robust enough to serve as the basis for decision-making. A sensitivity analysis is also crucial for identifying the models components with the highest impact on the model's results. This knowledge helps to assess how reliable the results obtained with the model are and to establish priorities for future research. As for the uncertainty analysis, it helps to identify those uncertainties that significantly influence the results obtained with a model.

In this chapter, the results obtained in Chapter 3 are compared against measured values in order to gain insight into the degree to which the results correspond to the pollutant dispersion system being modelled. The chapter goes on presenting the results of a sensitivity analysis carried out to illustrate the relative impact of changes in input variables on the estimations of pollutant concentrations. Finally, a discussion on the uncertainties is provided to identify those uncertainties with a relevant effect on the results obtained with the hybrid dispersion modelling approach.

4.1. Comparison against measured values

In order to implement an air quality modelling system with confidence, it is a good practice to evaluate model performance by means of a comparison of results against measured values. Thus, the performance of the two models developed in Chapter 3 was evaluated by means of comparing the concentration predictions against observations for the reference year 2005. For this purpose, modelled urban increment values were compared against measured urban increment (see Section 3.4.2.1) and modelled street increments were compared against urban traffic stations values retrieved from the European Air Quality database Airbase (Airbase, 2008).

4.1.1 Urban increment model

The urban increment model described comprehensively in Section 3.4 was developed using a multiple regression analysis. The predictor variables adopted were: the emissions released within the city; the urban morphology; and the average wind speed. Moreover, the dependent variable – the measured urban increment – was estimated as the difference between observational data from paired rural and urban background measuring stations. From a total of 24 stations pairs for PM_{10} and 26 stations pairs for NO_X, half of them were used for model development and the other half is used in this section for evaluating the model. The comparison of the modelled against the measured PM_{10} and NO_X urban increments are shown in Figure 4.1 and Figure 4.2. A first visual inspection of the results show an overall good agreement with measurements and the urban increments are basically captured by the second tier of the hybrid dispersion modelling approach. The city of Ingolstadt depicts the highest underestimation (around 30 %) and the highest overestimation was estimated for the city Lüneburg (25%). As for NOX, the city of Ingolstadt depicts the highest underestimation (around 25 %) and the highest overestimation was estimated for the city Böblingen (80%). It is therefore noted that the model performs better for PM_{10} than for NO_X, which may be explained by the higher uncertainty regarding NO_X emissions allocation for urban areas, which is the most relevant parameter influencing the model for urban increment.

The model performance was evaluated for its accuracy, bias and errors as well. The metrics applied for this purpose were: the root mean square error (RMSE), the mean fractional bias and error (MFB and MFE, respectively) and the correlation coefficient (R^2). MFB and MFE normalize the bias and error for each model-observed pair by the average of the model and observation before taking the average (Boylan and Russell, 2006). The metrics are presented in Table 4.1.

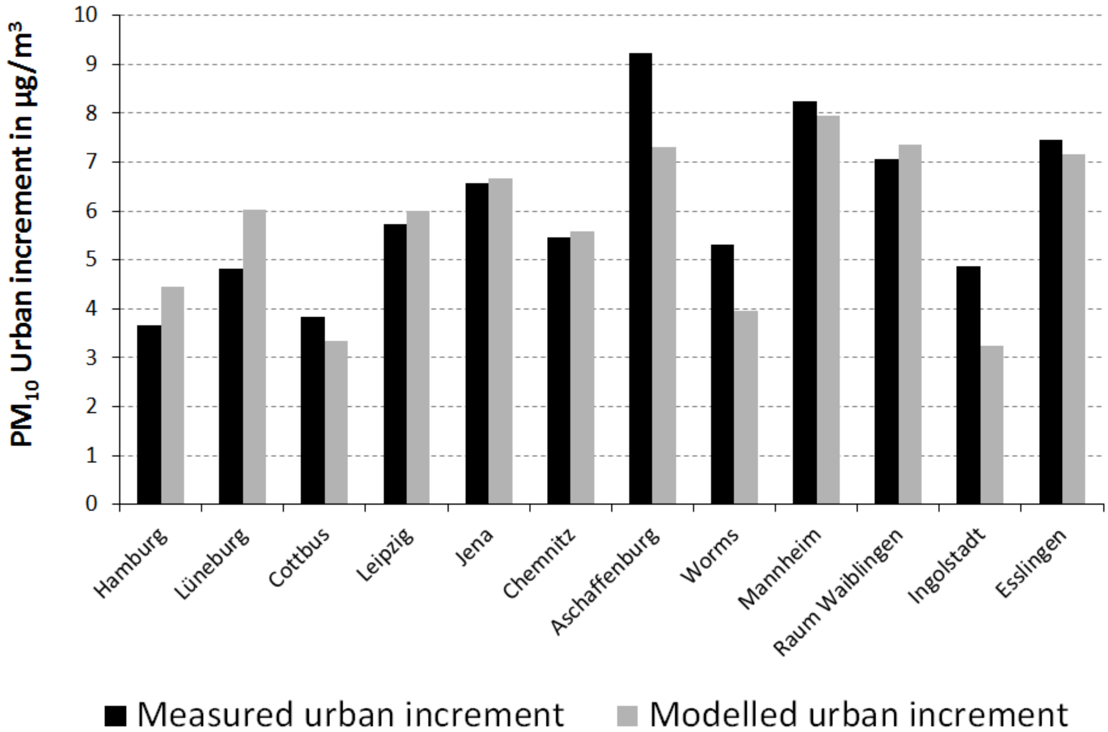

Figure 4.1 Comparison of modelled against measured PM_{10} urban increment concentrations.

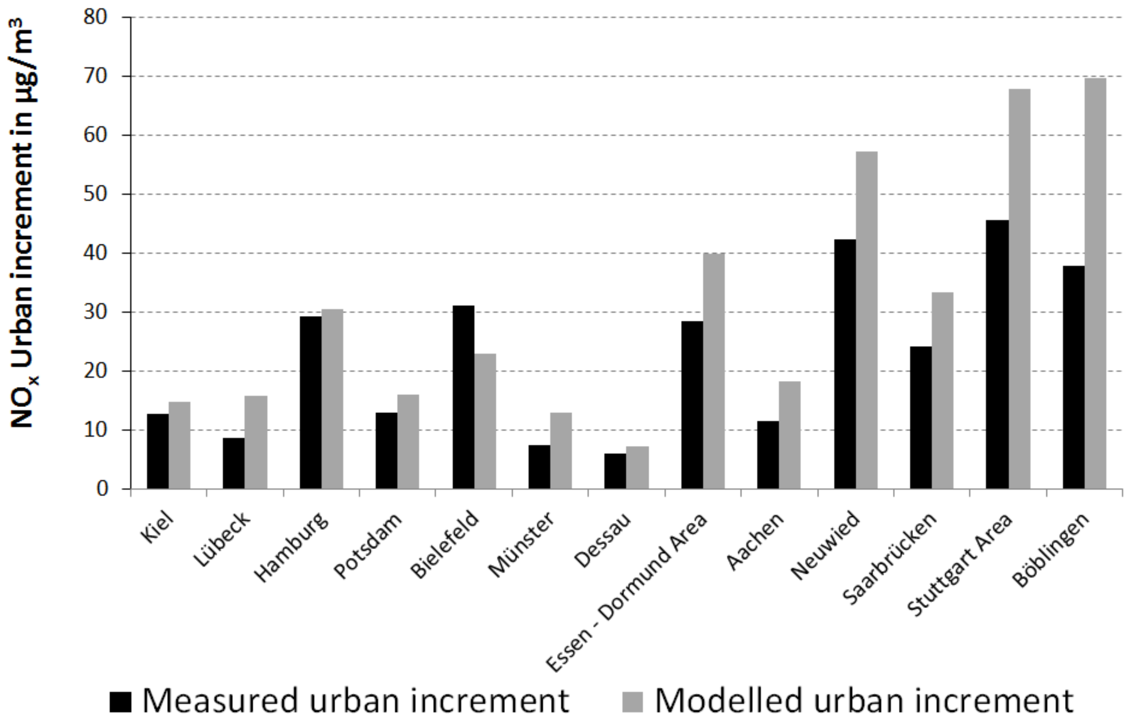

Figure 4.2 Comparison of modelled against measured NO_X urban increment concentrations.

Table 4.1 Statistics obtained comparing modelled and measured concentrations at urban background stations for PM_{10} and NO_X.

Pollutant	Measured mean [µg/m³]	Modelled mean [µg/m³]	RMSE [µg/m³]	MFB [%]	MFE [%]	R^2
PM_{10}	6.02	5.75	0.95	5	14	0.71
NO_X	22.90	31.20	12.84	29	34	0.84

RMSE: root mean square error; MFB: Mean fractional Bias; MFE: Mean fractional Error; R^2: Correlation coefficient

The correlation coefficient depicts a strong positive correlation between measured and modelled values for both pollutants. A slightly positive bias in the PM_{10} estimates can be also observed, although the bias for NOX is clearly larger. Boylan and Russell (2006) suggest, based on results from benchmark studies and examination of various bias and errors metrics, that the model performance goal (defined as the level of accuracy that is considered to be close to the best a model can be expected to achieve) for particulate matter has been met when both the MFB and MFE are less than or equal to ±30% and +50%, respectively. Furthermore, they also propose that the model performance criteria (defined as the level of accuracy that is considered to be acceptable for standard modelling applications) has been met when both MFB and MFE are less than or equal to ±60% and +70%, respectively. Using these criteria, the model goal performance is met and, although these criteria were developed for particulate matter, the model performance goal is also met for NO_X. Additionally, it is important to note that all modelled values fall within a factor of 2 of the measurements (Figure 4.3 and Figure 4.4) enforcing the notion that an overall acceptable model performance was accomplished.

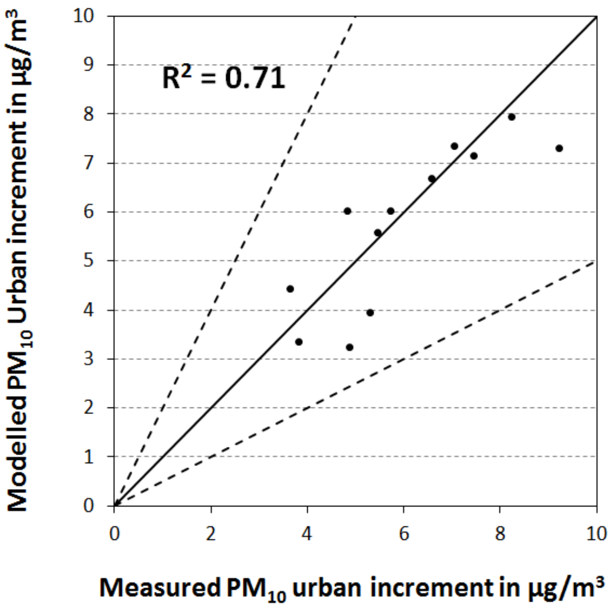

Figure 4.3 Comparison of modelled against measured PM_{10} urban increment concentrations.

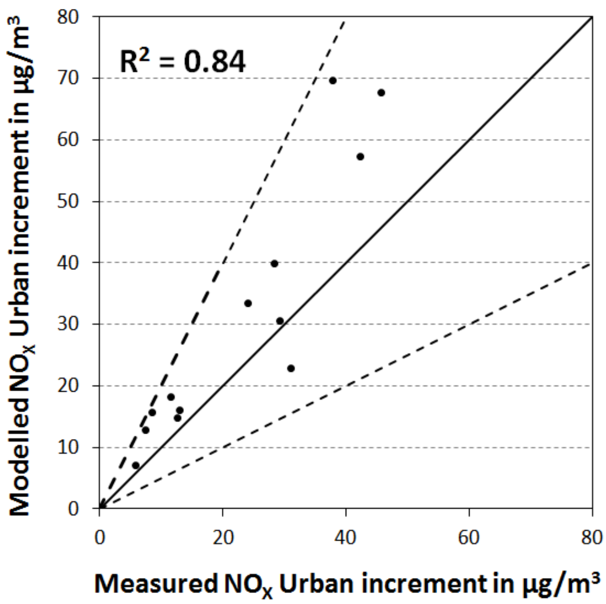

Figure 4.4 Comparison of modelled against measured NO_X urban increment concentrations.

4.1.2 Street increment model

The results of the street increment model are better compared against observational data provided by traffic stations, which are classified according to the type of area surrounding them, e.g. urban, suburban, or rural (Mol et al., 2008). Here it is important to keep in mind that additional concentrations were estimated for three different road types: roads that belong to the main network and outside urban areas; roads that belong to the main network and inside urban areas; and urban streets (see Section 3.5). From this typology it is evident that roads belonging to the first typology are not located within urban areas and, therefore, the third component of Equation 2.1 does not apply for this road type. As a consequence, total concentration of pollutants for these roads was estimated using a modified version of Equation 2.1, which is written as follows:

$$C_{i\ total} = C_{i\ regional} + C_{i\ roadside} \qquad \text{Equation 4.1}$$

The traffic stations considered in this comparison were restricted to urban areas with valid measured values from urban background stations. In this way, the performance of the street increment model can be better assessed as the uncertainty that could be introduced by the urban pollution increment model is avoided.

It is important to remember the heterogeneous nature of the stations: some of them are located within cities, near major roads or outside urban areas. Since this is relevant for comparison purposes, the stations were classified into three groups: stations located outside urban areas and near major roads; stations located inside urban entities; and stations located inside urban entities and at the same time within 30 metres of major roads. An overview of available data using the aforementioned classification is presented in Table 4.2.

Table 4.2 Available data from traffic stations by pollutant for Germany and the reference year 2005.

	Within urban areas	**Within urban areas and near major roads**	**Outside urban areas and near major roads**	**Total**
PM_{10}	35	27	2	64
$PM_{2.5}$	2	3	0	5
NO_X	27	19	0	46
NO_2	27	19	0	46

As can be seen from Table 4.2, only five stations provided data for $PM_{2.5}$ concentrations at traffic locations in the year 2005. As this limited number of traffic stations does not allow to draw definitive conclusions about the performance of the model for this specific pollutant, these stations are not further considered in the comparison. Furthermore, the same observation is valid for the two PM_{10} traffic stations located outside urban areas and near major roads and are therefore not considered as well.

Once the stations were classified, total pollutant concentrations expected to be found at these stations were estimated using the models and procedures already described in the previous sections. Concentrations obtained using the modelling approach for the main road network inside urban areas (see Section 3.5.2) were compared against traffic stations located within urban areas and near major roads. One parameter is especially relevant for this estimation: the distance between a station and the nearest road. Unfortunately, this distance could not be drawn from the Airbase georeferenced data due to their poor spatial accuracy, making a manual correction unavoidable. For this purpose, satellite images freely available from Google Earth mapping services were used to estimate an approximate value of this parameter.

In order to obtain NO_2 concentrations at street level, the Romberg model was used to convert NO_X into NO_2 (see Section 3.4.1). Using the modified function suggested by Bächlin et al., (2006), NO_2 concentrations at roadside were estimated from NO_X concentrations as follows:

$$U[NO_2] = \frac{A \cdot [NO_X]}{([NO_X] + B)} + C[NO_X]$$ Equation 4.2

where NO_2 and NO_X are the concentrations of those pollutants; A, B, and C are the correlation factors with values 43, 53, and 0.129, respectively. The comparison statistics for traffic stations located within urban areas and near major roads are presented in Table 4.3.

Table 4.3 Statistics obtained comparing modelled and measured concentrations at traffic stations within urban areas and near major roads for PM_{10}, NO_X, and NO_2.

Pollutant	Number of stations	Measured mean [µg/m³]	Modelled mean [µg/m³]	RMSE	MB	MFB [%]	MFE [%]	R^2
PM_{10}	27	31.9	32.7	4.6	0.9	3	13	0.65
NO_X	19	136.9	117.0	39.9	-19.9	-21	30	0.64
NO_2	19	51.9	58.8	12.27	6.88	10	17	0.71

From Table 4.3 can be drawn that the performance of the street increment model is slightly different for each pollutant. Concerning PM_{10}, a slightly positive bias with respect to the measured values can be observed. The NO_X and NO_2 mean fractional bias is larger than for PM_{10}, although both values are within the suggested by Boylan and Russell (2006). The same is true for the mean fractional error as well. Finally, the analysis shows that the correlation coefficient is good for all three pollutants. As for the spread of the results, Figure 4.5 shows that all modelled values for PM_{10} can be found within a factor two of the measured values. The agreement of the modelled concentrations of NO_2 and NO_X against measured values at traffic sites can also be described as satisfactory, although a larger spread than for PM_{10} can be observed. The main reason for this development can be the fact that the uncertainty in the NO_X emissions allocation is larger for this pollutant than for PM10, which certainly contributes to the larger spread. These issues are further explored in the sensitivity und uncertainty analysis chapter (see Section 4.2). Nevertheless, a scatter plot of the results shows that all NO_X and NO_2 modelled values can also be found within a factor two of the measured values.

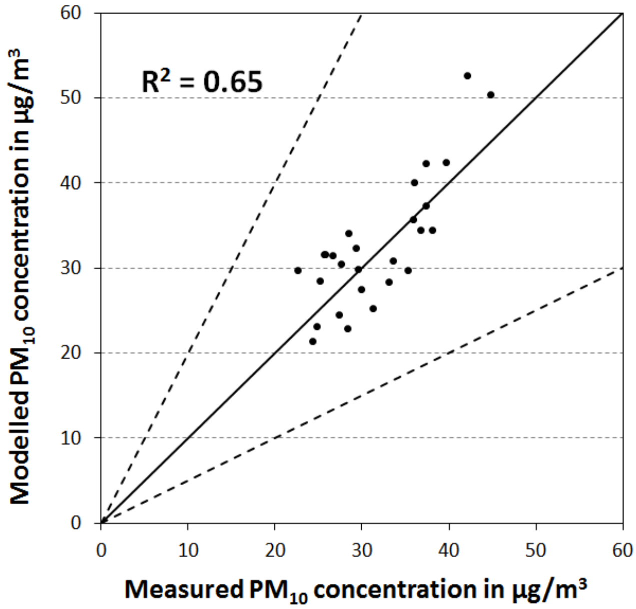

Figure 4.5 Comparison of modelled against measured PM_{10} concentrations at traffic stations.

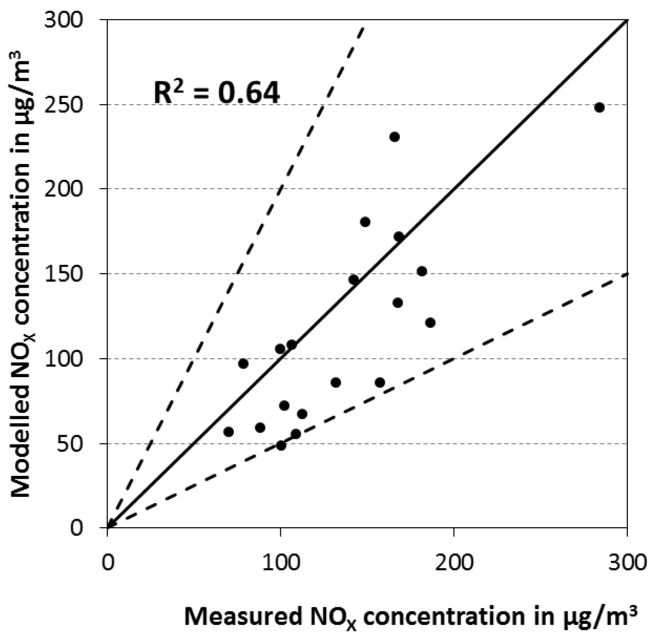

Figure 4.6 Comparison of modelled against measured NO_X concentrations at traffic stations.

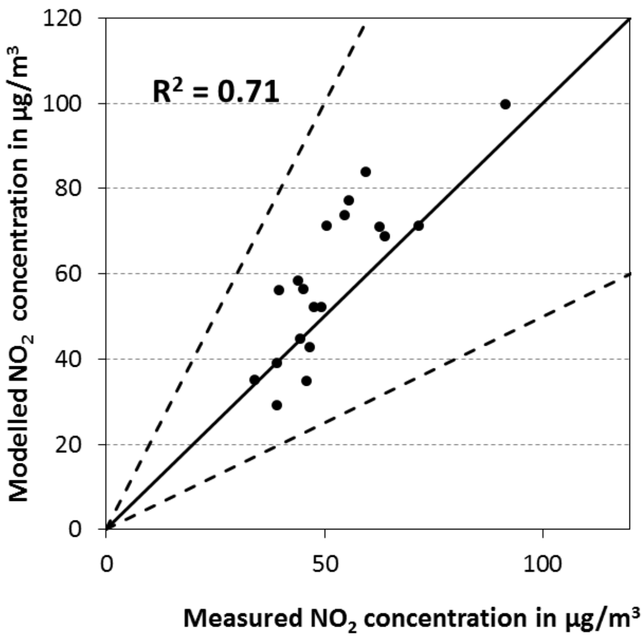

Figure 4.7 Comparison of modelled against measured NO_2 concentrations at traffic stations.

The above results take into account only stations located inside urban entities and at the same time within 30 metres of major roads. The stations inside urban entities that are located more than 30 metres away from a major road segment were compared against modelled values obtained applying the methodology for urban streets (see Section 3.6). Due to the probabilistic nature of the modelled additional concentration at street level, it is important to note that a direct comparison of these values against punctual measurements may not completely reflect the model performance. Indeed, the Monte Carlo simulation generates a large number of possible scenarios using all valid combinations of possible inputs to simulate all possible outcomes, resulting in a distribution of possible outcomes.

To illustrate this, consider the cumulative probability plot for Berlin presented in Figure 4.8. The cumulative probability provides the range of possible additional concentrations that could occur at any street roadside within Berlin (excepting major roads) and the likelihood of any concentration to occur. The same figure shows concentrations values measured at the traffic stations DEBE010 and DEBE067. According to these results, the PM_{10} concentration obtained at the traffic station DEBE010 would be likely to be found at about 10% of the streets within Berlin. On the other hand, lower values than the one reported for the station DEBE067 would have a significantly higher likelihood to be found at any street within Berlin (around 90%). In conclusion it can be said that the cumulative probability function gives a more detailed picture of the spatial variability of pollutant concentrations within an urban area. The advantage of this methodology is clearer when considering that a similar analysis is possible for each of the 114 UE analysed in this work.

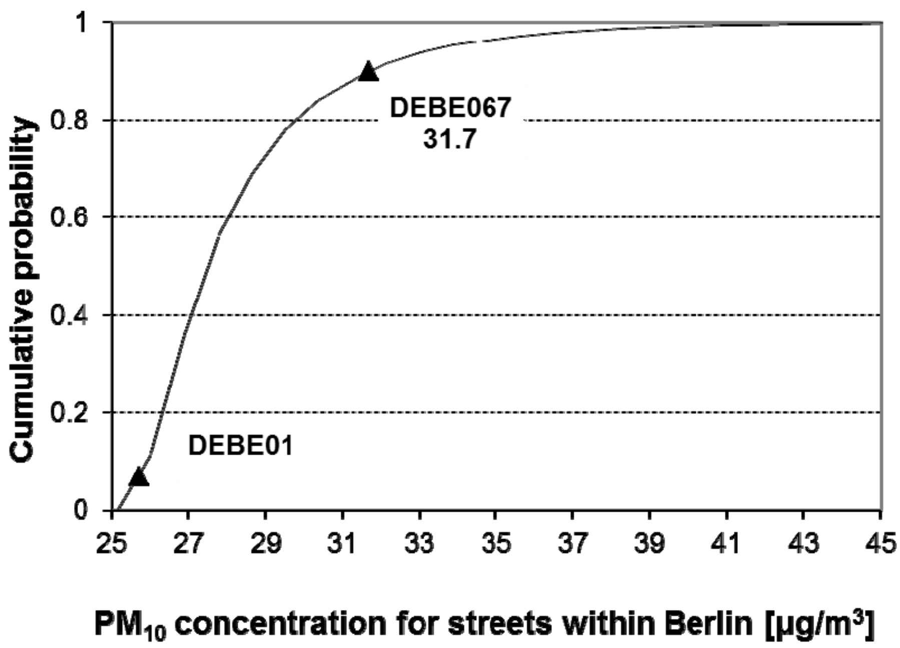

Figure 4.8 Comparison of the modelled cumulative distribution function for urban traffic concentrations of PM_{10} against measured values in Berlin.

Nevertheless, a comparison of the punctual measurements against the modelled concentrations is presented in the next figures. Figure 4.9 und Figure 4.10 present the comparison of PM_{10} modelled values against measured concentrations at traffic stations. Grey bars depict the modelled values for each urban area including the 95% confidence interval. The punctual measurements are depicted as red arrows to the right of each corresponding bar and two arrows mean that more than one station was available for the corresponding urban area.

