DOCTORAATSPROEFSCHRIFT

2009 | Interfacultair Instituut Verkeerskunde

An activity-based modelling framework for air pollution exposure assessment

Proefschrift voorgelegd tot het behalen van de graad van
Doctor in de Verkeerskunde, te verdedigen door:

Carolien BECKX

Promotor: prof. dr. Geert Wets
Copromotor: dr. Luc Int Panis (VITO)

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INSTITUUT VOOR MOBILITEIT

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D/2009/2451/41

"If we knew what we were doing, it wouldn't be called research"

Albert Einstein, theoretical physicist (1879-1955)

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SUMMARY

Transport has both positive and negative effects on health. On the one hand, transport connections help people to reach services, maintain contacts and interactions. On the other hand, transport causes annually hundreds of thousands of premature deaths in Europe, not only due to traffic accidents, but also due to air pollution problems. Transport related gaseous and particulate emissions are one of the main sources of air pollution and air pollution is estimated to cause around 370 000 premature deaths a year in the European Union.

Due to the negative effects of transport, one of the key challenges of the modern policy making consists of promoting a sustainable transportation system aiming at the prevention or reduction of the negative effects of the transportation system on health and environment. To give more accurate and complete estimates on the impact of (transport) policies on the environment, the use of a modelling framework, taking into account the different causal links between activities, trips, emissions, concentrations and exposure, is however required.

This dissertation describes the development and application of a modelling framework that enables the assessment of trips, emissions, concentrations and exposure in The Netherlands. Besides the use of an emission model (MIMOSA) and a dispersion model (AURORA), the research includes the application of an 'activity-based' transport model (ALBATROSS) to predict people's activity-travel behaviour.

The different research phases in this dissertation can be described as follows. In a first phase, the activity-based model ALBATROSS was used to predict activity-travel patterns for the Dutch population. The model started by developing a synthetic population for The Netherlands and activity-travel schedules were simulated for all the individuals within this population. Next, the predicted trips for the entire population were assigned to a road network and traffic flows were converted into vehicle emissions by applying the emission factor approach from

the MIMOSA emission model. A comparison between the modelled emissions and reported emission values demonstrated good correspondence. CO_2 emissions were overestimated by 11%. Differences between modelled and reported emissions of NO_x, VOC, SO_2 and PM varied between 3 and 26%. This result was not validated against measured values, because emissions cannot be measured at the national level. The mere replication of approximately the same emission values with a different model is however not really innovative. Compared to other travel or emission studies, though, this first step provides much more detailed temporal and spatial information on passenger car emissions instead of allowing only aggregated (yearly) emission values.

In a second phase, the activity-based emission approach was further explored by converting the emissions into pollutant concentrations. For this purpose, the AURORA dispersion model was applied to simulate the transport and conversion of the emissions into concentrations. An important advantage of this air quality modelling step is that it enables to validate the activity-based model predictions by comparing the simulated concentrations with measured values at Dutch monitoring stations. Both temporal and spatial validation analyses were performed. Results of the statistical analysis demonstrated a very good correspondence between the simulated and measured concentrations of O_3 (IA between 0.69 and 0.80). For NO_2 the IA value varied between 0.40 and 0.70. And for PM_{10} IA values between 0.48 and 0.64 were calculated. The comparison of concentrations constitutes an end-of-pipe validation of the accuracy of the entire model chain. We have specifically looked at the results for NO_2, a pollutant typical of transport which has both a strong spatial and temporal variation. NO_2 is the pollutant best suited to attempt a validation of the ALBATROSS-MIMOSA-AURORA model chain because its (modelled) concentrations will tend to be sensitive to errors in traffic streams, emission functions as well as atmospheric modelling. The analysis demonstrated that the activity-based air quality model chain was able to simulate the hourly concentration patterns in the Dutch study area with sufficient accuracy.

And finally, in the last phase of this research, population exposure analyses were performed. The predicted hourly concentration fields from the ALBATROSS-MIMOSA-AURORA modelling chain were combined with hourly information on people's location to calculate the exposure. By using the population information from the activity-based simulation, hourly population maps were simulated and dynamic exposure values could be estimated.
In a first exposure analysis, this dynamic exposure framework was applied on a Dutch urban area to demonstrate the importance of taking into account people's travel behaviour when calculating the exposure. The exposure study in the Dutch urban area demonstrated that large inflows of people occur during the day in the urban areas, causing people to be exposed to higher concentration values compared to their residential (static) situation. Traditional exposure studies that link concentration values with residential information therefore often underestimate the real exposure values.
In a second exposure analysis, these dynamic exposure values were calculated for the entire Dutch study area and further disaggregated according to different activity-based features like the gender of the person or the performed activity. Results demonstrate that, by neglecting people's travel behaviour, total average exposure to NO_2 will be underestimated by 4 % and hourly exposure results can be underestimated by more than 30 %. A more detailed exposure analysis revealed the intra-day variations in exposure estimates and the presence of large exposure differences between different activities (traffic > work > shopping > home) and between subpopulations (men > women, low socio-economic class > high socio-economic class). Understanding exposure variations among activities and subpopulations can be very useful for scientific and policy purposes. It can provide information on locations or population groups most at risk, or can indicate where and when the largest exposure values occur.

In summary, this dissertation demonstrated the advantages of an activity-based approach for air quality purposes by presenting three kinds of applications: the calculation of vehicle emissions, the simulation of pollutant concentration patterns and the assessment of the population exposure to air pollution.

SAMENVATTING

Transport heeft zowel positieve als negatieve effecten op de gezondheid van mensen. Aan de ene kant zorgen transportverbindingen ervoor dat mensen allerlei diensten kunnen bereiken, contacten kunnen onderhouden en sociale interacties kunnen aangaan. Aan de andere kant veroorzaakt transport jaarlijks enkele duizenden sterftes in Europa, niet alleen door verkeersongelukken, maar ook door de luchtverontreiniging die veroorzaakt wordt door het verkeer. Transportgerelateerde emissies zijn één van de belangrijkste bronnen van luchtverontreiniging, en men schat dat deze luchtverontreiniging jaarlijks ongeveer 370 000 vroegtijdige sterftes veroorzaakt in de Europese Unie.
Door de negatieve effecten van transport is het belangrijk om een duurzaam transportsysteem te stimuleren dat de negatieve effecten van transport op de gezondheid en het milieu vermijdt of reduceert. Om betere inzichten te verkrijgen in de impact van beleidsmaatregelen op de omgeving, is het echter noodzakelijk om de causale links tussen activiteiten, verplaatsingen, emissies, concentraties en blootstelling in kaart te kunnen brengen.

Dit proefschrift beschrijft de ontwikkeling en de toepassing van een modellenkader dat in staat is om de verplaatsingen, emissies, concentraties en blootstelling in Nederland in kaart te brengen. Naast het gebruik van een emissiemodel (MIMOSA) en een verspreidingsmodel (AURORA) wordt in dit kader gebruik gemaakt van een activiteitengebaseerd model (ALBATROSS) dat instaat voor de voorspelling van de activiteiten –en verplaatsingspatronen in het studiegebied.

De verschillende onderzoeksdelen in dit doctoraatsonderzoek kunnen als volgt samengevat worden. In een eerste onderzoeksfase werd het activiteitengebaseerde model ALBATROSS ingezet om de verplaatsingspatronen van de Nederlandse populatie te simuleren. Het model maakt hiervoor eerst een synthetische populatie aan en simuleert daarna activiteitenpatronen voor alle individuen die deel uitmaken van deze populatie. Vervolgens werden de voorspelde verplaatsingen toegedeeld op een verkeersnetwerk en werden de

resulterende verkeersstromen omgezet tot verkeersemissies met behulp van het emissiemodel MIMOSA. Een vergelijking tussen de gemodelleerde en de gerapporteerde emissies toonde een goede overeenkomst aan: CO_2 emissies werden ongeveer 11% te hoog geraamd, en de afwijkingen voor NO_x, VOC, SO_2 en PM varieerden tussen 3 en 26%. Dit resultaat kan echter niet echt gevalideerd worden met andere (gemeten) waardes vermits emissies niet gemeten worden op nationale schaal, enkel geschat. Het herberekenen van emissies met een alternatief model op zich is niet echt vernieuwend. In vergelijking met andere verplaatsings –en emissiestudies die voornamelijk geaggregeerde (jaarlijkse) waardes rapporteren, verschaft deze eerste stap echter wel meer gedetailleerde temporele en ruimtelijke informatie over de emissies van personenvoertuigen.

In een tweede onderzoeksfase werden de activiteitengebaseerde emissiewaardes omgezet tot concentraties. Het verspreidingsmodel AURORA werd aangewend om het transport en de conversie van emissies tot concentraties te berekenen. Een belangrijk voordeel van deze omrekeningsstap is dat het toelaat om de modelvoorspellingen te valideren met gemeten concentratiewaardes door Nederlandse meetstations. Zowel de temporele als de ruimtelijke voorspellingswaarde van het model werden geanalyseerd. De resultaten van de statistische analyse toonden goede overeenkomsten aan tussen de gesimuleerde en de gemeten O_3 concentraties (IA tussen 0.69 en 0.80). Voor NO_2 varieerde de IA waarde tussen 0.40 en 0.70; en voor PM_{10} werden IA waardes tussen 0.48 en 0.64 berekend. Deze vergelijkingsstudie kan beschouwd worden als een 'end-of-pipe' validatie van de nauwkeurigheid van de volledige modelketen. Daarnaast werd een meer gedetailleerde analyse uitgevoerd op NO_2, een typische verkeerspolluent met sterke temporele en ruimtelijke variaties. Aangezien de NO_2 concentraties sterk beïnvloed worden door fouten in de verkeersstromen (en de resulterende emissies en concentraties) is deze polluent het meest geschikt om de ALBATROSS-MIMOSA-AURORA modelketen te valideren. De analyse toonde aan dat het activiteitengebaseerde luchtkwaliteitsmodel in staat was om de concentratiepatronen in Nederland met voldoende nauwkeurigheid temporeel en ruimtelijk te kunnen voorspellen.