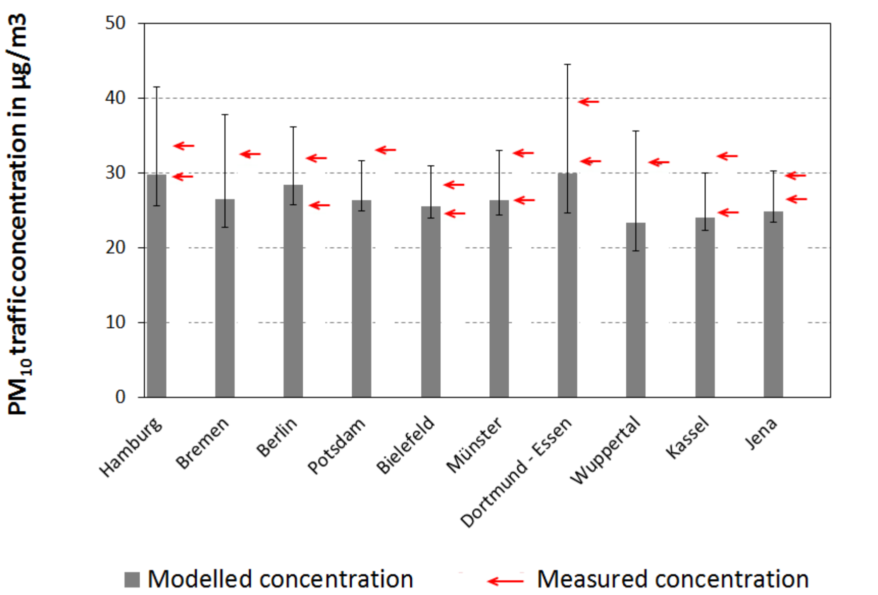

Figure 4.9 Comparison of modelled against measured PM_{10} concentrations at traffic stations.

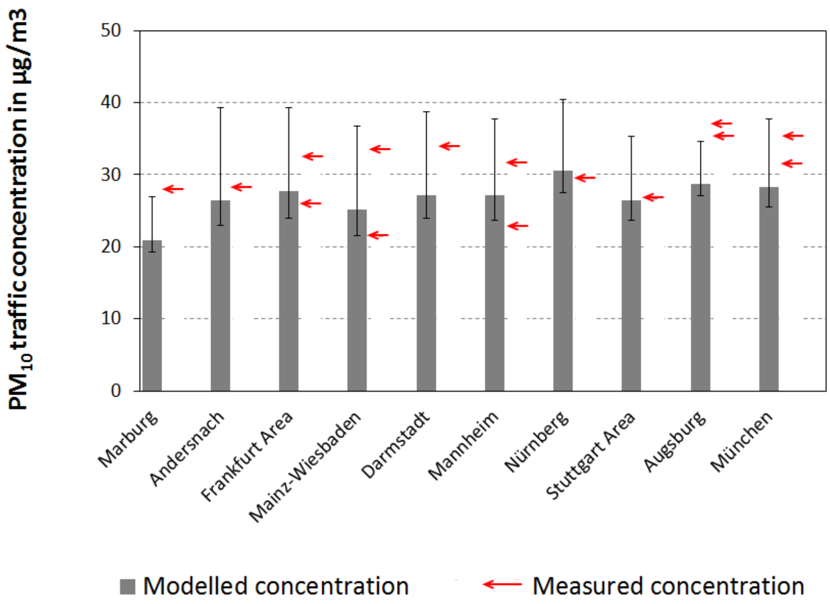

Figure 4.10 Comparison of modelled against measured PM_{10} concentrations at traffic stations.

As it can be read from the figures, all PM_{10} values measured at traffic stations can be found within the boundaries defined by the confidence interval, except four cases in which the measurements are slightly outside the aforementioned boundaries. An explanation for this behaviour may be the uncertainty in the emission factors and the parameters defining the probability distribution function for the average annual daily traffic (AADT). Concerning NO_2 concentration, the comparison is presented in Figure 4.11 and Figure 4.12.

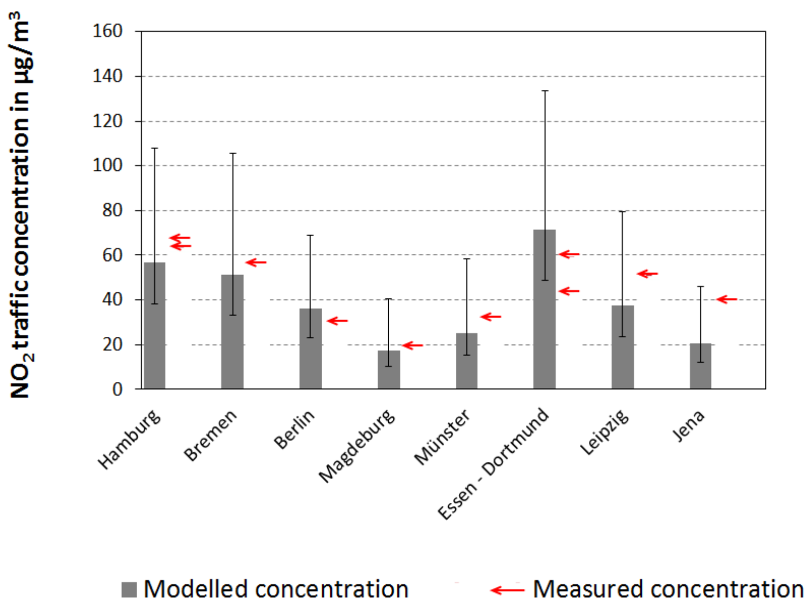

Figure 4.11 Comparison of modelled against measured NO_2 concentrations at traffic stations.

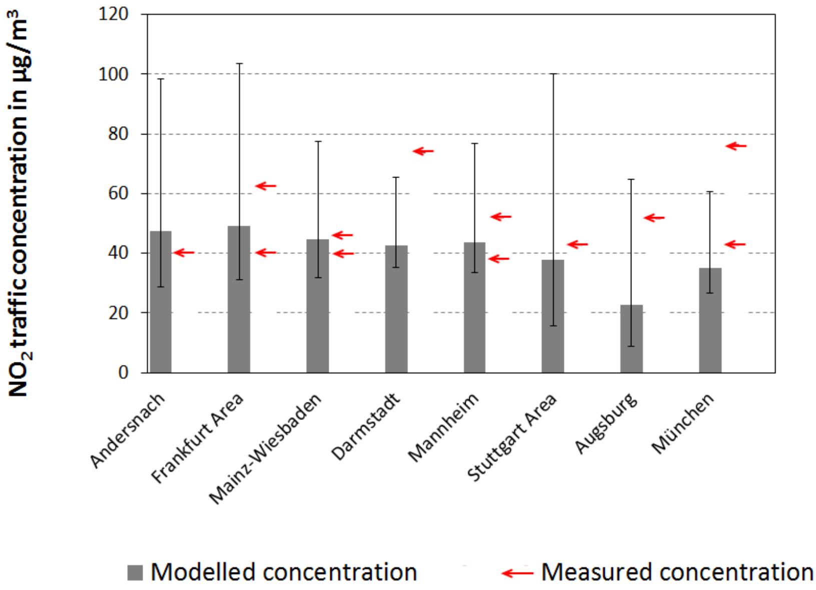

Figure 4.12 Comparison of modelled against measured NO_2 concentrations at traffic stations.

Similar to PM_{10}, almost all NO_2 values measured at traffic stations can be found within the boundaries defined by the confidence interval, except for one station in Darmstadt and one in München. Additionally to the uncertainties in the emission factors and parameters defining the probability distribution functions, the parametric model for converting NO_X concentrations into NO_2 concentrations may also play a role in the underestimation in some cases. Since the comparison of modelled NO_X concentration against measured values shows similar results as the NO_2 concentrations comparison, the NO_X results are not shown in this section.

4.1.3 Summary of the comparison findings

In view of the comparison against measured values presented in the last sections, it can be concluded that the hybrid dispersion modelling approach performs well at both urban and street scale. It provides estimates with an acceptable level of accuracy and within a fairly good performance range, according to the statistics parameters suggested by Boylan and Russell (2006). Results also indicate a better performance for PM_{10} than for NO_X and NO_2, which was expected due to the better insight into the PM_{10} formation mechanisms and emissions allocation, which is not entirely true for the other two pollutants. Unfortunately, only a limited number of stations with PM2.5 concentrations were available and, therefore, a comparison of results for this pollutant was not possible. Nevertheless, the results provided for PM_{10} could be considered as an indicator of the model performance for $PM_{2.5}$.

Another aspect to take into account is the lack of data regarding measure height, i.e., the height above the pavement at which pollutant concentrations were measured, which was not always available. This fact hindered an accurate correction by measure height (Eerens et al., 1993), which may have introduced a positive bias and hampered model performance. Using average emissions factors for estimating road emissions has certainly introduced uncertainty as those factors can only reflect average conditions for all German cities.

It is also recognised that the parameters of the distributions for the Monte Carlo simulation remain an important source of uncertainty. Then again, some of them may never be thoroughly known which is important to remember given that, even assuming that the underlying model is correctly specified, only good guesses of these parameters are currently available.

In summary it can be said that the models are useful for the estimation of pollutant concentrations within urban areas, allowing a good description of the concentration increment at roadside in a probabilistic way. Despite the validation of the modelling approach by means of comparison against measured values, some issues related to model sensitivity and uncertainty remain to be addressed. Due to their inherent importance to the evaluation of any air pollution modelling effort, both aspects are discussed in detail in the next section.

4.2. Sensitivity and uncertainty analysis

Lack of certainty is present at every step of the assessment depicted in this work. It would be surprising if this were not the case since, even in the most trivial aspects of daily life, uncertainty is omnipresent. Despite this fact, in the past a strong notion of determinism was deeply engrained in the civilization, certainly influenced to a large extent by religious beliefs (Gigerenzer, 2002) and now, at the beginning of the 21st century, society is still learning to accept uncertainty in every aspect of its lives and to deal with it in a reasonable way. Science has also experienced major changes over the last hundred years. In the past, comprehensive data collection and physical experimentation were needed to figure out relationships and laws consistent with the data. Modern science is nowadays more concerned with understanding and quantifying physical phenomena and implementing this knowledge in the form of numeric models. In this way, physical experimentation has been largely replaced by numerical modelling in many scientific disciplines. And still, absolute certainty cannot be achieved as incomplete data in addition to simplified models for describing a system cannot be avoided and, therefore, the ubiquitous nature of uncertainty has to be recognised and dealt with.

Thus, even though the model's validation presented in the last section showed that the hybrid dispersion modelling approach has a good overall performance, the uncertainty in relation to the model parameters and input data remain to be addressed and this section aims at studying the sensitivity and uncertainty of the hybrid modelling dispersion approach. Due to its flexibility and integration of qualitative and quantitative criteria, the Numeral Unit Spread Assessment Pedigree (NUSAP) method was chosen to characterize the model's uncertainty. A brief description of the NUSAP system is provided in the following.

4.2.1 The NUSAP system

The NUSAP method is 'a notational system whereby the different sorts of uncertainty in quantitative information are displayed in a standardized and perspicuous way.' (Funtowicz & Ravetz, 1992). The system combines quantitative and qualitative dimensions of uncertainty using the five categories found in the acronym: the first qualifier is related to a numeral, which can be an ordinary number; 'unit' is the second category, which is related to the unit expressed in the numeral category and it can be of the usual art, such as grams, metres or monetary values; the category 'spread' characterizes the random error or variance of statistics of the information in the numeral and unit categories; the fourth qualifier 'assessment' conveys qualitative judgments about the information gathered in the previous categories; and, finally, 'pedigree' aims at providing an evaluative description of the production of the information in order to identify strengths and weakness in the process. Pedigree is expressed by means of a pedigree matrix which codes qualitative expert judgements (Funtowicz & Ravetz, 1990). Using this information as input, a diagnosis diagram can be constructed to plot the pedigree and sensitivity of key uncertain variables. A diagnosis diagram discloses the critical knowledge basis of the variables used in a model with respect to the results obtained with it, helping to identify those parameters with the greatest need for improvement through research.

The NUSAP method has been used in a wide range of studies addressing complex issues, such as the assessment of uncertainty in CO_2 emission scenarios (Van der Sluijs et al., 2002), a greenhouse gas emission inventory (Ramírez, de Keizer, Van der Sluijs, Olivier, & Brandes, 2008), and cost data quality for eco-efficiency measures (Ciroth, 2009). For a comprehensive description of the methodology, the reader is referred to Funtowicz and Ravetz (1990) and Van der Sluijs et al. (2005).

The first two categories are easily to define as the information to be analysed is provided as pollutant concentrations expressed in µg/m^3. On the other hand, the remaining three qualifiers, i.e., Spread, Analysis, and Pedigree require a more detailed analysis, which is presented in the next sections.

4.2.2 Spread estimation

The qualifier spread can be addressed by means of sensitivity analysis which 'evaluates the effects of changes in input values or assumptions on a model's results.' (U.S. EPA, 2009). Sensitivity analysis can be classified into three categories: screening, local, and global (Van der Sluijs et al., 2004). Whereas the screening sensitivity analysis relies in a qualitative identification of the parameters with the largest influence on the model results, local sensitivity analysis focuses on quantifying the effect of the variation in an input variable when the others variables are kept constant. On the other hand, global sensitivity analysis aims at studying the full range of plausible value of key parameters and their interactions in order to assess how the uncertainty in the output of a mathematical model can be apportioned, qualitatively or quantitatively, to different sources of uncertainty in the input of a model (Saltelli, Tarantola, Campolongo, & Ratto, 2004).

Selecting the appropriate technique to determine the model's sensitivity is an important step which depends on a number of factors, such as the number of input variables, the computational effort it entails, the model's complexity, and the objective of the analysis. Thus, the choice of a sensitivity analysis method is usually a compromise between these sometimes conflicting factors. In this work, a global sensitivity analysis was carried out using Monte Carlo analysis. For this purpose, the commercial software crystal ball (Oracle, 2009) was used for both fitting the input data to probability distribution functions and for running the simulations. The sensitivity of the model to the different input variables is then expressed by means of the rank correlation coefficient, which provides a measure of the degree to which input variables and output change together. If an input variable and the output have a high correlation coefficient, it is deduced that the variable has a significant impact on the output. Positive coefficients indicate that an increase in the variable is related to an increase in the output and negative coefficients imply the opposite.

The modelling approach is able to estimate pollutant concentrations for three different road types: roads that belong to the main network and that are located outside urban areas; roads that belong to the main network and that pass through urban areas; and urban streets. Since the modelling approach is different for each road type, the sensitivity analysis was also performed according to this classification. In the next section, the results of the global sensitivity analysis for each model's component are presented.

4.2.2.1 Main road network outside urban areas

The model for estimating pollutant concentration near roads that belong to the main network and outside urban areas was introduced in section 3.5.1 and it is written as follows:

$$C_i(s) = c_n \cdot e_i \cdot g(s) \cdot f_u \qquad \text{Equation 3.6}$$

where

C_i (s) = concentration of pollutant i at a distance s (mg/m^3),

e_i = length-specific street emission (mg/m · h),

c_n = near-ground concentration standardised with respect to e_i (h/m^2),

g(s) = dispersion function (dimensionless) ; It is estimated using:

$$g(s) = 1- 1.166 \ln (1+s)$$

where s is the distance between road shoulder and an observation point

fu = function to consider wind speed (dimensionless); It is evaluates as follows:

$$f_u = \frac{2.3}{u_{avg}}$$

where u_{avg} is the annual average wind speed in m/s measured at 10 metres over the surface.

In order to determine the impact of changes in the input variables upon the estimation of the additional road increment, a global sensitivity analysis was carried out using Monte Carlo simulation. The sensitivity of the model to the different input variables is expressed by means of the rank correlation coefficients, which are presented in Figure 4.13. The sensitivity diagram shows that the model has the largest sensitivity to the transport emissions and it is also particularly sensitive to the distance between road shoulder and the receptor or observation point. This is not surprising as vehicle-related pollutant concentrations decrease rapidly with increasing distance from the source of the emissions. Furthermore, the model is less sensitive to the average wind speed.

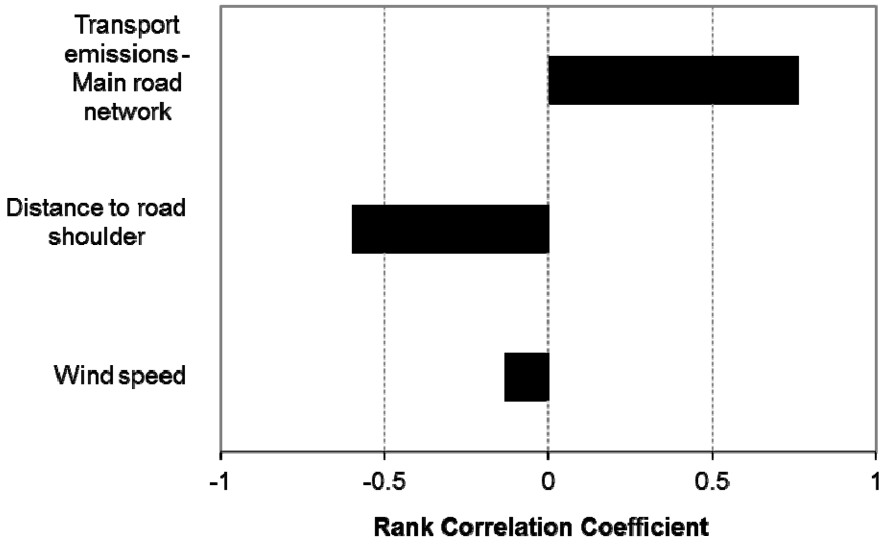

Figure 4.13 Sensitivity diagram of the model to estimate pollutant concentrations at roadside for the main road network outside urban areas.

4.2.2.2 Main road network inside urban areas

The model for estimating pollutant concentration near roads that belong to the main network and inside urban areas comprises two components: one for determining the urban increment (section 3.4) and a second to estimate the additional pollutant concentration near major roads and within urban areas (section 3.5.2). Combining both elements, the model is written as follows:

$$C_{i\ Main\,road} = \left[\varpi_i + \phi_i \frac{E_{i\,UE}}{A_{UE} \cdot u_{avg}} + \gamma\, C_{i\,rural} \right] + \left[E_{i\,Traffic} \cdot \theta \cdot W \right] \qquad \text{Equation 4.3}$$

where

$C_{i\ Main\ road}$ = Concentration of pollutant i near major roads within urban areas.

$E_{i\ UE}$ = Total emission of pollutant i within the UE in tons.

A_{UE} = Urban entity area in km^2.

u_{avg} = Urban entity average wind speed in m/s.

$C_{i\ rural}$ = Rural background concentration of PM_{10} in $\mu g/m^3$ (only for PM_{10}).

ω_i, ϕ_i, and γ_i = Multiple-regression parameters for pollutant i.

$E_{i\ Traffic}$ = Traffic emissions of pollutant i.

W = Wind factor, which is a function of u_{avg}.

θ = Dilution factor, which is calculated as follows:

$$\theta = aS^2 + bS + c$$

where a, b, and c are dilution parameters provided in Table 3.5 and S is the distance from the road axis to the receptor location in metres.

A global sensitivity analysis was carried out using Monte Carlo simulation and the sensitivity of the model to the different input variables is expressed by rank correlation coefficients. A visualization of the results for PM_{10} and NO_X is shown in Figure 4.14 and Figure 4.15, respectively. In the case of PM_{10}, the analysis indicates that the model has the highest sensitivity to the emissions data, particularly for the emissions attributed to transport activities. The model is also rather sensitive to the distance to road axis and the rural background PM10 concentrations. Moreover, the model is less sensitive to the urban area and the wind speed. As for NO_X, the model also has the highest sensitivity to the emissions, both from transport activities and from all sectors. The model for NO_X is also more sensitive to the definition of the urban areas than the model for PM_{10}. Finally, the variables with the lowest sensitivity are distance to road axis and average wind speed.

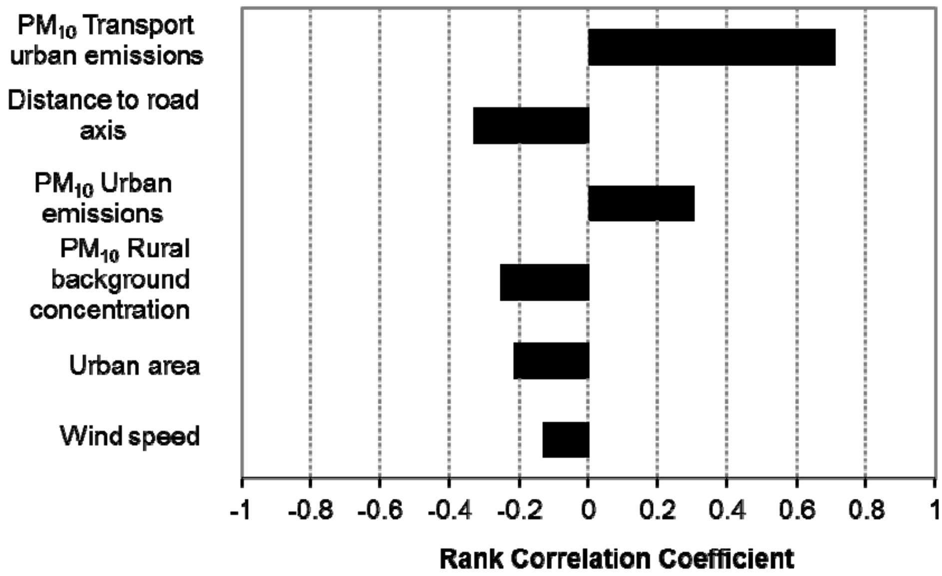

Figure 4.14 Sensitivity diagram of the model to estimate PM_{10} pollutant concentrations at roadside for the main road network within urban areas.

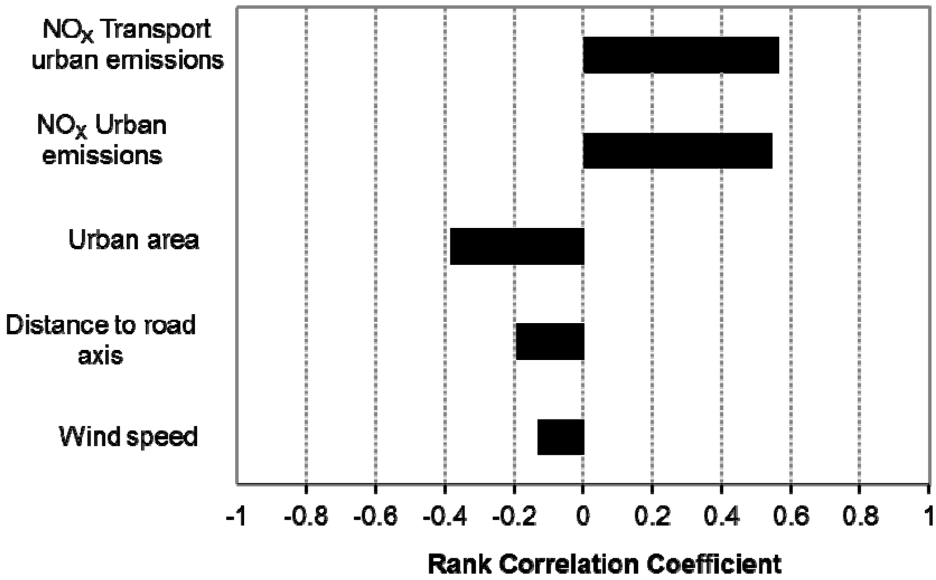

Figure 4.15 Sensitivity diagram of the model to estimate NO_X pollutant concentrations at roadside for the main road network within urban areas.

4.2.2.3 Urban streets

A global sensitivity analysis was also carried out to assess the model for estimating concentrations for urban streets. This model also comprises two parts: one for determining the urban increment (section 3.4) and a second to estimate the additional pollutant concentration near major roads and within urban areas, which was introduced in section 3.6. The resulting sensitivity diagrams for PM_{10} and NO_X are shown in Figure 4.16 and Figure 4.17, respectively.

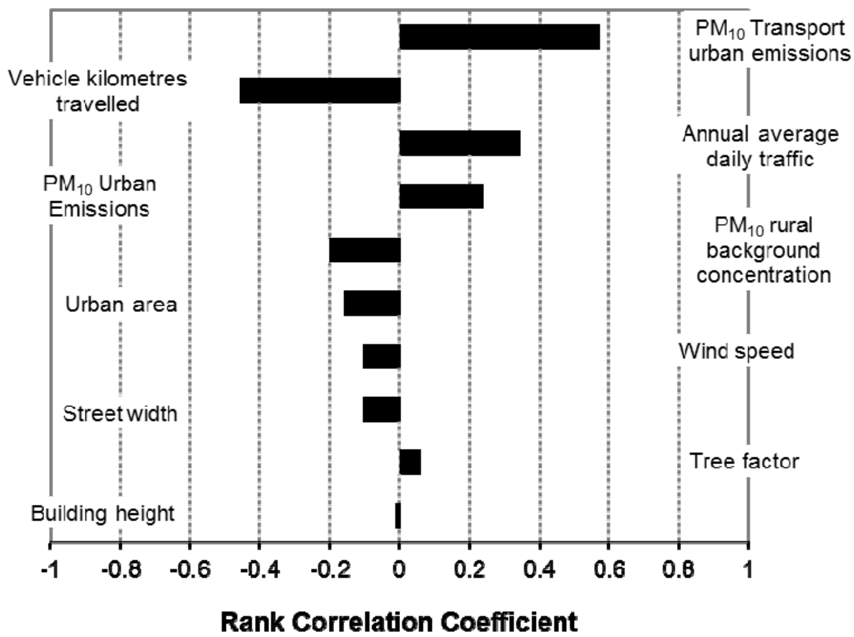

Figure 4.16 Sensitivity diagram of the model to estimate PM_{10} pollutant concentrations at roadside for urban streets.

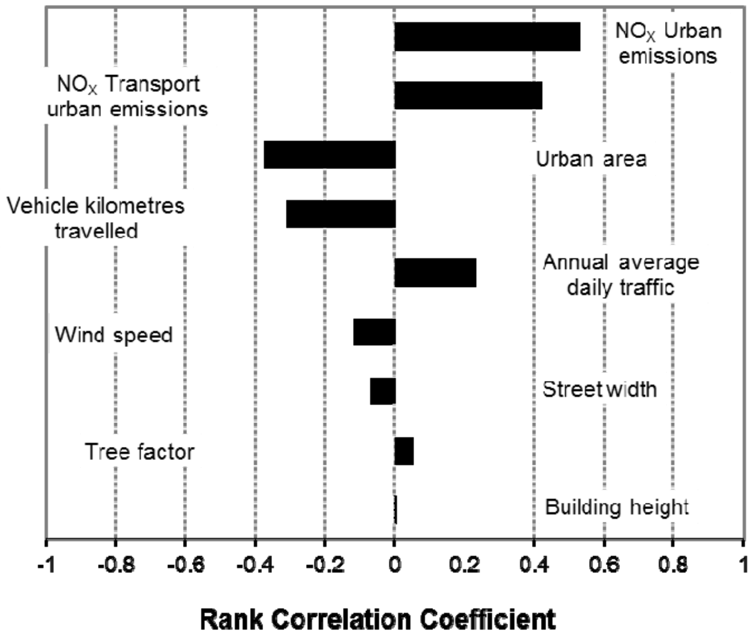

Figure 4.17 Sensitivity diagram of the model to estimate NO_X pollutant concentrations at roadside for urban streets.

Analysing both diagrams it can be concluded that the model has the highest sensitivity to changes in the emissions associated to the transport activity, presenting a lower sensitivity to the vehicle kilometres travelled and the average annual daily traffic. In the case of NO_X, the model has a higher sensitivity to the urban area definition for this pollutant than for PM_{10}, which is explained by the relevance of this input variable for determining the NO_X urban increment. Changes in the rural background concentration have a moderate influence on the PM_{10} concentrations at roadside for urban street. Moreover, the model is less sensitive to the average wind speed and the street width. Finally, the model is much less sensitive to the tree factor and building height.

4.2.3 Pedigree matrix

A pedigree matrix is a tool to evaluate the production process of information. According to Van der Sluijs et al. (2004), a pedigree matrix is used to 'code qualitative expert judgments for each criterion into a discrete numeral scale from 0 (weak) to 4 (strong) with linguistic descriptions (modes) of each level on the scale.'. In this context, the pedigree matrix provides a way of expressing the qualitative aspects of quantitative information. The matrix comprises multiple categories, which enable to easily score and code a wide range of evaluative descriptions. This information is relevant in that it provides insight into the strength of the basis of input data, enhancing the importance of quality in information. In this thesis, a matrix containing four pedigree criteria based on Funtowicz and Ravetz (1990) and adapted from Ellis et al. (2000) was used. The pedigree matrix is presented in Table 4.4.

Table 4.4 Pedigree criteria.

Score	Proxy representation	Empirical basis	Methodological rigour	Validation
4	An exact measure of the desired quantity	Controlled experiments and large sample direct measurements	Best available practice in well established discipline	Compared with independent measurements of the same variable over long domain
3	Good fit or measure	Historical/field data uncontrolled experiments small sample direct measurements	Reliable method Common within established discipline Best available practice in immature discipline	Compared with independent measurements of closely related variable over shorter period
2	Well correlated but not measuring the same thing	Modelled/derived data Indirect measurements	Acceptable method but limited consensus on reliability	Measurements not independent proxy variable limited domain
1	Weak correlation but commonalities in measures	Educated guesses indirect approx. Rule of thumb est.	Preliminary methods unknown reliability	Weak and very indirect validation
0	Not correlated and not clearly related	Crude speculation	No discernible rigour	No validation performed

Source: based on Funtowicz and Ravetz (1990) and adapted from Ellis et al. (2000).

Using the pedigree criteria depicted above, a pedigree scoring was carried out for each of the input variables with the largest sensitivity on the model's output. The input variables considered for pedigree analysis were:

a. Transport urban emissions
b. Urban emissions
c. Wind speed
d. Urban area definition
e. Average annual daily traffic
f. PM_{10} rural background concentration
g. Street width
h. Vehicle kilometres travelled
i. Tree factor
j. Building height

The pedigree scoring for wind speed, average annual daily traffic and urban area definition was carried out by the author using available documentation and the pedigree score cards containing the justification of the scores are provided as an annex in this work. Furthermore, as the variables from f to j were generated within the framework of this work, they were also scored by the author. Concerning the two first input variables, they were provided by the IER dataset, which was introduced in Chapter 3 of this work. Because the emission data are one of the most relevant inputs for the dispersion modelling approach, a more detailed pedigree analysis was made for this dataset. For this purpose, several interviews were carried out with experts from the Institute for Energy Economics and the Rational Use of Energy (IER from its initials in German), University of Stuttgart, to assess the quality of the emissions provided by the aforementioned dataset. A total of three experts were involved in the pedigree scoring and the results by SNAP (Selected Nomenclature for Air Pollution) sector are presented in Table 4.5.

Table 4.5 Pedigree scores by SNAP sector for the IER dataset.

Sector	Description	Pollutant	Emission factor	Activity rate
1	Combustion in energy and transformation industries (stationary sources)	PM	3.25	3.50
		Other but PM	4.00	3.50
2	Non-industrial combustion plants (stationary sources)	PM	3.25	2.63
		Other but PM	3.50	2.63
3	Combustion in manufacturing industry	PM	3.25	2.13
		Other but PM	4.00	2.13
4	Production processes (stationary sources)	PM	3.25	3.00
		Other but PM	4.00	3.00
5	Extraction and distribution of fossil fuels and geothermal energy	PM	1.00	3.50
		Other but PM	1.00	3.50
6	Solvent use and other product use	PM	1.00	2.00
		Other but PM	2.00	2.00
7	Road transport – Urban	PM Exhaust	3.25	1.75
		PM Non-exhaust	1.75	1.75
		NO_X	3.25	1.75
	Road transport – Non urban	PM Exhaust	3.25	3.50
		PM Non-exhaust	1.75	3.50
		NO_X	3.25	3.50
8	Other mobile sources and machinery	PM	2.75	2.75
		Other but PM	2.75	2.75
9	Waste treatment and disposal	PM	3.25	3.50
		Other but PM	4.00	3.50

As can be seen in Table 4.5, the quality of the information is heterogeneous: whereas activity data for the sector 1 (combustion in energy and transformation industries) are very good mostly due to reporting obligations, the same parameter present a lower value for sector 2 (Non-industrial combustion plants) and sector 3 (combustion in manufacturing industry) and even lower for transport activity within urban areas. This analysis gives insight into the strengths and weakness of the IER dataset and, at the same time, it helps to identify the critical sources of uncertainty in this dataset. Because several input variables comprise emissions from different sectors, such as the variable 'PM_{10} urban emissions', a normalized pedigree score (i.e., a weighted value between zero and one) was calculated for them (see Table 4.6). A summary of the pedigree scores relevant for the hybrid dispersion modelling approach is presented in Annex C.

Table 4.6 Normalized pedigree scores of input variables for the hybrid dispersion modelling approach.

Model component	Input variable	Normalized Pedigree
Concentrations at roadside for the main road network outside urban areas	Transport emissions – Main road network	0.78
	Wind speed	0.56
Concentrations at roadside for the main road network within urban areas	PM_{10} Transport urban emissions	0.53
	NO_X Transport urban emissions	0.63
	PM_{10} Urban emissions	0.66
	NO_X Urban emissions	0.73
	Urban area definition	0.69
	PM_{10} rural background concentration	0.75
	Wind speed	0.56
Concentrations at roadside for urban streets	PM_{10} Transport urban emissions	0.53
	NO_X Transport urban emissions	0.63
	Vehicle kilometres travelled	0.69
	Average annual daily traffic	0.81
	Tree factor	0.19
	Street width	0.50
	Building height	0.38

It is relevant to note that the pedigree criteria were weighted equally, even though it is possible that one criterion may be more relevant for a specific input variable than the other three criteria. The more detailed evaluation, however, demanded a greater involvement from experts in all areas relevant for the input variables, which was not attainable within the framework of this thesis. The scores for each input parameter obtained in this section were then put together with the spread expressed by the sensitivity rank correlation coefficient into diagnostic diagrams, which is a topic discussed in the next section.

4.3. Diagnostic diagrams

According to the NUSAP notation system introduced in Section 4.2.1, the qualitative and quantitative information obtained through the sensitivity analysis (spread) and the pedigree analysis (strength) are combined to produce diagnostic diagrams. The rationale behind a diagnostic diagram is that neither the spread nor the strength alone is enough to characterise the quality of the data. The diagram is constructed using both components: the strength axis displays the normalized results of the pedigree analysis with 1 at the origin and zero on the right; the sensitivity axis displays the results of the sensitivity analysis with zero at the origin and values increasing along the axis. In this way, the upper right side of the diagram is considered to be the danger zone, as it contains variables with a weak strength and, at the same time, a high sensitivity in the output. On the other hand, the lower left side of the diagram contains variables with a low sensitivity and very good results from the pedigree analysis and, therefore, this area is considered a safe zone. Figure 4.18 shows the structure of a diagnostic diagram (Van der Sluijs et al., 2004). It is important to note that there are no hard boundaries in the diagram and, therefore, the notations "safe zone" and "danger zone" should not be understood as absolute values but rather as terms to express combinations of sensitivity and strength. Thus, the diagnostic diagram helps to readily identify the model's weakness and the priorities for model improvement.

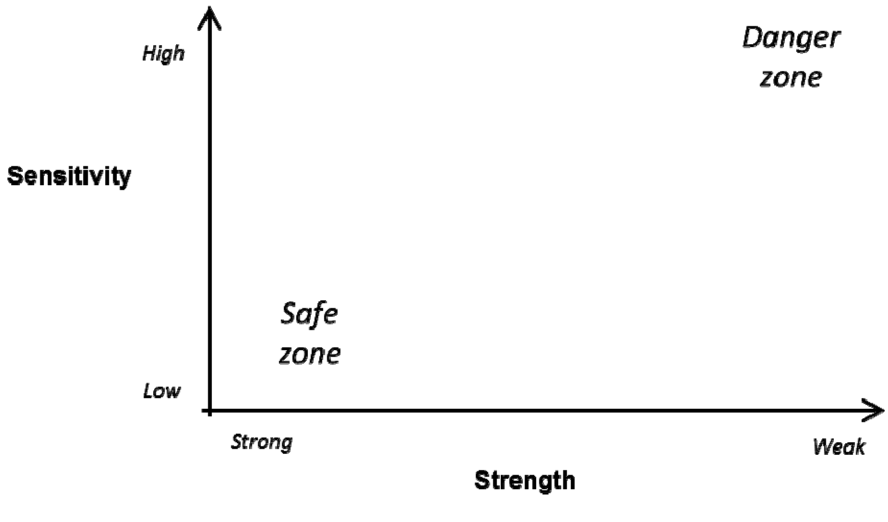

Figure 4.18 NUSAP diagnostic diagram. Source: Van der Sluijs et al. (2004)

Following the same procedure as with the sensitivity analysis, a diagnostic diagram was constructed for each component of the hybrid dispersion modelling approach. For this purpose, the results of the pedigree analysis presented in the last section and the absolute correlation coefficients obtained in the sensitivity analysis were used. Figure 4.19 shows the diagnostic diagram of the model to estimate pollutant concentrations at roadside for the main road network outside urban areas. Although the model comprises three input variables, only two are depicted in the diagram: the transport emissions for the main road and the wind speed. The third input variable, i.e., distance between road shoulder and receptor, was not included in the analysis because the exact location of the receptors along the roads is largely unknown. As a consequence, a distance of 100 metres from the road was set only for illustrative purposes to estimate the concentration increments in this thesis (see Section 3.4.5). Despite this shortcoming, this assumption can be easily modified as detailed data become available. According to the diagnostic diagram, both input variables can be considered as reliable, although the robustness of the model would benefit from an improvement in the quality of the wind speed data, for instance by means of a comparison with measured data.

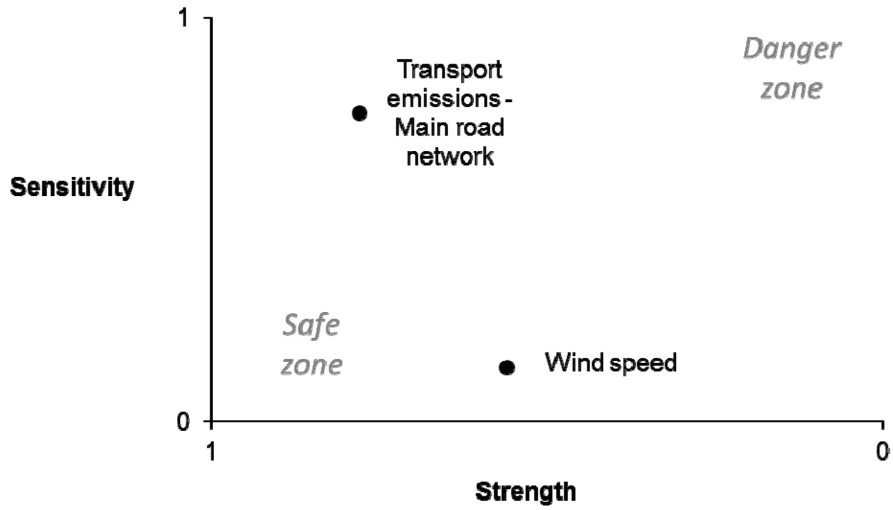

Figure 4.19 Diagnostic diagram of the model to estimate pollutant concentrations at roadside for the main road network outside urban areas.

The diagnostic diagrams of the model to estimate PM_{10} and NO_X pollutant concentrations for roads that belong to the main network and that pass through urban areas are shown in Figure 4.20 and Figure 4.21, respectively. Again, the distance of the receptor to the road axis was not included in the diagram as the exact location of the receptors along the roads is largely unknown. Therefore, receptor location was assumed to be around one metre from the carriageway. Here it is important to note that this assumption can be easily modified if detailed data are available.

The diagrams presented in this section reinforce the notion that the transport urban emissions play a relevant role on the model's results as they exhibit an average quality in their production process and, at the same time, a high sensitivity. As a consequence, the efforts for enhancing the model's performance should be focused on improving the emission factors and activity rates in urban areas, particularly for particulate matter. Here it is to note that, considering that the model for estimating $PM_{2.5}$ and NO_2 pollutant concentrations at roadside for the main road network within urban areas are largely derived from the models for PM_{10} and NO_X, the same conclusions are valid for the aforementioned pollutants.

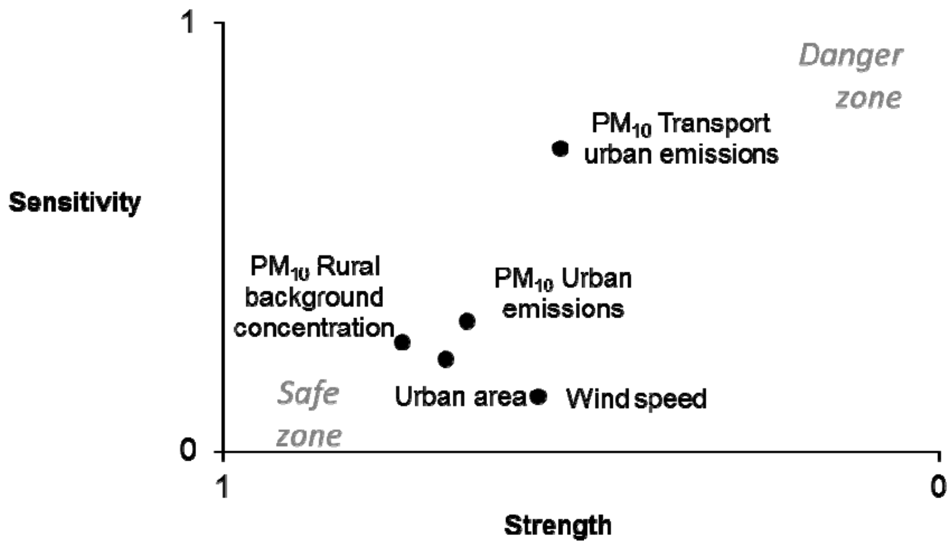

Figure 4.20 Diagnostic diagram of the model to estimate PM_{10} pollutant concentrations at roadside for the main road network within urban areas.

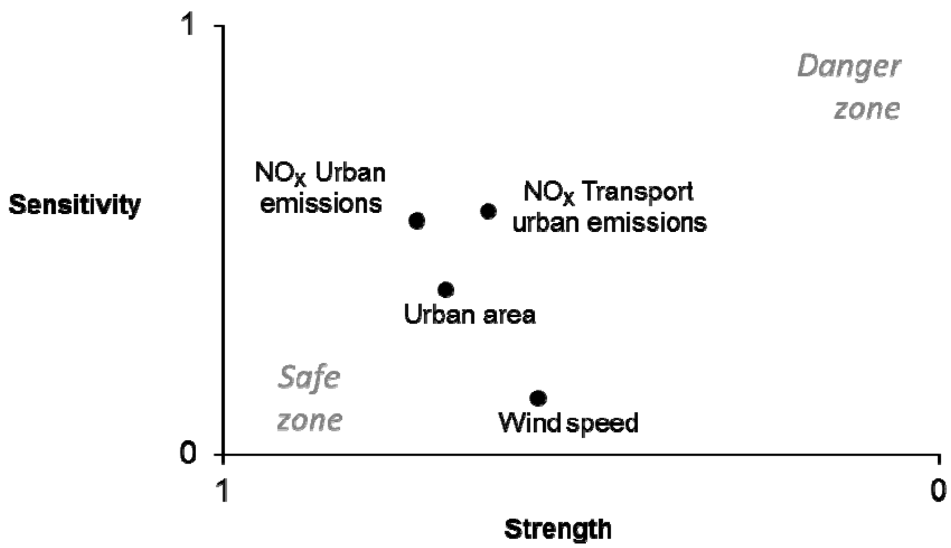

Figure 4.21 Diagnostic diagram of the model to estimate NO_X pollutant concentrations at roadside for the main road network within urban areas.

Finally, the diagnostic diagrams of the model for estimating PM_{10} and NO_X pollutant concentrations for urban streets are presented in Figure 4.22 and Figure 4.23, respectively. From these diagrams it can be observed that almost all variables tend to be located in the middle, lower right side of the diagram. This can be interpreted as an acceptable strength in the variables combined with middle sensitivity on the results. The model's robustness could be increased by improving the data concerning emissions and vehicle kilometres travelled. It is also to note that the tree factor and building height have a very low strength, which is a result of the lack of data for their determination and only educated guesses could be made about them. However, because changes in these variables have a very low influence on the output, the uncertainty introduced by them is likely to be very low.

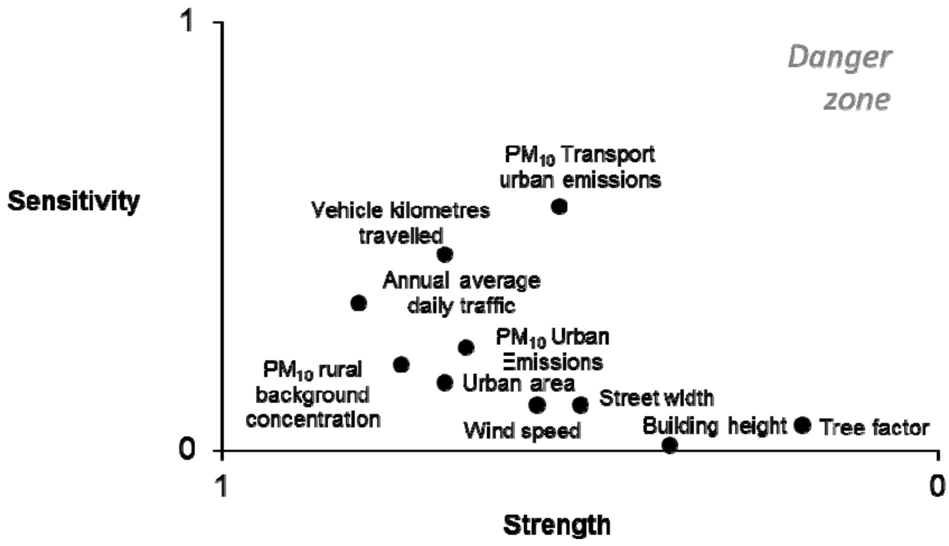

Figure 4.22 Diagnostic diagram of the model to estimate PM_{10} pollutant concentrations at roadside for urban streets.

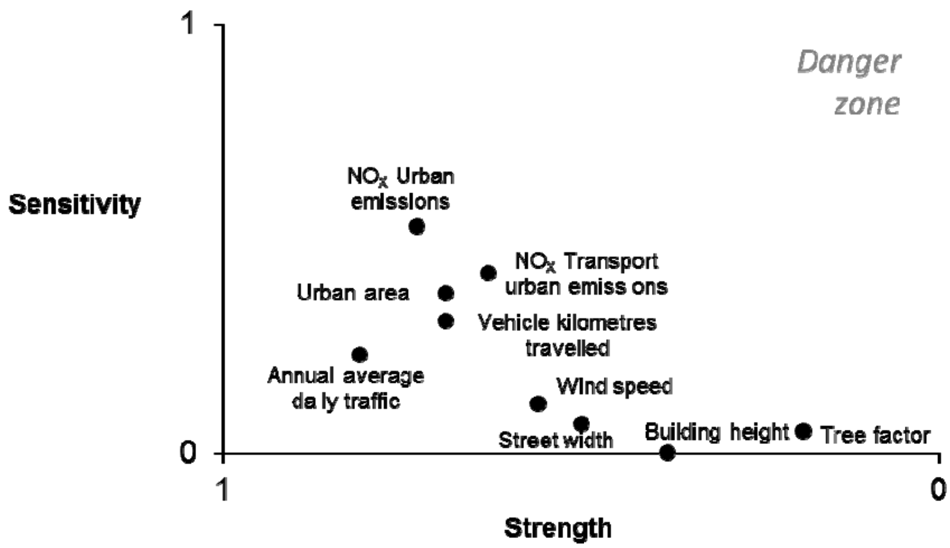

Figure 4.23 Diagnostic diagram of the model to estimate NO_X pollutant concentrations at roadside for urban streets.

Summarizing, the diagnostic diagrams for each component of the hybrid dispersion modelling approach provide evidence that the methodological framework of the model is robust and that the information used in its development is of good quality. At the same time, several weak links were identified, such as the emissions data. As this variable is relevant for all model tiers, it should be the focus of any improvement effort. This methodology also allowed to tests the fitness of the data for the specific needs of the modelling approach developed in this thesis. This is particularly important when trying to optimize the efforts for improving the model's performance by focusing on the weak links disclosed in the analysis.

Chapter 5

Model Application: health and climate change impacts of vehicle-related air pollutants in Germany

Growing environmental pollution has been identified as the source of a number of negative effects on human health, crops, ecosystems and materials. Accumulated scientific evidence points to a positive correlation between living near major roads and experiencing a significant higher risk of developing or worsening health problems (e.g., Ciccone et al., 1998; Holguin et al., 2007; Janssen et al., 2001). Considering that the road transport sector largely contributes to poor air quality, it is evident that there is a growing need for transparent and comprehensive information about the negative impacts on human health related to vehicle use.

Over the last few decades, environmental issues have become economic issues as well. With the growing world population and increasing living standards, natural resources are becoming scarcer and, therefore, more valuable. Considering that the welfare of society as a whole can decrease due to environmental effects, it follows that these effects have an economic value and that these values can be estimated using economic analysis. Indeed, when an impact on any party not directly involved in a decision about an activity is affected – positively or negatively – by that activity, it is said that an externality occurs. In a perfect market, the price paid for a good would reflect the social costs, which comprise private and external costs. In the real world, the production of some goods imposes burdens on society, which are not paid for by the originator. The price paid in the market is therefore less than the actual social costs, and, as a result, externalities arise.

This chapter is devoted to the estimation of health and climate change impacts related to air pollutants generated by road transport in Germany. In this context, the hybrid dispersion modelling approach developed in this thesis plays a crucial role by providing pollutant concentrations with a high spatial resolution. The chapter begins by highlighting the relevance of externalities in policy making and introducing the overall methodology for estimating physical damages and their associated external costs. The chapter goes on giving a description of each stage of the assessment, paying special attention to the Impact Pathway Approach (IPA), which constitutes the basis framework for the assessment. Using the IPA, the marginal and total physical damages attributed to vehicle operation in Germany are calculated and analysed in this chapter. Finally, marginal and total health and climate change costs associated to road transport are presented in this chapter. Here it is worth to note that not only the physical damages generated by vehicle use are considered for these calculations, but also those costs related to up- and down processes and climate change impacts are included as well.

5.1. Externalities and their relevance in policy making

In the middle of the information era, information about the environmental impacts of production and consumption of goods is still scarce, but interest in quantifying the actual social costs of economic activities has increased over the last decade. Indeed, this issue seems to concern not only economic sectors that are commonly related to environmental issues, such as transport activities and energy production, but also the externalities of a broad range of production and consumption activities have been assessed, for instance meat (Burke, Oleson, McCullough, & Gaskell, 2008) and livestock production (Delgado, Narrod, & Tiongco, 2003), to name a few. It could be then suggested that if information about the actual environmental effects generated by the production and supply of goods were available, individuals would be able to compare those impacts to competing products and make better choices (e.g., Bleda & Valente, 2009). Welfare economics show that the existence of externalities leads to outcomes that are not socially optimal. For instance, climate change, congestion and scarcity, accidents and health-related costs are some of the externalities associated to the transport sector. The assessment of these externalities has been the focus of scientists over the last decades, suggesting that although some of these externalities may not be easily measurable, they are nonetheless real.

Considering that the road transport sector contributes significantly to poor air quality, it is evident that there is a growing need for transparent and comprehensive information about the impacts related to vehicle use. For a number of years, the European Commission has been developing policies aimed at reducing the impacts of the transport sector and steering transport policies into a more environmentally friendly direction through market-based instruments, such as stricter environmental standards for new vehicles, encouraging technological innovation, and taxes charges. One of the initiatives promoted by the European Commission to incentivise changes in mobility behaviour is the internalisation of external costs (European Commission, 2008a), which means including external costs in the decision making process. This is necessary because when individuals make the decision about whether and how to travel, they usually do not take account of additional damages they inflict on society and, thus, giving the right price signals may play a role in changing mobility behaviour. While it is true that behaviour changes of one individual are negligible, when summated across millions of individuals making the similarly informed decision, the impact could be significant. Furthermore, the external costs may be included in cost-benefit analysis for the appraisal of transport projects and they may provide valuable information for supporting environmental policies.

Thus, it seems evident that a generally applicable, transparent, and comprehensive methodology to quantify external costs is needed to foster their integration into policy and decision making. This issue is further analysed in the next section, where the methodology applied in this analysis is presented.

5.2. The ExternE Methodology

External costs can be calculated using various methodologies, for instance “top-down” approaches (e.g., Hohmeyer, 1988; Ott, 1997) and extended Life Cycle Analysis (e.g., A. D. Owen, 2004). However, the methodology suggested by the European Research Network ExternE (External Costs of Energy) funded by the European Commission can be regarded as the most advanced approach for the estimation of air pollution costs and, thus, it is recommended as a best practice methodology (European Commission, 2008b).

The “bottom-up” methodology developed within the ExternE project series provides a robust and validated approach for estimating external costs, allowing different technologies to be compared (European Commission, 1995, 2005). Over the last fifteen years, the ExternE methodology has been extensively applied in a number of studies to estimate the external costs of energy systems and policies, such as CASES (Cost Assessment for Sustainable Energy Systems), NewExt (New Elements for the Assessment of External Costs from Energy Technologies), and NEEDS (New Energy Externalities Developments for Sustainability). As for the transport sector, this methodology has also been applied in European-funded projects, such as UNITE (Unification of Accounts and Marginal Costs for Transport Efficiency), RECORDIT (Real Cost Reduction of Door-to-door Intermodal Transport), HEATCO (Developing Harmonised European Approaches for Transport Costing and Project Assessment) and GRACE (Generalisation of Research on Accounts and Cost Estimation). Consequently, the methodology is being continually updated in order to incorporate the most recent scientific findings.

The ExternE methodology comprises several stages. The activity to be assessed and the corresponding background (or reference) scenario are defined in a first stage. Relevant externalities and impact categories are also defined in this stage. In a second stage, a detailed bottom-up approach, the Impact Pathway Approach, is carried out to define a reference scenario, followed by a second analysis using the same reference scenario but including the additional activity of interest (e.g., an additional kilometre travelled with a vehicle). The difference between both analysis is then interpreted as the impacts caused by the activity being assessed, which leads directly or indirectly (e.g., through health effects caused by air pollutants) to a change in the utility of the affected persons. Finally, the resulting welfare changes from these impacts are then transferred into monetary values. In the next section, the main components of the Impact Pathway Approach are outlined.

5.3. The Impact Pathway Approach, a bottom-up analysis

The impacts of vehicle-related pollutant emissions were estimated using the Impact Pathway Approach (IPA) developed within the ExternE projects. In this approach, pollutant emissions are followed in their journey through the air, taking into account their transformation due to physical, mechanical and/or chemical processes. In this way, pollutant concentrations can be estimated for a certain spatial and temporal reference scenario. A second simulation with perturbed emissions data allows the assessment of concentration changes due to the additional emissions. Making use of concentration-response functions, these concentration changes can then be associated with impacts on human health and the environment. A brief description of each stage of the IPA is presented in the following.

5.3.1 Emissions

Emissions can be defined as discharges into the atmosphere by natural and anthropogenic sources. Not all emissions contaminate per se, but when their levels, chemical nature or persistence generate harm or discomfort humans and other living organisms and materials, they become pollutants. Quantifying the amount of emissions considered in an analysis is an essential task since this parameter is one of the most strongly correlated to ambient concentration of pollutants. The emission datasets used in this assessment were described in detail in Chapter 2, along with the methodology followed for their spatial disaggregation.

5.3.2 Air dispersion modelling

Emissions are subjected to physical, chemical and mechanical processes in their journey through the atmosphere. A method for simulating this phenomenon uses dispersion models, which resort to a myriad of different approaches, ranging from simple empirical correlations to more computationally expensive and complex models. When analysing the dispersion of pollutants over a large domain such as Europe, long-range transport should be included in the analysis. As a result, a regional dispersion model was adopted in this work for estimating the changes in background concentrations on a European scale attributed to changes in the urban emissions. Using a regional dispersion model allows to consider important regional and continental atmospheric chemical effects, along with transboundary pollutant transport. The regional dispersion model applied was the Polyphemus system (Mallet et al. 2007). A detailed description of the model setup, configuration, and input data are provided en Annex D. The results provided by the urban increment model discussed at length in Section 3.4 were then coupled with the results provided by the regional dispersion model. This configuration allows to capture the transport of emissions released in Germany at a local level and the long-range pollutant transportation over the whole of Europe as well.

5.3.3 Estimation of physical impacts

Physical impacts attributed to a certain activity are estimated using Concentration Response Functions (CRF). A CRF associates an ambient air pollution concentration that affects a receptor (e.g., a human being, an ecosystem, a building) to the physical impact on this receptor. Since an impact can only be quantified if a CRF is known, considerable research efforts have been focused on understanding the effects of pollutants on the environment and living organisms. As a result, CRFs for the impacts caused by a range of pollutants on human health, buildings[14], and crops have been formulated and they are also continuously subjected to revision in order to draw the most recent epidemiological findings. Considering that results from studies focusing on the estimation of external costs generated by road transport have shown that health impacts contribute with the largest share of the total costs (e.g., Bickel et al., 2006; Schmid, 2005), the analysis presented in this thesis focuses on the impact of airborne pollutants on human health.

The effects of some pollutants have been more extensively researched than others and, as a result, they are better understood. For instance, damage from carbon monoxide and ozone in particular have been studied over the last three decades and they are now better understood, whereas knowledge about health impacts from the different fractions of particulate matter and nitrogen dioxide is still at an early stage. Within the framework of ExternE and other related projects, several CRFs were used for estimating the impacts of the energy production and other anthropogenic activities. More recently, a set of concentration-response functions has been updated and improved within the scope of the EU-financed project NEEDS (New Energy Externalities Developments for Sustainability). Table 5.1 gives an overview of the endpoints or health impacts developed within this project (NEEDS, 2007).

[14] Regarding materials, the International Cooperative Programme on Effects of Air Pollution on Materials, including Historic and Cultural Monuments (ICP Materials) has performed quantitative evaluations of the exposure of materials in a network of test sites in a wide geographical zone. As a result, a set of dose-response functions was developed describing the deterioration of material attributed to several air pollutants (Tidblad et al., 2001).

Table 5.1 Overview of the concentration response functions for particulate matter and ozone.

Endpoint	Pollutant	Age group	Risk group fraction	CRF (95% CI)	Units
Chronic Mortality					
Life expectancy reduction	$PM_{2.5}$	30+	1	651 (127; 1194)	YOLL[a] per 10 μg/m^3 per 100 000 people
Infant mortality					
Increased mortality risk	PM_{10}	0-1	0.4%	4% (2%; 7%) 18	Attributable cases per 10 μg/m^3 YOLL per 10 μg/m^3 per 100 000 people (all ages)
Acute mortality					
Increased mortality risk	O_3 / SOMO35	All	0.99%	0.3% (0.1%; 0.43%) 0.75	Attributable cases per 10 μg/m^3 YOLL per case
Morbidity					
New cases of chronic bronchitis	PM_{10}	27+	0.38%	26.5 (-1.9; 54.1)	Per year, per 10 μg/m^3, per 100 000 adults aged 27+
Respiratory hospital admissions	PM_{10}	All	1	7.03 (3.83; 10.3)	Per year, per 10 μg/m^3, per 100 000 people
Cardiac hospital admissions	PM_{10}	All	1	4.34 (2.17; 6.51)	Per year, per 10 μg/m^3, per 100 000 people
Medication use / bronchodilator use	PM_{10}	5-14	PEACE criteria[b] (15% N&E-EU)[c] (25% W-EU)[d] Medicatio use 10%	180 (-690; 1060)	Per year, per 10 μg/m^3, per 1000 children meeting the PEACE criteria
	PM_{10}	20+	Asthmatics 4.5% Daily medication use probability 50%	912 (-912; 2774)	Per year, per 10 μg/m^3, per 1000 adults 20+
Lower respiratory symptoms (LRS)	PM_{10}	Adults	Symptomatic adults (30%)	1.3 (0.15; 2.43)	Symptom days per year, per 10 μg/m^3, per adults with chronic respiratory symptoms
	PM_{10}	5-14		1.86 (0.92; 2.77)	Symptom days per year, per 10 μg/m^3, per child 5-14
Restricted activity days (RADs)	$PM_{2.5}$	15-64	1	902 (792; 1013)	per year, per 10 μg/m^3, per 1000 adults 15-64
Work lost days (WLDs)	$PM_{2.5}$	15-64	1	207 (176; 208)	per year, per 10 μg/m^3, per 1000 adults 15-64
Minor restricted activity days (MRADs)	$PM_{2.5}$	18-64	1	577 (468; 686)	per year, per 10 μg/m^3, per 1000 adults 18-64
Respiratory hospital admissions	O_3 / SOMO35	65+	1	12.5 (-5; 30)	per year, per 10 μg/m^3, per 100 000 people 65+
MRAD	O_3 / SOMO35	18-64	1	115 (44; 186)	per year, per 10 μg/m^3, per 1000 adults 18-64
Medication use / bronchodilator use	O_3 / SOMO35	20+	Asthmatics (4.5%)	730 (-225; 1570)	per year, per 10 μg/m^3, per 1000 asthmatics adults 20+
LRS excluding cough	O_3 / SOMO35	5-14	1	0.16 (-0.43; 0.81)	Days of LRS per year, per 10 μg/m^3, per child 5-14
Cough days	O_3 / SOMO35	5-14	1	0.93 (-0.19; 2.22)	Cough days per year, per 10 μg/m^3, per child 5-14

[a] YOLL – Years Of Life Lost
[b] PEACE (Pollution Effects on Asthmatic Children in Europe) is a multicity panel study conducted in 14 centres using a common protocol. The reader is referred to Roemer et al. (2000) for a comprehensive discussion on the PEACE criteria.
[c] N&E-EU – North and East Europe
[d] W-EU – West Europe
CI = Confidence Interval

Source: NEEDS, 2007.

The end points for acute and chronic mortality are expressed in terms of years of life lost (YOLL), which is a metric to calculate mortality impacts as a reduction in life expectancy. From Table 5.1 can be also concluded that the impact analysis is restricted to particulate matter and ozone, contrary to earlier studies where the effects of other pollutants, such as carbon monoxide, nitrogen dioxides and sulphur dioxide, were also included in the analysis. This difference lies in the fact that the effects of such gases are no longer considered to be independent from those attributed to particulate matter or ozone. Furthermore, evidence for the association between nitrogen dioxides and adverse health effects still remains inconclusive (NEEDS, 2007).

Using the concentration response functions presented in Table 5.1, the total physical damages of a certain vehicle activity can be estimated aggregating the damages over the population affected. The methodology for estimating the human health impacts is discussed in detail in section 5.4.

5.3.4 Monetary valuation

The theory of the measurement of welfare effects on the prices people pay for the goods they consume has been extensively discussed elsewhere (e.g., Boadway & Bruce, 1984; Johansson, 1987). Yet, welfare theory also states that damage to non-market goods represents welfare losses for individuals (Freeman, 2003). Given that competitive markets rarely exist from which benefit and costs can be directly measured in order to be used as values, special techniques are needed to place consumer preferences for environmental goods and human health on a common ground with demand for more conventional amenities.

It is important to note that whilst the use of monetary values for characterising environmental amenities may still be controversial and involve large uncertainties, expressing damage to human health or ecosystems in monetary values is an efficient practice which allows for including externalities into economic equations. Furthermore, they provide a valuable benchmarking tool, which can be implemented for a broad range of uses. Consistent comparison among energy systems, new technologies, policies and regulations for emission reduction – just to name a few – can be attained when the environmental effects are expressed in monetary metrics. In the next section, the non-market valuation techniques applied for human health and climate change – the two main impacts addressed in this study – are discussed.

5.3.4.1 Monetary valuation of health impacts

Evaluation of damages on human health can be ascertained by means of an individual’s preferences, namely the willingness to pay (WTP) for improving an existing environmental amenity (e.g., air quality) or their willingness to accept (WTA) compensation for non-improvement (e.g., increasing days of coughing due to air pollution). These values are commonly obtained using valuation methods suited for non-market goods. Navrud and Pruckner (1997) distinguish three types of procedures for valuating environmental goods and health impacts: household production function methods, hedonic price analysis and contingent valuation. According to the ExternE methodology and subsequent projects, the contingent valuation is the most used approach for valuating impacts on human health and, thus, the first two approaches are not discussed here further.

Contingent valuation is a stated preference method based on the simulation of market exchanges using survey questionnaires. The questions can be formulated in such a way that they elicit monetary values directly (the contingent valuation and trade off techniques) or elicit values indirectly (contingent ranking and rating, and the priority evaluator). In this way, intended behaviour of a sample of respondents can be analysed and transferred to whole populations (e.g., a country).

However, intentions are usually costless to express and the answers given by the respondents may be different under real conditions and, since the method is based on individual preferences, their valuation necessarily involves subjective choices. In fact, although according to economic theory the maximum WTP should be equal to the minimum WTA, evidence from contingent valuation studies shows that, along with large differences between people's responses, WTA is actually higher than WTP by a factor depending on the type of goods being analysed (see Horowitz and McConnell, 2000, for a comprehensive review of studies focusing on WTA/WTP ratio)[15].

Thus, very different WTP and WTA estimates for non-market goods are likely to result depending on how an issue is framed. Hanemann (1991) suggest that the choice between WTP and WTA depends generally on where the property right lies. For instance, if the recipients of an environmental service have a right to that service, the loss from eliminating such a service is the WTA. On the other hand, if no inherent right to use an environmental service can be recognized, it follows that its value to people is better measured by the WTP. As for human health, the experience accumulated within ExternE and related projects has shown that health impacts are more appropriately valued using contingent studies eliciting the WTP.

Generally, contingent valuation surveys are used to look at the WTP based on changes of Life Expectancy (LE)[16] to obtain the value of a life year (VOLY), which is one of the key parameters developed within ExternE. More recently, a questionnaire based on the change of LE was conducted in nine European countries (Czech Republic, Denmark, France, Germany, Hungary, Poland, Spain, Switzerland and the United Kingdom) within the framework of the NEEDS project. Consensus of a team of European experts and the results of the aforementioned questionnaire provided the scientific basis for the update of the VOLY, which now allows EU members and the new EU member countries to be differentiated between. However, for cost-benefit analysis of EU directives and policies, the authors suggest the use of a VOLY equal to 40 000 $€_{2006}$ (NEEDS, 2006).

It is important to note that the valuation of human health effects does not attempt to express the value of a human life in monetary terms, but rather to assess the benefit of risk reduction (e.g., reduction of the number of fatalities related to air pollution) due to air quality improvements. This methodology may not give a complete answer to the problem,

[15] Thaler (1980) suggested that the endowment effect is responsible for the divergence between WTP and WTA values. This effect posits that people demand much more to give up a possession than they are willing to spend to acquire it (See Kahneman et al., 1991, for an overview of experiments supporting this notion).

[16] Early contingent values surveys were based on the value of small changes in the probability of dying or the value of a prevented fatality. However, as demonstrated by Chilton et al. (2004), respondents seem to have problems understanding the concept of probability variations and, in consequence, more recent surveys are based on changes of Life Expectancy (LE).

yet it can be an especially efficient method when the required conditions for its effective use are available.

5.3.4.2 Monetary valuation of climate change

Climate change is probably one of the environmental issues that currently receive the most attention from all sectors of society. This is not surprising in view of the considerable scientific evidence linking greenhouse gases generated by anthropogenic activities to an uncommonly rapid increase in global temperatures. Given that road transport is responsible for almost a fifth of the EU's greenhouse gas emissions, it seems clear that any serious attempt to solve the climate change problem will necessary have to include this sector (EEA, 2009a).

In order to compare the impacts of climate change with mitigation costs, it is necessary to express the benefits of mitigated climate change in the same metrics as the costs of emission reduction – that being monetary values. Although current knowledge gaps still do not allow a detailed analysis of the impacts caused by climate change, this damage category can be evaluated by multiplying the amount of carbon dioxide equivalents[17] released by a cost factor, often called the social cost of carbon. Several approaches have been developed for estimating this factor, such as avoidance costs based on reduction scenarios of greenhouse gases, damage costs or shadow prices of an emission trading system. The approach used in this work is discussed in detail in section 5.5.3.

5.4. Estimation of human health impacts related to vehicle operation

In this section, the physical impacts on human health associated to vehicle operation are estimated using the Impact Pathway Approach. The emissions used in this analysis are: hot emissions, cold start emissions, resuspension, and non-exhaust emissions due to tyre, road surface and brake wear (see Section 5.4.1). Taking advantage of the high spatial resolution in the concentration gradients provided by the hybrid dispersion modelling approach, the results are presented not only as average marginal and total health impacts but also for each urban entity analysed in this work, comprising all large urban areas in Germany. In this context, the term 'marginal' refer to the physical impact attributed to one additional kilometre travelled with a vehicle. Further, as total vehicle kilometres travelled are known, it was possible to estimate the total physical impacts related to vehicle activities in Germany in the year 2005.

The physical impacts on human health associated to a certain vehicle activity were estimated carrying out two assessments using the hybrid dispersion modelling approach: one depicting a reference scenario and a second one including additional emissions associated with the activity under study, e.g., an additional kilometre travelled with a vehicle. The results of the first assessment, i.e., the reference scenario, have been already discussed at length in Chapter 3. As for the second assessment, emissions generated by an additional road transport activity were needed in order to run the dispersion modelling. These additional emissions were calculated using emission factors, which are presented later in this section.

[17] Carbon dioxide equivalent of a greenhouse gas is derived by multiplying the amount of the gas by the associated Global Warming Potential (GWP). For instance, the GWP for methane is 23, for nitrous oxide 296, and for carbon dioxide 1.

The difference between both analyses, which is expressed as delta concentration (ΔC), is then attributed to the transport activity being assessed. Once the delta concentration increment has been computed, population data are needed in order to estimate the population exposure according to the following equation:

$$Exposure = \Delta C(p) \cdot pop \qquad \text{Equation 5.1}$$

where ΔC depicts the delta concentration of a pollutant *p* and pop is the population affected by the delta concentration. The physical impacts, i.e., human health impacts, can then be estimated by multiplying the population exposure and the corresponding Concentration Response Functions (CRF), which were summarized in Table 5.1.

In this section, the emission factors used for estimating the emissions generated by additional road transport activities are presented. The procedure for estimating the population exposure is described in this section as well, along with the population data implemented for this purpose. Finally, an estimation of the impacts on human health related to vehicle operation for different vehicle technologies is presented.

5.4.1 Emissions generated during vehicle operation

The emissions generated during the operation of a vehicle comprise hot emissions, cold start emissions, resuspension, and non-exhaust emissions due to tyre, road surface and brake wear. The road vehicle types analysed comprise passenger cars, light duty vehicles (LDV) with both petrol and diesel fuelled engines and heavy duty vehicles (HDV) with diesel fuelled engines. Exhaust emission factors were extracted from the Handbook of Emission Factors for Road Transport (HBEFA from its initials in German).

The HBEFA is a highly detailed emission factor database which has been published as separate versions for Germany, Switzerland and Austria. The version provides emission factors for hot, excess cold start and evaporation emissions and uses specific information on slope, average trip length and traffic situations from those countries (HBEFA, 2004). Furthermore, emission factors for passenger cars, LDV and HDV were derived in measurement campaigns with real world test cycles up to EURO III and the model allows to differentiate among three types of roads: motorways, other roads, and urban. In this analysis, hot emissions factors were retrieved for average vehicle fleet, driving patterns, and traffic situations for each road type. Table 5.2 shows exhaust emission factors per vehicle kilometre for an average traffic composition for the year 2005.

Table 5.2 Hot emission factors in g/km.

Vehicle Type	Fuel type	Road type	Pollutant in g/km			
			CO_2	NMVOC	NO_X	$PM_{2.5}$
Heavy Duty Vehicle	Diesel	Motorway	708	0.322	7.010	0.144
		Other roads	607	0.274	6.369	0.138
		Urban	757	0.729	8.284	0.258
Light Duty Vehicle	Diesel	Motorway	273	0.022	0.901	0.096
		Other roads	196	0.029	0.557	0.052
		Urban	243	0.099	0.653	0.059
	Petrol	Motorway	283	0.231	0.992	0.000
		Other roads	191	0.155	0.550	0.000
		Urban	255	0.230	0.460	0.000
Passenger Car	Diesel	Motorway	185	0.031	0.605	0.045
		Other roads	136	0.025	0.420	0.029
		Urban	174	0.072	0.521	0.035
	Petrol	Motorway	199	0.043	0.214	0.000
		Other roads	151	0.037	0.165	0.000
		Urban	208	0.067	0.162	0.000

Source: HBEFA, 2004.

Additionally to hot emissions, the model provides factors for cold start emissions released in urban areas, although only in grams per start. In order to obtain emission factor by travelled kilometre, results from John (1999) and Wickert (2001) were adopted. Cold start emission factors for vehicle activities in urban areas are presented in Table 5.3.

Table 5.3 Cold start emission factors for vehicle activities in urban areas in g/km.

Vehicle Type	Fuel type	Pollutant in g/km			
		CO_2	NMVOC	NOx	$PM_{2.5}$
Light Duty Vehicle	Diesel	6.118	0.008	0.009	0.001
	Petrol	6.325	0.118	0.064	0.000
Passenger Car	Diesel	7.362	0.013	0.008	0.004
	Petrol	7.529	0.080	0.030	0.000

Source: HBEFA, 2004, John (1999) and Wickert (2001).

Non-exhaust emissions due to tyre, road surface and brake wear should be considered for an accurate calculation of fine particulate matter emissions generated by vehicles. In this work, the results obtained in a research project on behalf of the German Environment Agency (Jörß, Handke, Lambrecht, & Dünnebeil, 2007) were implemented and they are shown in Table 5.4. Finally, emission factors for resuspension (Table 5.5) were assumed as suggested by Schaap et al. (2009).

Table 5.4 Break, road surface, and tyre wear emission factors in kg/km.

Vehicle type	Emission	Pollutant in kg/km	
		PM_{10}	$PM_{2.5}$
Heavy Duty Vehicle	Break wear	0.0000320	0.0000127
	Road surface wear	0.0000380	0.0000205
	Tyre wear	0.0000270	0.0000189
Light Duty Vehicle	Break wear	0.0000115	0.0000046
	Road surface wear	0.0000075	0.0000041
	Tyre wear	0.0000101	0.0000071
Passenger Car	Break wear	0.0000074	0.0000029
	Road surface wear	0.0000075	0.0000041
	Tyre wear	0.0000064	0.0000045

Source: Jörß et al. (2009).

Table 5.5 Resuspension emission factors in g/km.

Vehicle Type	Road type	Pollutant in g/km	
		PM_{10}	$PM_{2.5}$
Heavy Duty Vehicles	Motorway	0.220	0.022
	Other roads	0.480	0.048
	Urban	0.480	0.048
Passenger Cars and Light Duty Vehicles	Motorway	0.024	0.002
	Other roads	0.053	0.005
	Urban	0.053	0.005

Source: Schaap et al. (2007).

5.4.2 Population exposure estimation

The emission factors described in the last sections were used to characterize additional vehicle activities and to carry out a second assessment to be compared against the reference scenario. The delta concentrations computed using both assessments were used for estimating population exposure.

As is common in this type of assessment, a grid, i.e. the Polyphemus system grid defined in Annex D, was used to compute the population exposure. Taking advantage of the highly spatial disaggregated pollutant concentrations provided by the hybrid dispersion modelling approach, it is possible to assess not only the delta concentrations in the rural background but also the deltas in urban background concentrations. Thus, Equation 5.1 can be rewritten as follows:

$$E_{Transport} = \sum_{i}^{n} \left(\Delta C_{i\,Rural}(p) * pop_i \right) + \left(\Delta C_{UE}(p) * pop_{UE} \right) \qquad \text{Equation 5.2}$$

where

$E_{Transport}$ = Total exposure attributed to a certain transport activity.

$\Delta C_{i\,Rural}$ = Rural background delta concentration of pollutant p in grid cell *i*.

Pop_i = Total population in grid cell *i*.

ΔC_{UE} = Urban delta concentration of pollutant p in an urban entity located in grid cell *i*

Pop_{UE} = Population in urban entity located in grid cell *i*.

For this kind of analysis, population datasets disaggregated by administrative entities (e.g., municipality, district, and commune) are commonly used as this information is readily available for most countries. Yet, this type of datasets fails to provide insight into where the people actually live and work, hardly resembling the actual spatial distribution of the population within an administrative entity. This is the same issue already discussed in Chapter 3.5.1, where the definition of urban areas was addressed. Thus, given that the concentration gradients obtained with the hybrid system allow to differentiate between urban and non-urban areas, it seems advisable to employ population data that take into account this issue as well. Such dataset was available for this assessment in the form of a population density grid generated at the European Commission Joint Research Centre (JRC). This dataset comprises population densities for the EU-27[18] countries with a spatial resolution of 100 metres. It is built on the basis of population data by commune, which was disaggregated using Corine Land Cover 2000, version 4.1 (Gallego & Peedell, 2001).

The estimation of the total population within a grid cell (pop_i) and the population in urban entities located in each grid cell (pop_{UE}) in Equation 5.2 is quite straightforward as the boundaries of each unit, i.e., grid cells and urban areas, are known. Furthermore, it is reasonable to assume that all inhabitants of urban areas are likely to be equally affected by an increment in the rural and urban background concentrations. This assumption allows the estimation of population exposure by multiplying the delta concentrations and the corresponding population.

5.4.3 Health impacts related to vehicle operation

The health impacts due to road vehicle operation were estimated taking into account the population exposure obtained with Equation 5.2 and the corresponding concentration response functions (CRF), which were summarized in Table 5.1. In this context, the emissions generated during the operation of a vehicle comprise hot emissions, cold start emissions, resuspension, and non-exhaust emissions due to tyre, road surface and brake wear. As suggested in the ExternE Methodology update 2005, primary particles from vehicles were assumed to have 1.5 times the toxicity of $PM_{2.5}$ (European Commission, 2005). With this

[18] EU-27 comprises Austria, Belgium, Bulgaria, Cyprus, Czech Republic, Germany, Denmark, Estonia, Spain, Finland, France, United Kingdom, Greece, Hungary, Ireland, Italy, Lithuania, Luxembourg, Latvia, Malta, Netherlands, Poland, Portugal, Romania, Sweden, Slovenia, and Slovakia.

information, human health impacts were estimated in terms of Disability Adjusted Life Years (DALY). This metric combines mortality and morbidity risks from air pollution and it is calculated as the sum of Years of Life Lost (YOLL), which is a metric to calculate mortality impacts as a reduction in life expectancy, and the Years Lost due to Disability (YLD) for incident cases of a health condition (NEEDS, 2007).

Taking advantage of the high spatial resolution in the concentration gradients provided by the hybrid dispersion modelling approach, not only the average marginal and total health impacts related to vehicle operation in Germany are presented in this section but also for each urban entity analysed in this work.

5.4.3.1 Marginal health impacts related to vehicle operation

The marginal DALYs, i.e. the DALYs attributed to one additional kilometre travelled with a certain vehicle, are presented in Figure 5.1. The emissions amount generated by each vehicle activity was determined using the emission factors introduced in Section 5.4.1. Here it is useful to note that these emission factors were estimated for average traffic composition, driving patterns, and traffic situations in Germany. Furthermore, as damages on human health vary across cities, the average damage for all cities was used to construct this figure.

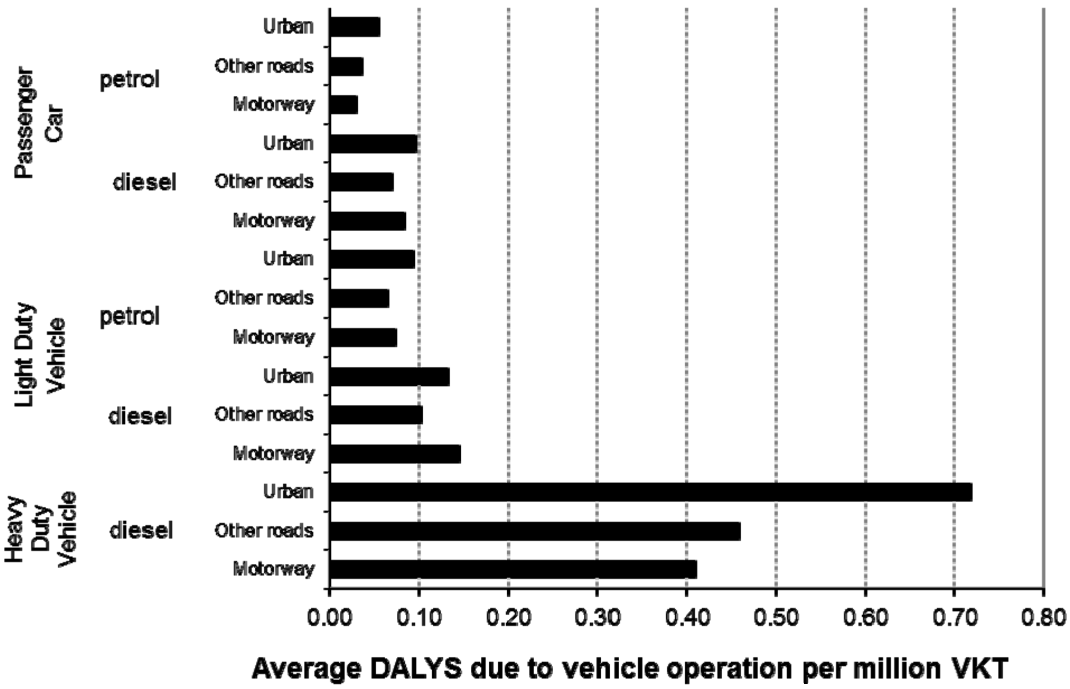

Figure 5.1 Average disability adjusted life years (DALYs) per million vehicle kilometre travelled in Germany in 2005 by vehicle and fuel type.

As it can be expected, the damages on human health are strongly correlated with the amount of emissions released per kilometre by a vehicle. Thus, heavy duty vehicle vehicles have the highest damage, especially when they pass through urban areas and passenger vehicles generate a lower number of DALYs than light duty vehicles. It can be noted that the highest number of DALYS for all vehicle types are generated when passing through urban areas, with the exception of diesel light duty vehicles. For this vehicle type, the number of DALYs is 8% higher in motorways than in urban areas. The reason for this development can be found in the fact that the $PM_{2.5}$ hot emissions generated by this vehicle type are around 60% higher in motorways than in urban areas (see Table 5.2). Looking at the hot emission factor provided in Table 5.2, it is also evident that the $PM_{2.5}$ hot emissions of diesel passenger cars are also higher in motorways than in urban areas. However, in this case the difference is smaller and it accounts for 30% more emissions in motorways than in urban areas.

In order to gain insight into the differences in DALYs across urban areas in Germany, results for a diesel passenger car driving through urban areas are presented in Figure 5.2. This figure helps to visualize the differences in DALYs across cities, which account for about 20% for this vehicle type. The urban areas with the largest DALYs per million VKT are Munich, Berlin, and the Stuttgart area (including Leinfelden), followed by Frankfurt and Düsseldorf. One of the most important factors influencing this development are likely the population affected by an increase in road vehicle emissions, along with the size of the area occupied by the urban entity. Furthermore, the lower average wind speed is another factor contributing to higher health damages attributable to a certain road transport activity.

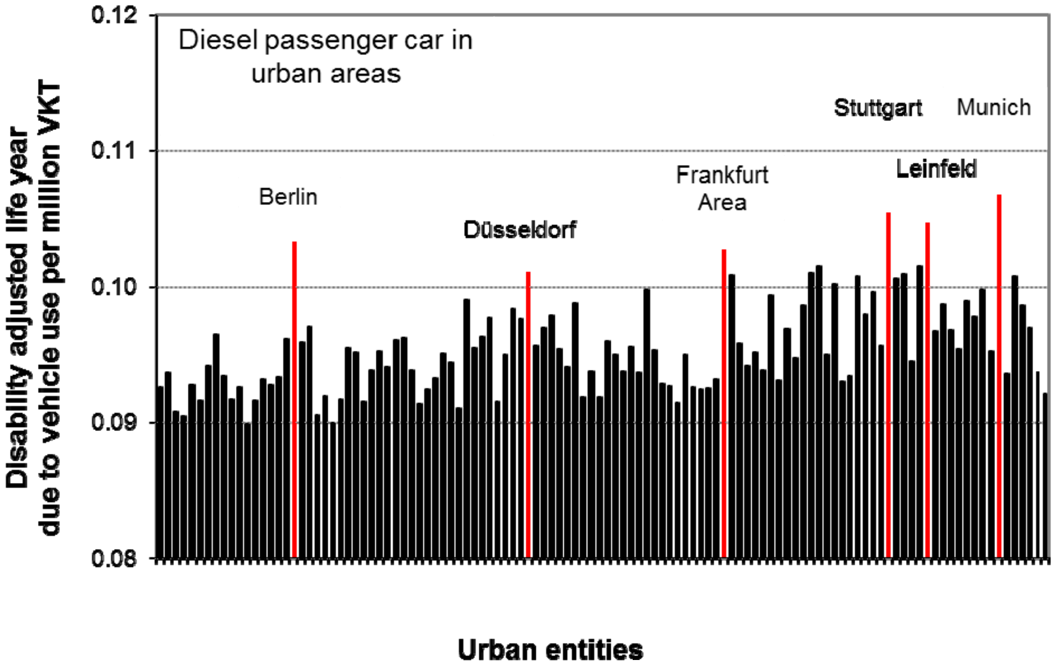

Figure 5.2 Disability adjusted life years due to the operation of a diesel passenger car in urban areas per million VKT in Germany in 2005.

5.4.3.2 Total health impacts related to vehicle operation

As the marginal health impacts related to vehicle operation are known, the total vehicle kilometres travelled by vehicle and type fuel are needed for estimating the total health impacts. For this purpose, mileage data for the main road network provided by Köble et al. (2009) and own calculations for urban mileage were used. Furthermore, the split between diesel and petrol vehicle kilometres travelled was drawn from national totals estimated by Kalinowska and Kunert (2007). The total vehicle kilometres travelled by vehicle and type fuel are presented in Table 5.6. Here it is important to note that although the mileage from motorized two-wheelers and other unspecified vehicles were not included in the analysis presented above, the mileage covered with the vehicle categories covered in Table 5.6 account for over 95 percent of the reported national total vehicle kilometres travelled.

The total health impacts related to vehicle operation expressed as DALYs are presented in Table 5.6. The results indicate that the health damages attributed to road vehicle operation in Germany in the year 2005 account for almost 60 thousand DALYs.

Table 5.6 Total health impacts due to vehicle operation in Germany in 2005.

Vehicle Type	Fuel type	Road type	Mileage in mill. VKT	Average DALYS due to vehicle operation per mill. VKT	DALYS due to vehicle operation
Heavy Duty Vehicle	Diesel	Motorway	30175	0.4090	12340
		Other roads	17044	0.4586	7816
		Urban	2904	0.7181	2085
Light Duty Vehicle	Diesel	Motorway	13633	0.1448	1974
		Other roads	10666	0.1015	1082
		Urban	15970	0.1317	2103
	Petrol	Motorway	453	0.0726	33
		Other roads	354	0.0639	23
		Urban	530	0.0933	49
Passenger Car	Diesel	Motorway	54796	0.0823	4507
		Other roads	69451	0.0693	4810
		Urban	58201	0.0956	5563
	Petrol	Motorway	114875	0.0300	3441
		Other roads	145598	0.0363	5284
		Urban	122013	0.0535	6526
				Total DALYs	**57637**

Source: own calculations, Köble et al. (2009) and Kalinowska and Kunert (2007).

Total DALYs for all large urban areas in Germany are presented in Figure 5.3. This figure helps to visualize the large differences in total DALYs across cities, which in some cases account for two orders of magnitude. The urban areas with the largest total DALYs attributed to vehicle use are located in the Essen-Dortmund area, Cologne-Bonn, and Berlin, followed by Hamburg, Frankfurt, Munich, and Stuttgart.

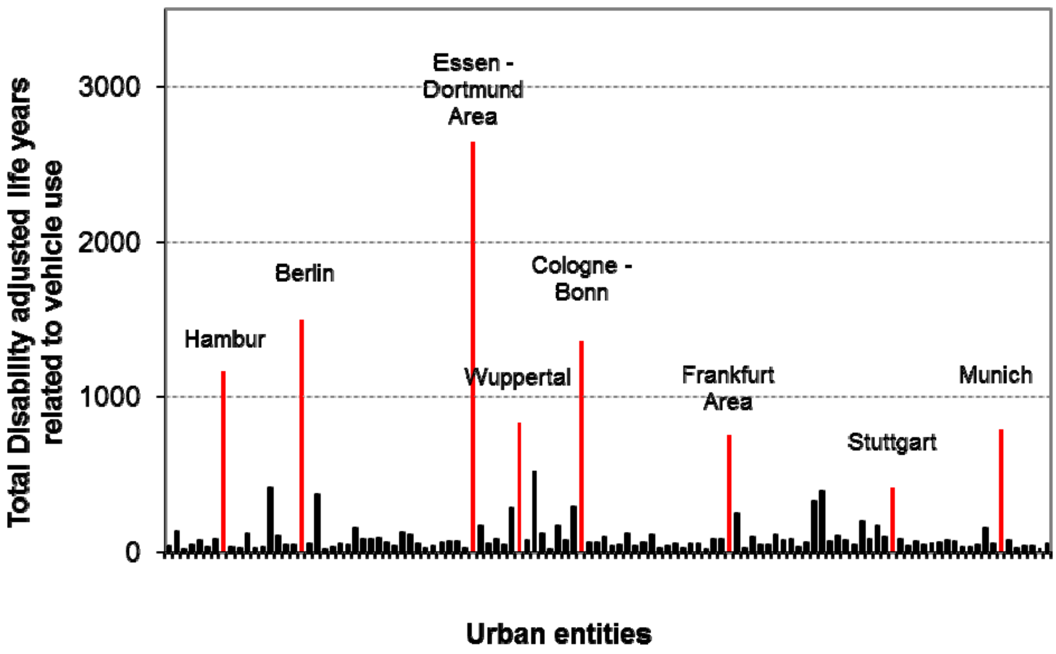

Figure 5.3 Total disability adjusted life years due to the operation of vehicles in urban areas.

5.5. Estimation of health and climate change costs of vehicle-related air pollutants

In this section, monetary values are used to derive human health costs associated to vehicle operation. Although vehicle operation consumes a large fraction of the total energy used by road transport, other up- and downstream processes are also relevant when calculating external costs since they yield the remaining fraction of the energy used and, therefore, have influence on the total costs. As a consequence, the processes that take place before and after the vehicle operation were taken into account in order to get the full picture of the health costs attributed to road transport. Furthermore, considering that climate change is probably the most pressing environmental issue facing our planet today and that the road transport sector has a large share on the overall CO_2 emissions, the costs associated to climate change are also drawn in this analysis.

Several EU research projects have come to the conclusion that the most efficient way of estimating damages associated to air pollution is by means of marginal costs (e.g., CAPRI, EXTERNE, HEATCO, GRACE). Marginal external costs of transport can be defined as 'those additional costs imposed on society by a person making an additional journey, which are not accounted for by that person.', (Nash, Sansom, & Matthews, 2001). In the environmental science, it is commonly accepted that total average costs are approximately equal to marginal costs. However, whilst this holds true for air pollution, it cannot be readily applied for other environmental effects, such as noise or crop losses. Thus, for the purposes of this assessment, the marginal cost is defined as the cost of an additional trip using a vehicle with a certain technology.

Given the physical impacts, appropriate monetary values are needed to derive damage costs. In this assessment, the monetary value chosen to derive damage costs was the one suggested in the NEEDS project (NEEDS, 2006). Within the framework of the NEEDS project, a questionnaire based on the change of life expectancy was conducted in nine European countries. Consensus of a team of European experts and the results of the aforementioned questionnaire provided the scientific basis for suggesting the use of a value of a life year (VOLY) equal to 40 000 €$_{2006}$ (NEEDS, 2006). This value was used to derive chronic and acute mortality damage costs. As for morbidity impacts, such as new cases of bronchitis and respiratory hospital admissions, the values suggested in Preiss et al. (2008) were used to derive morbidity damages costs.

5.5.1 Marginal costs due to vehicle operation

Marginal costs due to vehicle operation were estimated making use of the emission factors introduced in the last section. Table 5.7 presents the estimation of the average marginal health costs due to vehicle operation split into regional and average local costs in €$_{2000}$ per 100 vehicle kilometres travelled. Average marginal health costs are strongly correlated to the emissions released by a vehicle, for instance, the health costs attributable to heavy duty vehicles are seven times higher as a petrol passenger car when they diverge through an urban area. Given that there is a strong correlation between health impacts and the costs associated to them, the cities with the largest costs correspond to the cities with the largest damages expressed as DALYs in Figure 5.3, namely Munich, Berlin, and Stuttgart, followed by Frankfurt and Düsseldorf.

Table 5.7 Average marginal health cost due to vehicle operation in Germany in 2005.

Vehicle Type	Fuel type	Road type	Regional costs in € per 100 VKT			Average local costs in €$_{2000}$ per 100 VKT		Vehicle operation costs in €$_{2000}$ per 100 VKT
			PM $_{Coarse}$	$PM_{2.5}$	ozone	PM $_{Coarse}$	$PM_{2.5}$	
Heavy Duty Vehicle	Diesel	Motorway	0.052	1.081	0.002	n.a.	n.a.	1.135
		Other roads	0.102	1.179	0.002	n.a.	n.a.	1.283
		Urban	0.102	1.775	0.006	0.014	0.349	2.245
Light Duty Vehicle	Diesel	Motorway	0.008	0.565	0.000	n.a.	n.a.	0.573
		Other roads	0.013	0.361	0.000	n.a.	n.a.	0.374
		Urban	0.013	0.399	0.001	0.002	0.080	0.495
	Petrol	Motorway	0.008	0.090	0.002	n.a.	n.a.	0.099
		Other roads	0.013	0.104	0.001	n.a.	n.a.	0.118
		Urban	0.013	0.104	0.003	0.002	0.010	0.132
Passenger Car	Diesel	Motorway	0.007	0.294	0.000	n.a.	n.a.	0.301
		Other roads	0.012	0.227	0.000	n.a.	n.a.	0.240
		Urban	0.012	0.275	0.001	0.002	0.053	0.342
	Petrol	Motorway	0.007	0.069	0.000	n.a.	n.a.	0.076
		Other roads	0.012	0.083	0.000	n.a.	n.a.	0.096
		Urban	0.012	0.083	0.001	0.002	0.008	0.106

n.a. = Not applicable

5.5.2 Marginal costs due to up- and downstream processes

Whereas vehicle operation consumes a large fraction of the total energy consumed by road transport, other up- and downstream processes are also relevant when calculating externals since they yield the remaining fraction and, therefore, have influence on the total costs. For this reason, large research efforts have been invested over the last few decades to provide insight into the full range of environmental and social damages related to goods and services. Given that a detailed impact pathway approach comprising the whole life of a good or service (i.e., materials production, manufacturing, use, maintenance and end-of-life) remains unfeasible, simplified approaches have been developed. For instance, Life Cycle Assessment (LCA) addresses these issues by quantifying the environmental impact of goods and products in a generalised way. Thus, in order to get the full picture of the health impacts attributed to road transport, processes that take place before and after the vehicle operation should be taken into account. For this purpose, emission factors were taken from the Ecoinvent database, which is the result of a large effort by Swiss institutes to update and integrate several databases into a user-friendly platform (Ecoinvent Centre, 2008).

In addition to emissions released during vehicle operation, emissions due to the following up-and downstream processes were also considered: fuel provision, vehicle provision, maintenance and disposal. Table 5.8 and Table 5.9 show the emissions associated to vehicle provision, maintenance and disposal.

Table 5.8 Emissions generated by passenger vehicle provision, maintenance and disposal in kg/vehicle, including downstream processes.

Process	NO_X	PM_{coarse}	$PM_{2.5}$	Ozone	SO_2
Provision	3.166	0.242	0.514	0.020	1.566
Maintenance	0.531	0.015	0.023	0.004	0.026
Disposal	0.142	0.004	0.006	n.s.	0.013
Total	3.839	0.260	0.543	0.024	1.605

Table 5.9 Emissions generated by heavy duty vehicle provision, maintenance and disposal in kg/vehicle, including downstream processes.

Process	NO_X	PM_{coarse}	$PM_{2.5}$	Ozone	SO_2
Provision	21.131	0.728	2.894	0.066	8.481
Maintenance	20.025	0.039	0.752	0.043	1.048
Disposal	0.358	0.005	0.017	0.000	0.011
Total	41.514	0.772	3.664	0.109	9.540

The values provided in both tables are expressed in kg per vehicle. In order to obtain values in terms of grams per kilometre travelled, a life use of 12 and 15 years was assumed for passenger and heavy duty vehicle, respectively. Furthermore, an average of 12 500 and 22 000 km travelled per year were assumed (BASt, 2009).

Concerning fuel provision, the emissions generated by fuel provision are presented in Table 5.10. Here it is important to note that it is assumed that gasoline and diesel are produced in refineries under representative European conditions and with average production technology.

Table 5.10 Emissions generated by fuel provision at regional storage in g/kg fuel, including downstream processes.

Type of fuel	NO_X	PM_{coarse}	$PM_{2.5}$	Ozone	SO_2
Petrol	0.198	0.007	0.017	0.001	0.017
Diesel	0.185	0.006	0.016	0.001	0.016

The values in Table 5.10 are provided in terms of g/kg fuel and, therefore, data concerning fuel use (g/km) were also retrieved from the HBEFA (see Table 5.11). Using these data, the emissions generated by fuel provision were determined in terms of grams per kilometre travelled.

Table 5.11 Fuel use by vehicle type in g/km.

Vehicle Type	Fuel type	Street type	Fuel Use [g/km]
Heavy Duty Vehicle	Diesel	Motorway	223.02
		Other roads	191.20
		Urban	238.33
Light Duty Vehicle	Diesel	Motorway	86.01
		Other roads	61.83
		Urban	76.53
	Petrol	Motorway	89.03
		Other roads	60.27
		Urban	80.35
Passenger Car	Diesel	Motorway	58.19
		Other roads	42.84
		Urban	54.79
	Petrol	Motorway	62.72
		Other roads	47.59
		Urban	65.54

Emissions associated with up- and downstream processes were valued using damage factors based on recent findings reported by the NEEDS project. Given that neither source location nor release height for the different emissions and processes are known, damage factors were selected assuming average European conditions (EU-27) and average release height

(NEEDS, 2008). Furthermore, it is assumed that emission source is not located within densely populated areas. Damage factors for up- and downstream processes are shown in Table 5.12.

Table 5.12 Average EU-27 damage factors for pollutants assuming average release height. Only human health costs are considered.

	€$_{2000}$ per tonne emitted			
	NO_X	PM_{coarse}	$PM_{2.5}$	SO_2
EU-27	6082	1441	26559	6604

Source: NEEDS, 2008.

Using the damages factors provided in Table 5.12, the costs associated to fuel use and up- and downstream processes were estimated for each vehicle category. The results are provided in Table 5.13.

Table 5.13 Marginal costs associated to up- and downstream processes in €$_{2000}$ per 100 VKT.

Vehicle Type	Fuel type	Road type	Provision, maintenance and disposal in €$_{2000}$ per 100 VKT	Fuel Use in €$_{2000}$ per 100 VKT
Heavy Duty Vehicle	Diesel	Motorway	0.125	0.037
		Other roads	0.125	0.032
		Urban	0.125	0.040
Light Duty Vehicle	Diesel	Motorway	0.052	0.014
		Other roads	0.052	0.010
		Urban	0.052	0.013
	Petrol	Motorway	0.052	0.016
		Other roads	0.052	0.011
		Urban	0.052	0.014
Passenger Car	Diesel	Motorway	0.032	0.010
		Other roads	0.032	0.007
		Urban	0.032	0.009
	Petrol	Motorway	0.032	0.011
		Other roads	0.032	0.008
		Urban	0.032	0.012

5.5.3 Marginal costs associated to climate change

Climate change is probably the most pressing environmental issue facing our planet today, attracting wide attention and concern among all sectors of the society. This is not surprising in view of the considerable scientific evidence linking greenhouse gases generated by anthropogenic activities to an uncommonly rapid increase in global temperatures. As outlined by the Intergovernmental Panel on Climate Change (IPCC) in its Fourth Assessment report: 'it is likely that anthropogenic warming has had a discernible influence on many physical and biological systems.', (IPCC 2007b). As a result, global mean temperatures and temperature variability are expected to increase in the near future. The consequences of these changes cannot be yet foreseen, despite intensive research efforts focused on understanding the mechanisms and processes governing climate changes. On the other hand, while effects on natural and human environments have also been related to climate changes at the regional scale, it is still difficult to discern whether these changes are emerging due to adaptation or to non-climate drivers. Nevertheless, it seems to be a strong international consensus that non-action is no longer an option.

Following from these facts, the need arise to take into account the impacts of climate change for developing environmental policies and strategies. Furthermore, in order to compare the impacts of climate change with mitigation costs, it is necessary to express the benefits of mitigated climate change in the same metrics as the costs of emission reduction, that being monetary values. Thus, it can be suggested that the economic valuation of such impacts may be the most straightforward way to achieve this goal. Although current knowledge gaps still do not allow a detailed analysis of the impacts caused by climate change, this damage category can be evaluated multiplying the amount of carbon dioxide equivalents released by a cost factor (European Commission, 2005). Several approaches have been developed for estimating this factor, such as avoidance costs based on reduction scenarios of greenhouse gases, damage costs or shadow prices of an emission trading system.

Recent research on this subject conducted by the NEEDS project uses the Climate Framework for Uncertainty, Negotiation and Distribution (FUND) model to estimate damage and avoidance costs. The FUND model has been used for this purpose in a number of studies (e.g., Tol et al., 2003; Link and Tol, 2004; Guo et al., 2006). Two important issues have to be addressed when estimating marginal costs for climate change: one is the discount rate or the aggregation over time, and the second is equity weighing, which is the aggregation across countries or regions. Some studies show that using equity weighing results in higher marginal costs (e.g., Tol, 2003). Furthermore, when choosing the appropriate discount rate for climate change, ethical considerations relevant to the distant future are involved, as it implies how this generation values future generations.

For this assessment, the marginal costs of carbon dioxide emissions is assumed to be 23.5 $€_{2005}$ per tonne[19], which corresponds to the avoidance costs for achieving the reduction goals formulated in the Kyoto Protocol (NEEDS, 2009). Using the emission factors introduced in Section 5.4.1, the costs associated to climate change were estimated and the results are shown in Table 5.14.

[19] As this value is expressed in $EURO_{2005}$, it was deflated to $EURO_{2000}$ using the OECD Consumer Price Index (CPI).

Table 5.14 Marginal cost due to climate change in €$_{2000}$/100 VKT.

Vehicle Type	Fuel type	Road type	Climate change costs in €$_{2000}$ per 100 VKT
Heavy Duty Vehicle	Diesel	Motorway	1.537
		Other roads	1.317
		Urban	1.642
Light Duty Vehicle	Diesel	Motorway	0.593
		Other roads	0.426
		Urban	0.541
	Petrol	Motorway	0.613
		Other roads	0.415
		Urban	0.567
Passenger Car	Diesel	Motorway	0.415
		Other roads	0.295
		Urban	0.393
	Petrol	Motorway	0.432
		Other roads	0.328
		Urban	0.468

Although this value may change in the future, it seems adequate to use it to assess the current situation regarding climate change. Because of the global nature of the climate change impacts, the location at which a greenhouse emission is released do not play a role in the quantification of the damages, following that the same cost factor may be used across countries.

5.5.4 Marginal health and climate change costs related to road transport

The marginal costs presented in the last sections, i.e., vehicle operation, up- and downstream processes, and global warming, are summarised in Table 5.15. In this table, the total marginal health and climate change costs for different vehicles are shown, disaggregated by fuel and road type.

Heavy duty vehicles passing through urban areas have the largest damage costs with around 4 €$_{2000}$ per 100 VKT. This value is five times higher than the average damages attributed to a diesel passenger car for the same area. It can also be noted that petrol passenger cars cause lower cost per vehicle kilometre compared to diesel cars as they emit much less fine particles, leading to lower health impacts. A closer look at the costs distribution by damage categories reveals that the contribution of global warming to the total costs is significant, particularly for vehicles travelling through roads outside urban areas. Indeed, the share of global warming damages for these vehicles accounts for almost half of the total marginal costs. As for urban areas, vehicle operation accounts for half of the costs for diesel passenger cars and one fifth for petrol passenger cars. Concerning up and downstream processes, the costs estimated for this category account for four to ten percent of the marginal health and climate change costs.

Table 5.15 Marginal health and climate change costs related to road transport activities in Germany in 2005. All values in $€_{2000}$ per 100 VKT

Vehicle Type	Fuel type	Road type	Vehicle operation (Average)	Up- and downstream processes	Climate change	Marginal costs in $€_{2000}$ per 100 VKT
Heavy Duty Vehicle	Diesel	Motorway	1.135	0.163	1.537	2.83
		Other roads	1.283	0.157	1.317	2.76
		Urban	2.245	0.165	1.642	4.05
Light Duty Vehicle	Diesel	Motorway	0.573	0.066	0.593	1.23
		Other roads	0.374	0.062	0.426	0.86
		Urban	0.495	0.064	0.541	1.10
	Petrol	Motorway	0.099	0.067	0.613	0.78
		Other roads	0.118	0.062	0.415	0.60
		Urban	0.132	0.066	0.567	0.76
Passenger Car	Diesel	Motorway	0.301	0.042	0.415	0.76
		Other roads	0.240	0.040	0.295	0.57
		Urban	0.342	0.042	0.393	0.78
	Petrol	Motorway	0.076	0.044	0.432	0.55
		Other roads	0.096	0.041	0.328	0.46
		Urban	0.106	0.044	0.468	0.62

The marginal costs for a diesel passenger car driving through an urban area are shown in Figure 5.4. The three damage categories components of marginal costs are presented for each urban entity: the lower bar segment depicts the global warming costs; the second bar segment represent the costs attributable top- and downstream processes, which include fuel provision, vehicle provision, maintenance, and disposal; and the costs due to vehicle operation are represented by the third bar segment. The first two damage categories have the same value for all urban entities and differences across urban entities can be observed only due to their vehicle operation costs. The variation in the marginal health and climate change costs is rather low which can be explained by the larger contribution of the global warming costs in comparison with the differences in vehicle use costs across cities.

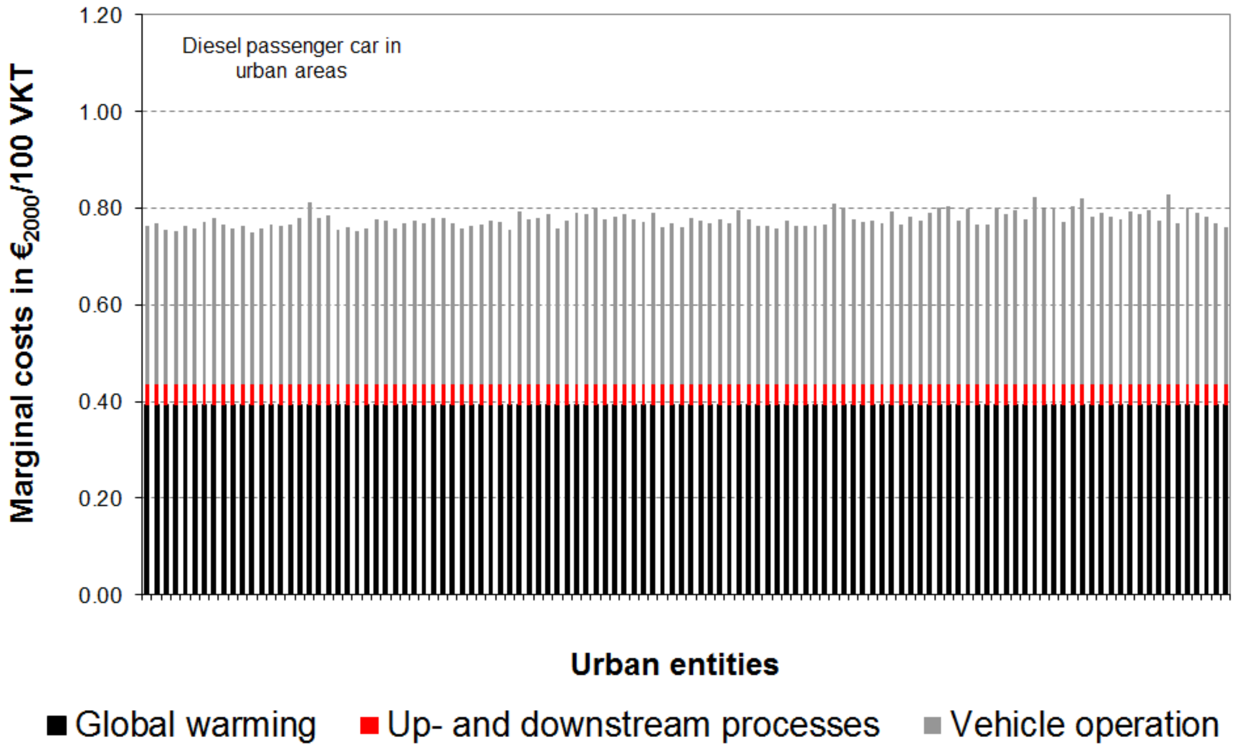

Figure 5.4 Marginal health and climate change costs related to a travel with a diesel passenger car in urban areas in Germany in 2005. Values are in $€_{2000}$ per 100 VKT.

5.5.5 Total health and climate change costs related to road transport

As the marginal health costs related to road transport are known, the total vehicle kilometres travelled by vehicle and type fuel are needed for estimating the total health impacts. For this purpose, the mileage data introduced in Section 5.4.3.2 was used. The total health impacts related to vehicle operation expressed as $€_{2000}$ are presented in Table 5.16. It was estimated that the total health and climate change costs attributable to vehicle-related air pollutants in Germany in the year 2005 amounted to 5.2 thousand millions $EURO_{2000}$. Analysing the results, it can be noted that whereas heavy duty vehicles did only 8% of the total mileage, they are responsible for 28% of the total costs. On the other hand, petrol passenger cars did almost 60% of the total mileage and their share of the total costs is only 40%. Furthermore, diesel passenger vehicles do almost 30% of the total mileage and their contribution to the total costs was estimate to be around 25%. Both diesel and petrol passenger account for about 86% of the total mileage and they are responsible for two thirds of the total costs.

Table 5.16 Total health and climate change costs due to road transport in $€_{2000}$.

Vehicle Type	Fuel type	Road type	Mileage in mill. VKT	Marginal costs in $€_{2000}$ per 100 VKT	Total costs in Mill. $€_{2000}$
Heavy Duty Vehicle	Diesel	Motorway	30175	2.83	855
		Other roads	17044	2.76	470
		Urban	2904	4.05	118
Light Duty Vehicle	Diesel	Motorway	13633	1.23	168
		Other roads	10666	0.86	92
		Urban	15970	1.10	176
	Petrol	Motorway	453	0.78	4
		Other roads	354	0.60	2
		Urban	530	0.76	4
Passenger Car	Diesel	Motorway	54796	0.76	416
		Other roads	69451	0.57	399
		Urban	58201	0.78	452
	Petrol	Motorway	114875	0.55	634
		Other roads	145598	0.46	677
		Urban	122013	0.62	754
				Total costs	**5220**

Source: own calculations, Köble et al. (2009) and Kalinowska and Kunert (2007).

5.6. Discussion on results

In this chapter, the ExternE methodology was applied for estimating health and climate change impacts associated to road vehicle activities in Germany in the year 2005. A vital component of this assessment was the calculation of changes in rural and urban background concentrations attributable to an additional vehicle activity, which was carried out with the hybrid dispersion modelling approach.

The results showed that the damages on human health are strongly correlated to the emissions released by a vehicle, the location in which they are released, the meteorological conditions, and the number of receptors that can be potentially affected by vehicle-related pollution. Moreover, heavy duty vehicle vehicles have the highest damage, especially when they pass through urban areas and passenger vehicles generate a lower number of DALYs than light duty vehicles. The results indicate that the total health damages attributed to road vehicle operation in Germany in the year 2005 account for almost 60 thousand DALYs and the urban areas with the largest total DALYs attributed to vehicle use are located in the Essen-Dortmund area, Cologne-Bonn, and Berlin, followed by Hamburg, Frankfurt, Munich, and Stuttgart.

Concerning the marginal health and climate change costs, it was found that heavy duty vehicles passing through urban areas have the largest damage costs with 4 $€_{2000}$ per 100 VKT. This value is five times higher than the average damages attributed to a diesel passenger car for the same area. Furthermore, it was found that the cities with the largest health impacts are also the cities with the largest costs related to road transport. This is not surprising as there is a strong correlation between health impacts and the costs associated to them. The contribution of global warming to the total costs is significant, particularly for vehicles travelling through roads outside urban areas. Indeed, the share of global warming damages for these vehicles accounts for almost half of the total marginal costs. As for urban areas, vehicle operation accounts for half of the costs for diesel passenger cars and one fifth for petrol passenger cars. Concerning up and downstream processes, the costs estimated for this category account for four to ten percent of the marginal health and climate change costs.

The total health and climate change costs attributed to road vehicle operation in Germany in the year 2005 were estimated to be around 5.2 thousand millions $EURO_{2000}$. The total costs obtained in this work are lower than those obtained in a similar analysis carried out by Schmid (2005). The main reason for this difference may be the fact that Schmid used a Gaussian-line-source model for the local dispersion modelling, which accounted for changes in pollutant concentrations to up to 25 km far from the road segment where the emissions were released. This means that, as changes in urban background concentrations attributable to an additional vehicle activity were not determined, the delta concentrations may have been overestimated in the Schmid study. Furthermore, urban morphology (i.e., land use, building geometry, and street patterns, among others) was not accounted for in the calculation. Since urban morphology has a significant influence on urban pollutant gradients, it is vital to include this aspect for depicting pollutant concentrations within urban environments. Finally, Schmid accounted for damages not considered in this work, such as damages on materials and crops. Although these costs categories are not relevant compared with health and climate change costs, they also contribute to the differences between Schimd's results and the results obtained in this work.

It is also worth to note that, although the analysis presented in this chapter was focused on emissions released by the road transport sector, the hybrid dispersion modelling approach can be used for assessing emissions released by activities from other sectors as well. This is possible because the hybrid dispersion modelling approach is able to estimate changes in urban background concentrations attributable to any additional emissions released from low sources within urban areas.

Considering that the methodology presented here is a restricted idealization of a real system, uncertainties can be found at every analysis stage. While the uncertainty related to the hybrid dispersion modelling approach was comprehensively addressed in Chapter 4 in this work, additional uncertainty sources may arise at every step of the analysis process. For instance, the effects of some pollutants on human health are not completely understood and, therefore, assumptions are needed for quantifying those effects. Furthermore, the assignment of economic values to non-market goods is another relevant issue. Here it is important to note that whilst the use of monetary values for characterising environmental amenities may still be controversial and involve large uncertainties, expressing damage to human health or ecosystems in monetary values is an efficient practice which allows for including externalities into economic equations.

Thus, despite the uncertainties involved in this kind of analysis, it should be recognized that the information provided by the external costs reflect, with an acceptable accuracy, damages that otherwise could only be qualitatively analysed, providing a reliable tool for supporting decision makers in the process of evaluating new directives and regulations concerning the environment.

Chapter 6

Conclusions and outlook

Air pollution control strategies have helped to improve air quality over Europe over the last thirty years. Despite this success, the improvements have been insufficient to protect health of those who spend most of their time within urban areas and particularly near major roads. Considering that an urban street network is a structuring component of the city, a detailed analysis of its interaction with the environment and inhabitants is relevant for assessing policy measures aiming at improving urban air quality. However, given the inherent complexity of urban environments and the incomplete understanding of the physical and chemical processes involved in pollutant dispersion, it is a challenging task to estimate urban air quality.

The objective of this thesis was to develop a modelling approach to resolve not only the long-range pollution dispersion but also to capture the higher pollutant concentrations commonly found within urban areas and at kerbside for assessing the localized effects associated to vehicle-related pollutants. A major challenge was to provide estimates not only for specific streets and cities but for the major road network and all streets within major cities in Germany. For this purpose, a hybrid dispersion modelling approach was developed for predicting air quality across different spatial scales: from regional to urban and kerbside scale, accounting for the intrinsic and distinctive urban morphology of urban areas. In this context, a Monte Carlo model was developed for estimating the cumulative probability of additional concentration at kerbside within urban entities. The cumulative probability provides the range of possible additional concentrations that could occur at any street roadside within an urban area and the likelihood of any concentration to occur.

The hybrid dispersion modelling approach was used for estimating annual concentrations of PM_{10}, $PM_{2.5}$, and NO_2 for all urban areas with more than 50 000 inhabitants in Germany for the reference year 2005. The results showed that there are large differences on air quality levels across urban areas in Germany, which may be relevant when planning or evaluating emission control strategies. An empiric regression function to estimate the number of days exceeding the daily limit value of 50 µg/m^3 of PM_{10} by means of the annual mean PM_{10} concentrations was also developed in this work. Using this function, it was estimated that an annual mean PM_{10} concentration above 31 µg/m^3 may lead into not meeting the standard related to the number of days exceeding the daily limit value of 50 µg/m^3 of the same pollutant, which can only be exceeded 35 times. Furthermore, taking advantage of the high spatial resolution in the air quality results, it was possible to analyse the compliance with the 24-hour limit value of 50 µg/m^3 of PM_{10} in the main road network. It was estimated that this directive is not complied in around half of the almost 6 000 kilometres of main road network passing through urban areas and that the compliance in over 95% of the length of the main road network would need a reduction of 10 µg/m^3 in the annual PM_{10} concentrations.

Lack of certainty is present at every step of the modelling approach developed in this work. This is not surprising since even the most sophisticated air dispersion models can only provide a simplified representation of the reality due to an incomplete understanding of the physical and chemical processes involved in pollutant dispersion. Thus, absolute certainty cannot be achieved and the ubiquitous nature of uncertainty has to be recognised and dealt with. In order to assess the model's reliability and accuracy, the results were compared against observational data. Furthermore, a sensitivity and uncertainty analysis were carried out as well in order to identify the parameters with the largest uncertainties and the strengths and weaknesses in the data generation process. The results of this comprehensive analysis provided reasonable evidence of satisfactory performance of the hybrid dispersion modelling approach. Furthermore, the diagnostic diagrams analysis carried out reinforce the notion that transport urban emissions play a relevant role on the model's results and, as a consequence, the efforts for enhancing the model's performance should be focused on improving the emission factors and activity rates, particularly for urban areas.

The air quality reference scenario was also applied to estimate health and climate change impacts associated to road vehicle activities in Germany in the year 2005. A vital component of this assessment was the calculation of changes in rural and urban background concentrations attributable to an additional vehicle activity, which was carried out with the hybrid dispersion modelling approach. The modelling approach enabled a differentiation not only by vehicle types and technologies but also across urban areas within a geographically referenced framework. In this way, external costs for individual cities and technologies were obtained, rather than generalised national values. The results showed that the damages on human health are strongly correlated to the emissions released by a vehicle, the location in which they are released, the meteorological conditions, and the number of receptors that can be potentially affected by vehicle-related pollution. The results indicate that the total health damages attributed to road vehicle operation in Germany in the year 2005 account for almost 60 thousand DALYs. The urban areas with the largest total DALYs attributed to vehicle use are located in the Essen-Dortmund area, Cologne-Bonn, and Berlin, followed by Hamburg, Frankfurt, Munich, and Stuttgart.

The total health and climate change costs attributed to road vehicle operation in Germany in the year 2005 were estimated to be around 5.2 thousand millions $EURO_{2000}$. Analysing the results, it can be noted that whereas heavy duty vehicles did only 8% of the total mileage, they are responsible for 28% of the total costs. On the other hand, both diesel and petrol passenger account for about 86% of the total mileage and they are responsible for two thirds of the total costs.

In summary, the results presented in this thesis show the advantages of applying a hybrid approach for assessing urban air quality, taking cognizance of the strengths of several modelling approaches working at different scales. The hybrid modelling approach developed in this work was applied for analysing urban air quality and the health and climate change impact and their associated costs of vehicle activities in Germany in the year 2005. In this context, the hybrid dispersion modelling approach showed its flexibility regarding changing initial conditions and building different scenarios for a large spatial domain. There are, however, other potential uses of the hybrid dispersion modelling approach for addressing environmental issues, such as exposure assessment. In this context, accurate data on pollutant concentrations at the boundary between a human and the environment and the duration of the contact are crucial to exposure assessment. As the modelling approach is able to provide insight into the levels of pollutant concentrations within urban areas and at kerbside with a high spatial resolution, it could be used in future research addressing the assessment of human exposure to vehicle-related pollutants.

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Annex A - Urban entities

UE ID	City Name	State
12396	Flensburg	Schleswig-Holstein
13371	Kiel	Schleswig-Holstein
13469	Stralsund	Mecklenburg-Vorpommern
13594	Rendsburg	Schleswig-Holstein
14083	Rostock	Mecklenburg-Vorpommern
14384	Neumünster	Schleswig-Holstein
15218	Bad Schwartau	Schleswig-Holstein
15218	Lübeck	Schleswig-Holstein
15218	Stockelsdorf	Schleswig-Holstein
16115	Hamburg	Hamburg
16115	Glinde	Schleswig-Holstein
16115	Halstenbek	Schleswig-Holstein
16115	Henstedt-Ulzburg	Schleswig-Holstein
16115	Norderstedt	Schleswig-Holstein
16115	Pinneberg	Schleswig-Holstein
16115	Reinbek	Schleswig-Holstein
16115	Schenefeld	Schleswig-Holstein
16601	Schwerin	Mecklenburg-Vorpommern
16729	Neubrandenburg	Mecklenburg-Vorpommern
16849	Bremerhaven	Bremen
16849	Langen	Niedersachsen
17151	Wilhelmshaven	Niedersachsen
19074	Lüneburg	Niedersachsen
19372	Bremen	Bremen
19372	Schwanewede	Niedersachsen
19596	Oldenburg	Niedersachsen
20489	Delmenhorst	Niedersachsen
22660	Hennigsdorf	Brandenburg
22770	Berlin	Berlin
22770	Falkensee	Brandenburg
22770	Kleinmachnow	Brandenburg

UE ID	City Name	State
22770	Neuenhagen	Brandenburg
22770	Teltow	Brandenburg
24638	Potsdam	Brandenburg
24642	Garbsen	Niedersachsen
24642	Hannover	Niedersachsen
24642	Hemmingen	Niedersachsen
24642	Laatzen	Niedersachsen
24642	Langenhagen	Niedersachsen
24642	Seelze	Niedersachsen
24671	Brandenburg	Brandenburg
24767	Wolfsburg	Niedersachsen
25006	Königs Wusterhausen	Brandenburg
25736	Minden	Nordrhein-Westfalen
25868	Braunschweig	Niedersachsen
25914	Osnabrück	Niedersachsen
26759	Bad Oeynhausen	Nordrhein-Westfalen
26759	Lohne	Nordrhein-Westfalen
26759	Vlotho	Nordrhein-Westfalen
26920	Magdeburg	Sachsen-Anhalt
27280	Hildesheim	Niedersachsen
27377	Herford	Nordrhein-Westfalen
28088	Bielefeld	Nordrhein-Westfalen
28088	Oerlinghausen	Nordrhein-Westfalen
28533	Münster	Nordrhein-Westfalen
29264	Gütersloh	Nordrhein-Westfalen
29743	Dessau	Sachsen-Anhalt
29770	Cottbus	Brandenburg
30565	Borchen	Nordrhein-Westfalen
30565	Paderborn	Nordrhein-Westfalen
31076	Marl	Nordrhein-Westfalen
31077	Hamm	Nordrhein-Westfalen
31249	Bitterfeld	Sachsen-Anhalt
31249	Wolfen	Sachsen-Anhalt

UE ID	City Name	State
31785	Bochum	Nordrhein-Westfalen
31785	Bottrop	Nordrhein-Westfalen
31785	Castrop-Rauxel	Nordrhein-Westfalen
31785	Dinslaken	Nordrhein-Westfalen
31785	Dortmund	Nordrhein-Westfalen
31785	Duisburg	Nordrhein-Westfalen
31785	Essen	Nordrhein-Westfalen
31785	Gelsenkirchen	Nordrhein-Westfalen
31785	Gladbeck	Nordrhein-Westfalen
31785	Hattingen	Nordrhein-Westfalen
31785	Herne	Nordrhein-Westfalen
31785	Herten	Nordrhein-Westfalen
31785	Holzwickede	Nordrhein-Westfalen
31785	Krefeld	Nordrhein-Westfalen
31785	Lünen	Nordrhein-Westfalen
31785	Moers	Nordrhein-Westfalen
31785	Mülheim	Nordrhein-Westfalen
31785	Oberhausen	Nordrhein-Westfalen
31785	Recklinghausen	Nordrhein-Westfalen
31785	Schwerte	Nordrhein-Westfalen
31785	Witten	Nordrhein-Westfalen
32162	Kamen	Nordrhein-Westfalen
32162	Unna	Nordrhein-Westfalen
32700	Göttingen	Niedersachsen
32987	Halle	Sachsen-Anhalt
33686	Arnsberg	Nordrhein-Westfalen
33974	Leipzig	Sachsen
33974	Markkleeberg	Sachsen
34002	Altena	Nordrhein-Westfalen
34002	Ennepetal	Nordrhein-Westfalen
34002	Gevelsberg	Nordrhein-Westfalen
34002	Haan	Nordrhein-Westfalen
34002	Hagen	Nordrhein-Westfalen

UE ID	City Name	State
34002	Hemer	Nordrhein-Westfalen
34002	Herdecke	Nordrhein-Westfalen
34002	Hilden	Nordrhein-Westfalen
34002	Iserlohn	Nordrhein-Westfalen
34002	Remscheid	Nordrhein-Westfalen
34002	Schwelm	Nordrhein-Westfalen
34002	Solingen	Nordrhein-Westfalen
34002	Wermelskirchen	Nordrhein-Westfalen
34002	Wetter	Nordrhein-Westfalen
34002	Wuppertal	Nordrhein-Westfalen
34624	Heiligenhaus	Nordrhein-Westfalen
34624	Velbert	Nordrhein-Westfalen
34813	Dusseldorf	Nordrhein-Westfalen
34813	Kaarst	Nordrhein-Westfalen
34813	Meerbusch	Nordrhein-Westfalen
34813	Monheim	Nordrhein-Westfalen
34813	Ratingen	Nordrhein-Westfalen
34925	Kassel	Hessen
34925	Vellmar	Hessen
35391	Görlitz	Sachsen
35805	Mönchengladbach	Nordrhein-Westfalen
36001	Lüdenscheid	Nordrhein-Westfalen
36658	Coswig	Sachsen
36658	Dresden	Sachsen
36658	Freital	Sachsen
36658	Heidenau	Sachsen
36658	Pirna	Sachsen
36658	Radebeul	Sachsen
38383	Alfter	Nordrhein-Westfalen
38383	Bad Honnef	Nordrhein-Westfalen
38383	Bergisch Gladbach	Nordrhein-Westfalen
38383	Bonn	Nordrhein-Westfalen
38383	Bornheim	Nordrhein-Westfalen

UE ID	City Name	State
38383	Brühl	Nordrhein-Westfalen
38383	Hürth	Nordrhein-Westfalen
38383	Köln	Nordrhein-Westfalen
38383	Königswinter	Nordrhein-Westfalen
38383	Leichingen	Nordrhein-Westfalen
38383	Leverkusen	Nordrhein-Westfalen
38383	Niederkassel	Nordrhein-Westfalen
38383	Sankt Augustin	Nordrhein-Westfalen
38383	Troisdorf	Nordrhein-Westfalen
38383	Wesseling	Nordrhein-Westfalen
38383	Remagen	Rheinland-Pfalz
38383	Sinzig	Rheinland-Pfalz
38906	Bergneustadt	Nordrhein-Westfalen
38906	Gummersbach	Nordrhein-Westfalen
38906	Wiehl	Nordrhein-Westfalen
39516	Erfurt	Thüringen
39840	Hilchenbach	Nordrhein-Westfalen
39840	Kreuztal	Nordrhein-Westfalen
39840	Netphen	Nordrhein-Westfalen
39840	Siegen	Nordrhein-Westfalen
40599	Jena	Thüringen
40906	Gera	Thüringen
41328	Chemnitz	Sachsen
41913	Düren	Nordrhein-Westfalen
41913	Kreuzau	Nordrhein-Westfalen
41964	Eschweiler	Nordrhein-Westfalen
41964	Stolberg	Nordrhein-Westfalen
42019	Aachen	Nordrhein-Westfalen
42397	Marburg	Hessen
42723	Hohenstein-Ernstthal	Sachsen
43489	Zwickau	Sachsen
45635	Suhl	Thüringen
46439	Giessen	Hessen

UE ID	City Name	State
47006	Fulda	Hessen
47006	Künzell	Hessen
47548	Plauen	Sachsen
48163	Andernach	Rheinland-Pfalz
48163	Neuwied	Rheinland-Pfalz
48779	Bendorf	Rheinland-Pfalz
48779	Koblenz	Rheinland-Pfalz
48779	Lahnstein	Rheinland-Pfalz
52769	Bad Soden	Hessen
52769	Eschborn	Hessen
52769	Florsheim	Hessen
52769	Frankfurt	Hessen
52769	Hainburg	Hessen
52769	Hanau	Hessen
52769	Heusenstamm	Hessen
52769	Hofheim	Hessen
52769	Maintal	Hessen
52769	Mühlheim	Hessen
52769	Obertshausen	Hessen
52769	Offenbach	Hessen
52769	Rüsselsheim	Hessen
52769	Seligenstadt	Hessen
53465	Ginsheim-Gustavsburg	Hessen
53465	Wiesbaden	Hessen
53465	Mainz	Rheinland-Pfalz
54128	Schweinfurt	Bayern
54942	Aschaffenburg	Bayern
54942	Goldbach	Bayern
54942	Hosbach	Bayern
55209	Bayreuth	Bayern
55995	Bamberg	Bayern
56196	Darmstadt	Hessen
56196	Pfungstadt	Hessen

UE ID	City Name	State
56196	Weiterstadt	Hessen
56861	Trier	Rheinland-Pfalz
57336	Würzburg	Bayern
59653	Worms	Rheinland-Pfalz
60637	Erlangen	Bayern
61273	Mannheim	Baden Württemberg
61273	Schwetzingen	Baden Württemberg
61273	Frankenthal	Rheinland-Pfalz
61273	Ludwigshafen	Rheinland-Pfalz
61890	Fürth	Bayern
61890	Lauf	Bayern
61890	Nürnberg	Bayern
61890	Oberasbach	Bayern
61890	Röthenbach	Bayern
61890	Stein	Bayern
61890	Zirndorf	Bayern
62687	Kaiserslautern	Rheinland-Pfalz
63191	Heidelberg	Baden Württemberg
63191	Leimen	Baden Württemberg
63191	Wiesloch	Baden Württemberg
63604	Dillingen	Saarland
63604	Saarlouis	Saarland
63832	Bexbach	Saarland
63832	Neunkirchen	Saarland
63832	Schiffweiler	Saarland
64427	Saarbrücken	Saarland
64427	Sulzbach	Saarland
64427	Völklingen	Saarland
64427	Wadgassen	Saarland
66160	Heilbronn	Baden Württemberg
66160	Neckarsulm	Baden Württemberg
68600	Ettlingen	Baden Württemberg
68600	Karlsruhe	Baden Württemberg

UE ID	City Name	State
68600	Pfinztal	Baden Württemberg
68662	Lappersdorf	Bayern
68662	Neutraubling	Bayern
68662	Regensburg	Bayern
70975	Ditzingen	Baden Württemberg
70975	Gerlingen	Baden Württemberg
70975	Korntal-Münchingen	Baden Württemberg
70975	Kornwestheim	Baden Württemberg
70975	Leonberg	Baden Württemberg
70975	Ludwigsburg	Baden Württemberg
70975	Remseck	Baden Württemberg
70975	Stuttgart	Baden Württemberg
71005	Pforzheim	Baden Württemberg
71993	Waiblingen	Baden Württemberg
71993	Weinstadt	Baden Württemberg
72771	Ingolstadt	Bayern
73647	Esslingen	Baden Württemberg
73901	Leinfelden-Echterdingen	Baden Württemberg
74164	Ebersbach	Baden Württemberg
74164	Eislingen	Baden Württemberg
74164	Göppingen	Baden Württemberg
74180	Böblingen	Baden Württemberg
74180	Sindelfingen	Baden Württemberg
74910	Nürtingen	Baden Württemberg
74910	Wendlingen	Baden Württemberg
76457	Ergolding	Bayern
76457	Landshut	Bayern
77198	Tübingen	Baden Württemberg
77437	Pfullingen	Baden Württemberg
77437	Reutlingen	Baden Württemberg
78692	Augsburg	Bayern
78692	Friedberg	Bayern
78692	Gersthofen	Bayern

UE ID	City Name	State
78692	Königsbrunn	Bayern
78692	Stadtbergen	Bayern
78876	Ulm	Baden Württemberg
78876	Neu-Ulm	Bayern
81894	Eichenau	Bayern
81894	Gräfelfing	Bayern
81894	Gröbenzell	Bayern
81894	Grünwald	Bayern
81894	Haar	Bayern
81894	Karlsfeld	Bayern
81894	München	Bayern
81894	Neubiberg	Bayern
81894	Olching	Bayern
81894	Ottobrunn	Bayern
81894	Planegg	Bayern
81894	Puchheim	Bayern
81894	Taufkirchen	Bayern
81894	Unterhaching	Bayern
84470	Freiburg	Baden Württemberg
86833	Kolbermoor	Bayern
86833	Rosenheim	Bayern
86833	Stephanskirchen	Bayern
87408	Ravensburg	Baden Württemberg
87408	Weingarten	Baden Württemberg
88288	Kempten	Bayern
89499	Konstanz	Baden Württemberg
89906	Lörrach	Baden Württemberg
89906	Weil	Baden Württemberg

Annex B – Air Quality Results

B1. PM_{10} concentrations in µg/m3

UE ID	PM_{10} Rural Background	PM_{10} Urban Background	PM_{10} Urban Streets			PM_{10} Main road network		
			Mean	2.5% CI	97.5% CI	Mean	2.5% CI	97.5% CI
12396	19.6	24.7	26.0	24.8	30.2	29.1	28.6	30.9
13371	19.6	24.7	26.1	24.8	30.6	32.8	28.7	36.2
13469	17.8	23.7	24.7	23.8	27.7	26.4	25.9	28.2
13594	20.2	25.0	28.0	25.3	37.7	30.8	27.0	34.3
14083	19.4	24.5	25.6	24.6	29.3	30.5	26.6	32.0
14384	19.9	24.8	26.2	24.9	30.9	28.7	26.8	29.2
15218	19.7	24.7	26.2	24.8	30.8	31.8	27.4	34.5
16115	20.4	25.1	30.1	25.9	41.9	34.3	28.7	43.3
16601	20.1	24.9	26.0	25.0	29.7	28.7	28.0	29.8
16729	17.5	23.6	24.8	23.7	28.6	27.0	24.9	28.4
16849	22.1	26.0	28.5	26.2	36.8	31.6	29.1	32.0
17151	22.7	26.0	27.1	26.1	30.7	29.5	29.4	29.8
19074	19.5	24.6	26.2	24.7	31.3	31.8	29.9	33.1
19372	22.2	25.9	30.1	26.5	41.5	36.9	26.9	40.9
19596	25.3	27.4	29.8	27.6	37.3	33.1	30.4	38.1
20489	22.7	26.1	28.6	26.3	36.5	37.5	37.4	37.5
22660	20.7	25.3	28.0	25.5	36.8	36.2	35.8	37.2
22770	22.0	25.9	29.2	26.4	36.8	37.3	29.5	52.8
24638	21.4	25.5	27.0	25.6	32.3	28.8	28.6	30.4
24642	17.6	23.8	26.9	24.2	35.8	35.9	26.6	43.1
24671	20.8	25.2	26.3	25.3	30.0	28.3	28.3	28.4
24767	17.9	23.9	25.8	24.1	31.9	31.8	30.6	33.7
25006	22.0	25.8	28.7	26.0	38.2	34.1	27.9	39.2
25736	17.2	23.6	25.7	23.8	32.6	28.3	26.3	29.5
25868	17.5	23.8	26.7	24.0	36.4	32.0	26.6	39.5
25914	19.1	24.5	26.8	24.7	34.4	33.7	25.9	36.5
26759	16.7	23.5	28.3	23.9	43.9	31.7	25.7	35.3
26920	19.1	24.4	25.8	24.5	30.6	28.2	26.2	33.5
27280	16.9	23.5	26.3	23.8	35.1	31.7	26.8	33.7
27377	16.5	23.3	25.8	23.5	34.1	28.6	27.8	30.1
28088	16.1	23.1	24.9	23.2	30.2	34.0	27.1	36.8
28533	18.4	24.2	26.4	24.4	33.0	32.6	28.1	34.5
29264	17.0	23.7	27.4	24.0	39.7	31.3	28.4	33.1
29743	20.5	25.0	26.6	25.2	31.6	30.1	28.6	30.4
29770	21.4	25.5	27.0	25.6	31.8	29.3	27.4	30.6
30565	15.3	22.7	25.1	22.9	32.6	31.3	28.5	31.6
31076	18.3	24.6	28.0	24.9	38.8	31.6	30.0	35.3
31077	18.8	24.3	26.2	24.5	32.5	31.2	27.2	31.8
31249	20.0	24.9	26.3	25.0	30.7	29.0	27.3	30.8
31785	18.9	24.6	31.0	25.7	45.5	35.5	27.8	44.5
32162	18.3	24.6	33.5	25.4	62.3	33.5	27.6	39.3

UE ID	PM_{10} Rural Background	PM_{10} Urban Background	PM_{10} Urban Streets			PM_{10} Main road network		
			Mean	2.5% CI	97.5% CI	Mean	2.5% CI	97.5% CI
32700	15.2	22.8	24.5	22.9	30.3	29.3	27.8	32.8
32987	18.7	24.2	25.4	24.3	29.4	30.0	26.6	33.6
33686	18.7	24.4	27.5	24.7	37.9	29.1	26.0	31.7
33974	19.4	24.6	27.6	24.9	35.8	33.3	27.2	37.3
34002	16.9	23.6	27.8	24.1	40.1	32.5	26.3	39.9
34624	17.7	24.0	27.2	24.3	38.1	31.4	29.6	32.8
34813	17.8	24.1	28.0	24.5	39.0	35.6	27.5	43.6
34925	14.9	22.5	24.4	22.7	30.3	30.3	24.4	34.6
35391	19.3	24.5	25.4	24.6	28.3	27.4	26.7	27.9
35805	19.3	24.7	27.8	24.9	38.3	33.0	27.6	38.0
36001	15.8	23.0	26.7	23.4	38.1	30.5	25.3	35.4
36658	23.2	26.4	28.8	26.7	35.3	33.8	28.9	39.1
38383	15.5	23.0	30.8	24.3	48.8	35.0	25.6	51.9
38906	14.8	22.4	25.1	22.7	37.5	29.0	24.5	31.8
39516	15.0	22.5	23.9	22.6	28.9	26.7	25.3	28.7
39840	13.4	21.8	23.9	21.9	30.9	28.6	24.3	31.9
40599	16.5	23.2	24.9	23.4	30.4	31.5	25.7	36.4
40906	17.6	23.8	25.9	23.9	32.6	29.2	25.4	28.0
41328	21.1	25.4	27.2	25.5	32.9	33.1	27.1	36.9
41913	17.3	23.7	26.2	23.9	34.1	27.4	26.0	30.2
41964	17.2	23.8	28.0	24.2	41.0	32.2	27.9	36.5
42019	17.6	23.8	25.6	24.0	31.3	29.8	26.4	34.3
42397	14.7	22.8	24.6	23.0	30.6	31.8	31.8	31.8
42723	20.1	25.0	27.9	25.3	37.5	27.5	26.7	27.9
43489	19.0	24.4	26.3	24.6	32.7	30.8	26.8	32.9
45635	12.6	21.3	23.6	21.5	30.5	25.0	23.3	26.9
46439	14.8	22.6	26.1	22.9	36.9	32.6	27.3	35.0
47006	12.5	21.5	25.2	21.9	36.9	29.8	25.0	30.9
47548	18.0	23.9	25.3	24.0	30.1	26.4	25.1	28.5
48163	14.0	22.4	26.2	22.7	39.1	31.9	27.8	33.0
48779	13.7	22.0	24.1	22.2	30.8	31.0	23.8	35.1
52769	18.5	24.5	28.8	25.1	40.4	36.9	28.6	50.1
53465	18.2	24.2	28.3	24.7	39.9	34.3	27.7	40.0
54128	15.2	22.7	24.3	22.9	29.3	30.9	26.9	32.2
54942	16.9	23.6	28.7	24.1	45.0	34.4	27.3	39.8
55209	18.3	24.2	27.1	24.5	36.4	33.1	28.1	37.3
55995	16.0	23.2	25.8	23.4	34.7	30.6	26.5	34.7
56196	20.6	25.8	29.4	26.1	40.9	41.2	28.8	49.9
56861	16.5	23.3	26.1	23.6	35.1	30.2	24.1	33.8
57336	16.2	23.2	25.6	23.4	33.3	35.3	28.6	38.2
59653	18.4	24.4	27.1	24.6	36.1	29.9	27.4	32.5
60637	16.8	23.6	26.8	23.9	36.3	36.6	34.8	41.4
61273	17.2	24.5	28.4	25.0	39.0	37.3	32.5	40.4
61890	17.4	23.8	27.4	24.3	37.3	33.9	28.8	41.6
62687	15.4	22.8	26.8	23.2	39.8	30.8	25.6	34.2
63191	16.8	23.6	26.1	23.8	34.2	36.6	30.8	42.0
63604	18.0	25.3	30.8	25.8	48.1	32.2	26.8	36.8

UE ID	PM$_{10}$ Rural Background	PM$_{10}$ Urban Background	PM$_{10}$ Urban Streets			PM$_{10}$ Main road network		
			Mean	2.5% CI	97.5% CI	Mean	2.5% CI	97.5% CI
63832	17.3	23.6	26.0	23.8	33.6	32.4	29.5	35.9
64427	19.5	24.7	28.1	25.2	37.4	32.6	27.7	39.4
66160	17.1	23.8	26.3	24.0	34.3	37.7	28.7	42.6
68600	21.7	25.9	28.6	26.2	37.2	42.0	31.7	48.4
68662	22.1	26.0	29.3	26.3	39.7	35.0	29.5	39.0
70975	16.8	23.7	26.9	24.1	35.8	40.3	32.4	44.8
71005	18.6	24.6	28.1	24.9	39.6	35.0	27.4	38.8
71993	16.4	23.7	26.7	23.9	36.6	38.0	36.6	39.1
72771	21.8	25.9	29.0	26.2	38.8	37.4	35.7	41.3
73647	16.4	23.5	25.1	23.6	30.5	39.7	38.2	40.5
73901	16.7	23.6	26.3	23.9	35.4	41.0	35.6	46.4
74164	16.4	23.5	25.7	23.7	32.6	33.3	28.5	36.4
74180	16.8	24.0	27.6	24.3	39.2	38.0	31.6	43.8
74910	16.3	23.7	29.0	24.1	46.8	37.0	30.2	39.7
76457	21.5	25.7	28.1	25.9	36.2	31.3	29.7	35.9
77198	16.2	23.3	25.3	23.5	31.6	31.7	26.7	34.4
77437	16.1	23.3	25.0	23.5	30.1	32.2	29.8	35.4
78692	17.6	23.9	25.7	24.1	31.6	35.1	27.9	38.0
78876	16.6	23.4	25.2	23.6	30.8	31.5	26.8	39.6
81894	17.4	23.9	27.0	24.2	36.4	34.7	28.9	42.5
84470	10.2	20.3	21.9	20.4	27.3	32.0	29.2	35.7
86833	18.4	24.3	25.8	24.4	30.7	33.8	33.6	34.1
87408	16.5	23.8	27.0	24.1	38.0	32.1	29.8	36.7
88288	16.7	23.5	26.3	23.8	35.6	30.3	26.3	31.6
89499	17.1	23.6	25.8	23.8	32.8	31.9	30.7	32.7
89906	10.7	20.6	23.1	20.8	31.2	28.3	24.8	33.1

B2. PM2.5 urban and road increment concentrations in µg/m3
Note that no rural background values were available for modelling air quality. For this reason, only urban and street increments are presented in this table.

UE ID	$PM_{2.5}$ Urban Increment	$PM_{2.5}$ Urban streets increment			$PM_{2.5}$ Main road network increment		
		Mean	2.5% CI	97.5% CI	Mean	2.5% CI	97.5% CI
12396	3.78	0.53	0.05	2.27	1.67	1.12	1.97
13371	3.80	0.57	0.05	2.42	3.13	1.14	4.45
13469	4.44	0.39	0.03	1.63	0.75	0.61	1.26
13594	3.66	1.22	0.10	5.18	2.50	0.56	4.54
14083	3.82	0.45	0.04	1.87	2.44	0.58	3.48
14384	3.67	0.59	0.05	2.49	1.10	0.57	1.25
15218	3.79	0.63	0.06	2.68	2.98	0.75	4.80
16115	3.54	2.07	0.35	7.00	3.92	1.01	8.89
16601	3.54	0.49	0.04	2.10	1.10	0.88	1.39
16729	4.58	0.49	0.04	2.00	0.95	0.35	1.36
16849	2.87	1.02	0.09	4.24	2.34	0.89	2.48
17151	2.51	0.43	0.04	1.81	0.99	0.96	1.06
19074	3.84	0.63	0.05	2.71	2.02	1.51	2.39
19372	2.83	1.72	0.21	6.70	4.18	0.28	7.32
19596	1.55	0.99	0.08	4.20	2.59	1.47	3.03
20489	2.58	1.00	0.09	4.08	5.54	5.53	5.55
22660	3.45	1.11	0.10	4.82	5.30	5.11	5.79
22770	2.91	1.35	0.24	4.45	4.78	1.03	13.18
24638	3.09	0.63	0.06	2.68	0.94	0.93	1.40
24642	4.66	1.26	0.16	4.80	5.03	0.78	9.45
24671	3.23	0.50	0.04	2.17	0.89	0.88	0.90
24767	4.53	0.75	0.06	3.18	3.14	1.90	4.78
25006	2.84	1.26	0.11	5.37	3.74	0.60	6.55
25736	4.82	0.86	0.08	3.67	1.34	0.76	1.67
25868	4.71	1.23	0.11	5.30	3.51	0.80	7.68
25914	4.03	0.92	0.08	3.70	3.72	0.39	5.86
26759	5.05	1.96	0.18	8.14	3.40	0.62	5.77
26920	3.97	0.57	0.05	2.44	1.07	0.51	2.58
27280	5.01	1.13	0.10	4.83	3.35	0.93	4.98
27377	5.08	1.03	0.09	4.34	1.52	1.29	1.93
28088	5.21	0.71	0.06	2.95	4.50	1.14	6.68
28533	4.39	0.86	0.07	3.57	3.37	1.10	4.74
29264	5.00	1.56	0.15	6.66	2.16	1.33	2.65
29743	3.38	0.61	0.06	2.57	1.44	1.02	1.51
29770	3.04	0.61	0.06	2.54	1.62	0.55	2.49
30565	5.58	1.01	0.09	4.27	3.33	1.65	3.83
31076	4.70	1.37	0.12	5.79	2.87	1.54	5.26
31077	4.17	0.78	0.07	3.34	3.04	0.80	2.70
31249	3.68	0.58	0.05	2.48	1.15	0.67	1.66
31785	4.29	2.58	0.45	8.37	4.61	0.90	9.58
32162	4.73	3.64	0.33	15.68	3.65	0.92	6.62
32700	5.64	0.74	0.07	3.20	2.38	2.29	4.90

UE ID	$PM_{2.5}$ Urban Increment	$PM_{2.5}$ Urban streets increment			$PM_{2.5}$ Main road network increment		
		Mean	2.5% CI	97.5% CI	Mean	2.5% CI	97.5% CI
32987	4.15	0.50	0.04	2.08	1.64	0.69	2.67
33686	4.29	1.27	0.12	5.29	2.00	0.47	3.56
33974	3.89	1.26	0.15	4.87	3.61	0.75	6.14
34002	5.01	1.74	0.21	6.75	3.85	0.78	7.98
34624	4.67	1.29	0.12	5.27	2.91	1.58	2.74
34813	4.73	1.58	0.20	5.81	4.75	0.96	9.19
34925	5.70	0.76	0.07	3.22	3.36	0.55	5.92
35391	3.87	0.35	0.03	1.47	1.15	0.62	1.51
35805	4.00	1.27	0.12	5.63	3.59	0.84	6.51
36001	5.45	1.51	0.13	6.45	3.29	0.65	6.02
36658	2.37	1.02	0.12	3.82	3.20	0.72	6.20
38383	5.64	3.18	0.54	10.70	5.30	0.74	14.10
38906	5.74	1.11	0.10	4.80	2.85	0.58	4.59
39516	5.64	0.59	0.05	2.43	1.49	0.79	1.75
39840	6.28	0.91	0.08	3.89	2.98	0.73	4.95
40599	5.08	0.69	0.06	2.82	3.67	0.69	6.40
40906	4.60	0.87	0.07	3.53	2.37	0.48	1.46
41328	3.20	0.77	0.07	3.28	3.38	0.48	5.66
41913	4.80	1.00	0.10	4.14	1.03	0.66	1.83
41964	4.93	1.71	0.15	7.06	3.69	1.16	6.21
42019	4.70	0.70	0.06	2.91	2.52	0.74	5.13
42397	6.10	0.72	0.07	2.94	2.54	2.53	2.56
42723	3.72	1.18	0.10	5.22	0.71	0.48	0.82
43489	4.07	0.78	0.07	3.26	2.67	0.69	4.11
45635	6.56	0.91	0.08	3.95	1.33	0.60	2.28
46439	5.84	1.37	0.12	5.66	4.09	1.32	6.03
47006	6.76	1.50	0.13	6.26	3.28	0.00	2.66
47548	4.39	0.59	0.05	2.49	0.71	0.35	1.32
48163	6.27	1.61	0.14	6.97	3.80	1.51	2.99
48779	6.22	0.83	0.07	3.56	3.76	0.52	5.69
52769	4.53	1.78	0.23	6.43	5.27	1.14	12.48
53465	4.49	1.60	0.19	5.96	4.30	0.97	7.70
54128	5.62	0.66	0.06	2.80	3.28	1.18	4.64
54942	5.09	2.07	0.19	8.81	4.46	1.02	7.89
55209	4.46	1.16	0.11	4.98	3.88	1.11	6.42
55995	5.36	1.07	0.09	4.49	3.13	0.94	5.64
56196	3.90	1.44	0.13	6.27	6.73	0.84	11.77
56861	5.10	1.11	0.10	4.59	2.96	0.22	5.11
57336	5.27	0.98	0.09	4.16	4.97	1.54	6.86
59653	4.50	1.10	0.10	4.54	1.54	0.83	2.28
60637	5.09	1.27	0.11	5.38	5.14	3.17	8.69
61273	5.43	1.58	0.19	5.99	4.98	2.27	6.47
61890	4.85	1.46	0.18	5.57	4.33	1.41	8.69
62687	5.55	1.63	0.15	7.01	3.40	0.79	5.54
63191	5.08	1.02	0.09	4.42	5.32	2.03	8.98
63604	5.42	2.29	0.20	9.64	2.99	0.43	5.62

UE ID	$PM_{2.5}$ Urban Increment	$PM_{2.5}$ Urban streets increment			$PM_{2.5}$ Main road network increment		
		Mean	2.5% CI	97.5% CI	Mean	2.5% CI	97.5% CI
63832	4.74	0.97	0.09	4.05	3.71	1.65	6.01
64427	3.92	1.36	0.16	5.26	3.32	0.82	7.16
66160	5.03	1.06	0.09	4.56	5.87	1.39	9.17
68600	3.18	1.09	0.10	4.57	6.79	1.64	11.00
68662	2.92	1.31	0.11	5.55	3.84	0.98	6.34
70975	5.18	1.31	0.16	4.85	6.86	2.46	10.29
71005	4.49	1.42	0.13	6.13	4.42	0.79	6.96
71993	5.47	1.24	0.11	5.29	4.06	3.66	4.35
72771	3.05	1.24	0.11	5.14	4.93	3.66	4.35
73647	5.33	0.65	0.06	2.83	4.60	4.15	4.82
73901	5.21	1.12	0.09	4.81	6.83	4.37	11.13
74164	5.34	0.89	0.07	3.77	2.77	1.41	3.63
74180	5.34	1.49	0.14	6.38	5.69	2.17	9.69
74910	5.51	2.16	0.19	9.31	5.41	1.84	7.85
76457	3.14	0.97	0.09	4.26	1.59	1.14	2.89
77198	5.33	0.86	0.08	3.58	2.38	0.95	3.15
77437	5.45	0.70	0.06	2.99	2.50	1.83	3.42
78692	4.71	0.74	0.07	3.11	4.49	1.13	6.32
78876	5.11	0.76	0.07	3.29	2.30	0.97	4.58
81894	4.88	1.30	0.16	4.97	4.64	1.43	9.09
84470	7.58	0.67	0.06	2.89	3.32	2.51	4.36
86833	4.40	0.62	0.05	2.65	2.68	2.65	2.78
87408	5.46	1.34	0.12	5.56	2.35	1.72	3.66
88288	5.12	1.15	0.10	4.82	2.74	0.78	3.85
89499	4.87	0.88	0.08	3.76	2.35	2.00	2.57
89906	7.44	0.99	0.09	4.08	3.13	1.18	6.10

B3. NO_2 concentrations in µg/m^3

UE ID	NO_2 Rural Background	NO_2 Urban Background	NO_2 Urban Streets			NO_2 Main road network		
			Mean	2.5% CI	97.5% CI	Mean	2.5% CI	97.5% CI
12396	10.19	19.00	26.25	19.70	41.55	45.22	37.49	50.15
13371	11.99	22.78	29.95	23.48	44.71	60.79	41.54	72.05
13469	9.24	13.59	18.90	14.09	31.32	27.23	25.14	33.64
13594	12.10	28.08	43.00	29.82	65.99	59.38	38.87	77.92
14083	9.46	16.14	22.40	16.76	36.22	48.39	27.18	59.23
14384	12.12	20.23	28.47	21.11	45.22	38.42	31.16	40.19
15218	11.31	22.73	31.03	23.60	48.03	58.21	36.43	74.07
16115	13.30	32.71	54.44	37.70	77.78	74.13	49.81	104.99
16601	10.29	17.69	24.01	18.33	37.49	35.91	33.19	39.17
16729	8.07	13.99	20.40	14.62	34.16	30.33	21.29	35.13
16849	12.66	31.13	43.49	32.51	64.34	62.29	46.74	65.75
17151	13.11	15.80	21.59	16.34	34.91	32.66	32.26	33.48
19074	10.88	21.02	29.38	21.88	46.57	48.50	43.72	51.52
19372	12.36	31.78	51.73	35.03	76.93	76.52	37.66	96.49
19596	12.94	26.16	38.07	27.47	58.17	56.63	41.20	80.00
20489	12.42	26.22	39.59	27.66	62.11	81.72	81.62	81.74
22660	12.81	32.22	45.39	33.77	67.09	86.41	85.33	89.07
22770	13.46	31.93	46.91	35.10	65.40	78.81	49.25	123.60
24638	13.43	24.85	32.89	25.68	49.29	40.98	40.98	46.46
24642	8.80	27.27	43.21	29.60	65.80	75.78	41.38	102.14
24671	10.23	13.77	20.34	14.40	34.73	29.33	29.22	29.54
24767	9.01	27.49	36.83	28.45	54.91	65.15	53.91	78.68
25736	12.85	22.99	38.52	24.84	62.64	61.49	34.45	83.80
25868	10.59	26.57	37.71	27.76	57.99	47.51	40.42	50.85
25914	8.14	29.33	44.57	31.07	67.14	68.26	43.72	95.81
26759	13.59	30.60	43.25	32.02	64.29	71.83	38.57	87.81
26920	10.76	34.41	57.01	37.43	87.26	73.38	46.20	91.12
27280	8.99	17.80	25.58	18.56	41.72	35.65	27.81	49.70
27377	8.12	29.31	44.07	31.05	67.43	67.86	45.41	81.68
28088	11.23	28.74	41.97	30.24	63.67	51.55	49.14	55.42
28533	11.63	27.08	36.96	28.09	55.24	72.73	45.78	88.58
29264	15.71	25.20	36.21	26.45	56.16	64.37	43.37	76.17
29743	12.84	38.75	57.82	41.21	84.66	67.41	59.59	71.16
29770	9.95	15.87	24.12	16.73	40.40	37.87	33.08	38.63
30565	11.02	18.42	26.50	19.25	42.87	43.18	29.03	54.23
31076	11.14	29.14	41.77	30.55	63.14	68.43	53.25	73.67
31077	17.90	40.75	57.44	42.71	82.62	76.18	63.79	94.67
31249	15.49	29.29	39.30	30.35	58.27	63.86	43.64	64.64
31785	10.45	17.13	24.58	17.91	39.65	35.99	29.66	41.34
32162	17.00	40.26	66.02	46.72	92.06	85.85	56.03	115.76
32700	15.53	56.54	90.18	61.96	132.73	97.24	72.53	117.71
32987	8.40	24.38	34.72	25.44	53.61	57.01	54.08	76.30
33686	9.60	19.74	26.13	20.39	39.93	43.79	32.53	52.30
33974	14.96	33.90	49.99	35.76	75.00	61.67	43.21	77.56

UE ID	NO_2 Rural Background	NO_2 Urban Background	NO_2 Urban Streets			NO_2 Main road network		
			Mean	2.5% CI	97.5% CI	Mean	2.5% CI	97.5% CI
34002	11.39	26.30	41.81	28.68	63.94	66.53	39.93	84.98
34624	14.41	38.06	57.35	41.36	81.14	78.51	52.12	106.00
34813	16.03	40.46	55.47	42.22	78.47	76.78	63.94	78.19
34925	16.53	51.13	69.02	53.97	92.40	98.16	67.60	124.82
35391	9.50	23.29	33.53	24.42	52.11	60.71	33.86	80.84
35805	10.83	18.24	23.32	18.74	35.81	38.58	29.99	44.69
36001	19.16	42.02	57.59	43.81	81.81	81.05	56.88	102.65
36658	13.82	39.73	59.17	42.15	86.08	75.85	51.97	97.79
38383	15.90	28.53	41.14	30.45	60.76	65.15	41.81	87.55
38906	13.81	45.29	74.33	53.02	102.81	93.46	58.85	140.99
39516	12.90	28.36	42.06	29.91	74.71	62.15	39.43	78.43
39840	9.45	20.87	28.49	21.67	44.44	45.23	35.06	46.10
40599	11.04	24.27	36.11	25.61	56.15	58.99	37.62	76.45
40906	9.97	23.20	32.26	24.11	49.24	61.38	36.04	83.26
41328	11.25	25.61	37.05	26.85	57.49	55.69	35.02	49.42
41913	13.39	26.03	36.23	27.19	54.81	63.35	35.59	82.14
41964	11.49	31.80	45.09	33.29	66.56	49.16	44.09	57.58
42019	10.72	35.90	55.79	38.45	83.17	74.92	54.86	94.98
42397	11.59	24.81	34.49	25.84	52.22	56.80	38.28	78.01
42723	14.84	34.71	44.71	35.73	64.12	66.33	66.27	66.44
43489	13.00	32.41	46.97	34.05	69.85	45.45	41.97	47.04
45635	12.62	24.04	34.62	25.18	54.33	57.55	36.83	71.22
46439	9.41	18.89	30.58	20.13	50.64	41.51	30.27	52.88
47006	22.62	45.48	62.15	47.44	86.89	88.87	66.25	103.61
47548	9.64	31.68	50.54	33.96	77.49	70.35	48.42	66.79
48163	13.09	20.49	28.51	21.30	45.23	33.52	27.71	41.26
48779	12.28	41.91	60.70	44.24	87.93	83.87	64.70	76.73
52769	12.18	34.63	45.30	35.83	63.82	75.69	44.84	90.91
53465	12.52	39.85	59.14	43.04	83.15	89.07	58.58	128.44
54128	14.07	38.50	56.38	41.44	79.80	82.06	55.12	105.06
54942	10.91	27.92	36.93	28.86	54.54	66.41	47.06	78.33
55209	10.86	39.20	62.47	42.47	93.51	84.44	56.49	106.69
55995	9.33	30.08	45.30	31.82	68.89	70.62	48.46	90.21
56196	9.49	30.25	44.17	31.81	67.33	66.64	46.51	86.29
56861	14.33	40.25	57.41	42.31	82.33	96.24	55.13	125.70
57336	11.53	30.95	44.86	32.50	67.43	65.99	35.66	84.03
59653	10.84	30.25	43.21	31.67	64.43	78.70	53.32	92.02
60637	13.25	38.80	52.28	40.29	74.41	61.84	53.61	68.40
61273	8.99	37.98	53.97	39.82	78.34	87.91	73.94	109.30
61890	12.72	40.72	58.32	43.59	81.73	89.92	70.26	101.12
62687	9.86	36.49	53.77	39.30	77.02	80.16	58.20	107.81
63191	10.79	32.82	52.07	35.26	79.73	71.03	47.03	88.30
63604	13.13	33.89	46.56	35.27	67.88	84.31	61.45	106.60
63832	10.73	40.04	64.42	43.31	95.59	74.89	48.72	95.98
64427	10.12	25.57	38.16	26.90	59.78	65.99	49.74	83.57
66160	8.71	29.47	45.97	32.09	68.45	67.11	44.13	93.38

UE ID	NO_2 Rural Background	NO_2 Urban Background	NO_2 Urban Streets			NO_2 Main road network		
			Mean	2.5% CI	97.5% CI	Mean	2.5% CI	97.5% CI
68600	11.38	36.93	50.11	38.42	71.77	89.64	58.46	110.51
68662	11.90	36.33	50.28	37.86	72.87	93.65	60.41	118.30
70975	9.91	33.56	50.13	35.58	74.42	74.47	50.36	93.30
71005	9.52	42.18	57.78	44.70	79.83	100.36	73.20	120.94
71993	10.67	39.66	57.55	41.79	83.81	84.22	53.88	102.54
72771	11.36	41.31	55.26	42.92	77.54	82.64	80.32	84.22
73647	11.05	33.09	49.38	34.93	74.65	80.30	72.10	76.00
73901	10.77	34.43	42.97	35.26	60.22	78.66	76.26	79.84
74164	9.65	38.31	52.11	39.76	74.69	96.93	81.34	120.86
74180	10.45	32.07	43.08	33.28	63.04	65.37	53.78	70.93
74910	8.69	41.91	58.94	43.87	84.69	94.44	70.61	117.92
76457	8.56	43.43	67.08	46.57	98.99	94.42	69.37	110.74
77198	12.64	28.62	41.08	29.99	62.04	52.20	47.37	62.71
77437	10.24	30.56	41.42	31.72	61.31	60.97	46.93	66.39
78692	10.17	30.93	39.63	31.86	56.65	62.26	56.72	68.49
78876	9.30	28.25	38.20	29.29	57.30	74.32	46.82	87.89
81894	11.14	26.05	35.81	27.06	54.40	55.84	42.65	70.20
84470	9.44	33.87	48.52	36.20	69.71	79.40	55.78	107.09
86833	9.32	18.13	26.86	19.01	44.09	55.08	49.55	61.09
87408	10.72	28.22	36.00	29.00	51.70	60.85	60.63	61.57
88288	9.47	37.81	53.11	39.51	76.75	67.96	62.57	76.81
89499	7.09	27.85	41.23	29.39	63.53	62.61	41.97	73.41
89906	11.38	22.17	33.02	23.33	52.11	52.34	49.50	54.01
12396	12.08	22.87	35.66	24.27	57.36	60.18	42.05	81.36

Annex C – Pedigree Scores

Name of input variable: Wind speed at 10 metres

Criteria		0	1	2	3	4		Elaboration - Justification
Proxy	Not related				X		Exact measure	Wind speed and direction were explicitly modelled.
Empirical basis	Weak			X			Strong	Wind speed data were modelled for the European domain and for four years with a resolution of one hour.
Methodological rigour	Low				X		High	Meteorological data is commonly generated using atmospheric models. The model used for calculating this variable (MM5) is widely used in air quality modelling studies.
Validation	No		X				Complete	Although no validation was carried out for this dataset, the MM5 model provides reliable estimates of this parameter.

Normalized score: 0.56

Name of input variable: Urban area definition

Criteria		0	1	2	3	4		Elaboration - Justification
Proxy	Not related				X		Exact measure	Urban areas were identified on the basis of land use data with a high spatial resolution.
Empirical basis	Weak				X		Strong	Urban areas were determined for a sample comprising 27 European countries.
Methodological rigour	Low			X			High	Although a clearly defined methodology was used for generating the UMZ dataset, there is no consensus in scientific community as to whether the definition of urban areas in this way is adequate.
Validation	No				X		Complete	The underlying data (CORINE2000) were compared with the LUCAS (Land Use and Cover Area frame sample Survey) database for testing its thematic accuracy, obtaining a good agreement.

Normalized score: 0.69

Name of input variable: **PM_{10} background concentration**

Pedigree scores for input variable

Criteria		0	1	2	3	4		Elaboration - Justification
Proxy	Not related				X		Exact measure	PM10 concentration were modelled
Empirical basis	Weak			X			Strong	PM10 background concentrations were modelled for the European domain using a full-chemical-transport model.
Methodological rigour	Low				X		High	Commonly used methodology within the scientific community for generating this type of data.
Validation	No					X	Complete	Monitoring data of the same variable from the European network Airbase were used for validation within the framework of this thesis.

Normalized score: 0.75

Name of input variable: **Vehicle kilometres travelled**

Pedigree scores for input variable

Criteria		0	1	2	3	4		Elaboration - Justification
Proxy	Not related			X			Exact measure	Population data was used as proxy for estimating urban VKT. Correlation between these two parameters has been demonstrated.
Empirical basis	Weak				X		Strong	Recent data were used for constructing a model to predict VKT as a function of population.
Methodological rigour	Low				X		High	Commonly used methodology within the scientific community for generating this type of data.
Validation	No				X		Complete	Data were validated against two detailed datasets within the framework of this thesis.

Normalized score: 0.69

Name of input variable: **Tree factor**

Pedigree scores for input variable

Criteria		0	1	2	3	4		Elaboration - Justification
Proxy	Not related		X				Exact measure	A proxy was used for the definition of this variable.
Empirical basis	Weak		X				Strong	Educated guess was used.
Methodological rigour	Low		X				High	Because data on this variable were not available, only a preliminary method was used to define it.
Validation	No	X					Complete	This parameter has not been validated.

Normalized score: 0.19

Name of input variable: **Average annual daily traffic**

Pedigree scores for input variable

Criteria		0	1	2	3	4		Elaboration - Justification
Proxy	Not related				X		Exact measure	The actual vehicle volume was addressed
Empirical basis	Weak				X		Strong	Modelled data using small sample of direct measurements
Methodological rigour	Low					X	High	Commonly used methodology within the scientific community for generating this type of data.
Validation	No				X		Complete	Although the data were not validated, the model used for their modelling has been validated.

Normalized score: 0.81

Name of input variable: **Street width**

Pedigree scores for input variable

Criteria		0	1	2	3	4		Elaboration - Justification
Proxy	Not related				X		Exact measure	The street width was measured using satellite imagery with a very high resolution.
Empirical basis	Weak				X		Strong	A comparatively small sample of streets was used for determining the probability density function of this parameter.
Methodological rigour	Low			X			High	Considering the large size of the domain, it is considered that the methodology applied for defining this variable was acceptable.
Validation	No	X					Complete	This parameter has not been validated.

Normalized score: 0.50

Name of input variable: **Building height**

Pedigree scores for input variable

Criteria		0	1	2	3	4		Elaboration - Justification
Proxy	Not related				X		Exact measure	Several studies were used where this parameter was directly measured.
Empirical basis	Weak			X			Strong	Only a small sample of measured data was used for constructing the probability density function for this variable.
Methodological rigour	Low		X				High	Considering the large size of the domain, it is considered that the methodology applied for defining this variable was acceptable.
Validation	No	X					Complete	This parameter has not been validated.

Normalized score: 0.38

Annex D – Regional dispersion modelling

D.1. Polyphemus – System description and configuration

Polyphemus is a modular system designed to assess and forecast emission-reduction strategies over Europe. It was developed at ENPC (École Nationale des Ponts et Chaussées) within the framework of several national and EU projects, and since its creation it has been continuously revised, improved and updated. Its modular structure allows for flexibility, accommodating different model configurations according to the user modelling needs. The following lines provide a brief overview of the Polyphemus system. More details on Polyphemus parameterizations and equations, including the numerical methods used to solve the model equations, can be found in Mallet et al. (2007).

Four independent components assemble the Polyphemus system: physical parameterizations, the so-called drivers, the actual models, and post-processing tools, which can be configured according to user's requirements. The configuration used for this research mainly comprises the Eulerian three-dimensional chemistry-transport model Polair3d for gaseous dispersion and chemistry, and the size-resolved aerosol model (SIREAM) for solving aerosols dynamics.

Polair3d uses the Regional Atmospheric Chemistry Mechanism (RACM) using a second-order Rosenbrock method for time integration (Stockwell, Kirchner, Kuhn, & Seefeld, 1997). The photochemical model includes approximately 237 thermal and photochemical reactions between 72 species. Advection is based on a third-order direct space-time scheme with a Koren-Sweby flux limiter and diffusion relies on a second-order Rosenbrock method. Dry deposition velocities are pre-processed using the revised parameterization of Zhang et al. (2003). Below-cloud scavenging is based on the microphysical properties of the species following Sportisse and Dubois (2002), and using effective Henry coefficients for addressing ion dissociation during below-cloud scavenging.

Atmospheric aerosols consisting of a suspension of solid or liquid particles in air (Holton, Curry, & Pyle, 2003) are solved with the model SIREAM, which is based on a sectional description of the aerosol distribution. The model depicts the time evolution of the aerosol distribution in a box under nucleation, condensation/evaporation and Brownian coagulation. The aerosol model is fully described in Debry et al. (2007). The dry deposition of the particles uses the resistance approach as described by Zhang et al. (2001). Both the representative diameter for the rain as a function of rain density and the raindrop velocity as a function of raindrop diameter are computed following Loosmore and Cederwal (2004).

D.2 Model setup and input data

In order to consider the influence of long-range transport during the formation of secondary pollutants and aerosols, the domain was chosen to cover Central Europe from 12.5°W to 30°E longitude and from 35°N to 72.5°N with a 0.5 x 0.5 arc degree horizontal resolution (about 35 by 55 km), as shown in Figure D.1. In the vertical direction, five height levels are used: from the surface to 40, 200, 600, 1400 and 3000 metres.

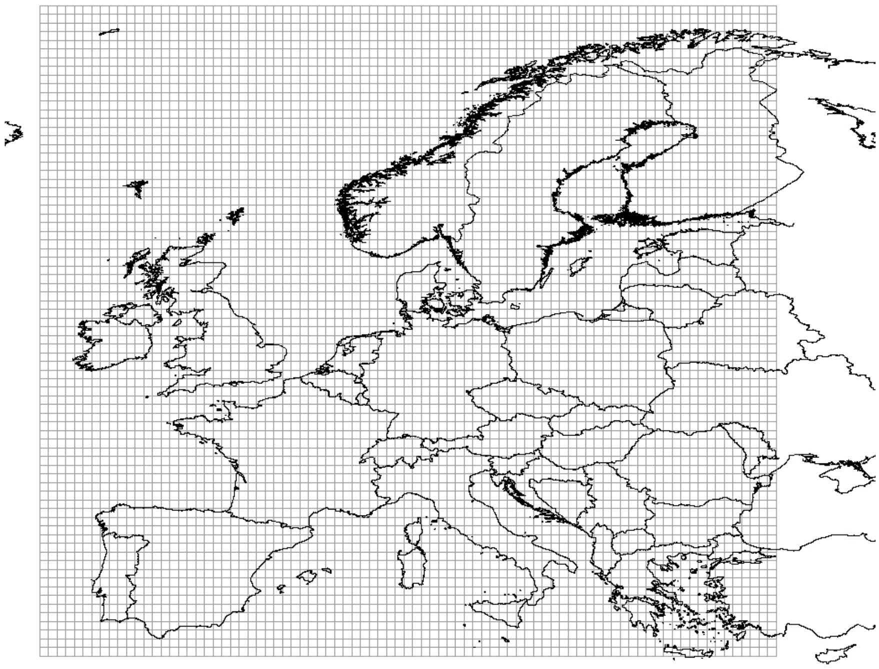

Figure D.1 Polyphemus system domain.

Ground data are generated using land-use data from the US Geological Survey (USGS) with 24 categories and 1 km spatial resolution. Boundary and initial conditions for the reference year are interpolated from outputs of the Laboratoire de Meteorologie Dynamique General Circulation Model (LMDz). Boundary conditions are updated daily. A detailed description of the anthropogenic emission dataset for Europe and Germany was already provided in Chapter 2. Biogenic emissions are computed on the basis of meteorological fields and land-use cover following Simpson et al. (1999) and the Monahan parameterisation (Monahan, Spiel, & Davidson, 1986) is used for sea salt emissions. For each emissions sector, a typical time distribution given for each month, day and hour is imposed using the temporal factors derived from the GENEMIS (Generation and Evaluation of Emission Data) project (Friedrich et al., 1999). Monthly and hourly emission factors for the agriculture sector are applied following Schaap (2003). The inventory species are disaggregated into real species using speciation coefficients following Passant (2002). Temporal, chemical and granulometrical aerosol speciation is configured following Sartelet et al. (2007).

Meteorological fields are provided offline by ECMWF (European Centre for Medium Range Weather Forecast). The dataset has a longitude-latitude grid projection with 31 vertical levels with a horizontal resolution of 0.36° by 0.36° and a temporal resolution of 3 hours. The Troen and Mahrt parameterization (1986) is used for calculating the vertical diffusion within the boundary layer, which is provided by the ECMWF, and for the area above it, the Louis parameterization is implemented (Louis, 1979).

Annex E – Supplementary Information

Table E.1 Selected Nomenclature for Air Pollution (SNAP) categories of the European emissions.

SNAP	Description
1	Combustion in energy and transformation industries (stationary sources)
2	Non-industrial combustion plants (stationary sources)
3	Combustion in manufacturing industry
4	Production processes (stationary sources)
5	Extraction and distribution of fossil fuels and geothermal energy
6	Solvent use and other product use
7	Road transport
8	Other mobile sources and machinery
9	Waste treatment and disposal
10	Agriculture
11	Other sources and sinks

Source: EEA, 2007b.

Table E.2 CORINE Land Cover classes.

CLC CODE	LABEL	CLC CODE	LABEL
111	Continuous urban fabric	311	Broad-leaved forest
112	Discontinuous urban fabric	312	Coniferous forest
121	Industrial or commercial units	313	Mixed forest
122	Road and rail networks and associated land	321	Natural grasslands
123	Port areas	322	Moors and heathland
124	Airports	323	Sclerophyllous vegetation
131	Mineral extraction sites	324	Transitional woodland-shrub
132	Dump sites	331	Beaches, dunes, sands
133	Construction sites	332	Bare rocks
141	Green urban areas	333	Sparsely vegetated areas
142	Sport and leisure facilities	334	Burnt areas
211	Non-irrigated arable land	335	Glaciers and perpetual snow
212	Permanently irrigated land	411	Inland marshes
213	Rice fields	412	Peat bogs
221	Vineyards	421	Salt marshes
222	Fruit trees and berry plantations	422	Salines
223	Olive groves	423	Intertidal flats
231	Pastures	511	Water courses
241	Annual crops associated with permanent crops	512	Water bodies
242	Complex cultivation patterns	521	Coastal lagoons
243	Land principally occupied by agriculture with significant areas of natural vegetation	522	Estuaries
244	Agro-forestry areas	523	Sea and ocean

Source: EEA, 2002.

Table E.3 Corine Land Cover version 2000 (CLC2000) classes used in the Urban Morphological Zones (UMZ) dataset.

CLC code	CLC Class	Criteria
111	Continuous urban fabric	Core Classes
112	Discontinuous urban fabric	
121	Industrial or commercial units	
141	green areas	
123	Port areas	Included when they neighbourhood to core classes
124	Airports	
142	Sport and leisure facilities	
122	Road and rail networks and associated land	Included when they neighbourhood to core classes and cut by a 300 metres buffer
511	Water courses	
311	Broad-leaved forest	Forest and scrub - Included when they are completely within the core classes
312	Coniferous forest	
313	Mixed forest	
322	Moors and heathland	
323	Sclerophyllous vegetation	
324	Transitional woodland-shrub	

Source: Milego, 2007.