Finaal, in de laatste onderzoeksfase werden blootstellingsanalyses uitgevoerd. Hiervoor werden de voorspelde concentratievelden van de ALBATROSS-MIMOSA-AURORA modelketen (per uur) gecombineerd met informatie over de locatie van de populatie. Door gebruik te maken van de activiteitengebaseerde simulatie van de populatie werden dynamische bevolkingskaarten opgesteld (eveneens per uur) en kon de blootstelling op een dynamische manier berekend worden.
In een eerste blootstellingsanalyse werd het dynamische blootstellingskader toegepast op een stedelijk gebied in Nederland. Deze blootstellingsstudie bevestigde de grote toestroom van mensen gedurende de dag in het stedelijke gebied waardoor mensen overdag blootgesteld worden aan hogere concentraties in vergelijking met hun residentiële situatie. Traditionele blootstellingsstudies, die concentratiewaardes combineren met residentiële informatie, zullen de werkelijke blootstelling dus vaak onderschatten.
In een tweede blootstellingsanalyse werden de dynamische blootstellingswaardes berekend voor gans Nederland en verder opgesplitst naar verschillende activiteitengebaseerde kenmerken zoals het geslacht van de persoon of de uitgevoerde activiteit. De resultaten van deze studie toonden aan dat, door geen rekening te houden met het verplaatsingsgedrag van mensen, de gemiddelde blootstelling aan NO_2 met ongeveer 4% onderschat wordt en de uurlijkse blootstelling zelfs tot 30% onderschat kan worden. Een opsplitsing van deze blootstelling toonde aan dat er grote blootstellingsverschillen kunnen optreden tussen verschillende activiteiten (transport > werk > winkelen > thuis) en tussen verschillende subpopulaties (man > vrouw; lage socio-economische klasse > hoge socio-economische klasse). Het in kaart brengen van blootstellingsvariaties tussen activiteiten en tussen subpopulaties kan zeer nuttig zijn voor wetenschappelijke en beleidsdoeleindes. Het kan informatie verschaffen over de locaties of de groepen die het meeste risico lopen of aangeven waar en waneer de hoogste blootstellingswaardes voorkomen.

Samengevat toonde dit proefschrift de voordelen aan van een activiteitengebaseerde aanpak voor luchtkwaliteit door het presenteren van drie toepassingen: het berekenen van voertuigemissies, de simulatie van concentraties en het berekenen van de blootstelling aan luchtverontreiniging.

LIST OF SYMBOLS AND ABBREVIATIONS

CFD	Computational Fluid Dynamics
C_o	Observed concentration level
CO_2	Carbon dioxide
C_p	Predicted concentration level
FB	Fractional Bias
GIS	Geographic Information System
IA	Index of Agreement
IFDM	Immission Frequency Distribution Model
IPF	Iterative Proportional Fitting
NMSE	Normalised Mean Square Error
NO_2	Nitrogen dioxide
NTS	National Travel Survey
O_3	Ozone
OD	Origin-Destination
PCA	PostCode Area
PM	Particulate Matter
PM_{10}	Particulate Matter, particles less than 10 μm in diameter
$PM_{2.5}$	Particulate Matter, particles less than 2.5 μm in diameter
r	Correlation coefficient
SEC	Socio-Economic Class
SNAP	Selected Nomenclature for sources of Air Pollution
SO_2	Sulphur dioxide
TCM	Transportation Control Measures
TDM	Transportation Demand Measures
VKT	Vehicle Kilometres travelled
VOC	Volatile Organic Compounds
σ_o	Standard deviation of observed values
σ_p	Standard deviation of predicted values

LIST OF ORIGINAL PUBLICATIONS

This thesis is based on the following articles, published in peer reviewed scientific journals. The articles are referred to in the text by Roman numerals I-V.

I Beckx C., Arentze T., Int Panis L., Janssens D. Vankerkom J., Wets G., 2009. An integrated activity-based modelling framework to assess vehicle emissions: approach and application. Environment and Planning B: Planning and Design. In press.

II Beckx C., Int Panis L., Van De Vel K., Arentze T., Janssens D., Wets G., 2009. The contribution of activity-based transport models to air quality modelling: a validation of the ALBATROSS - AURORA model chain. Science of the Total Environment 407, 3814-3822.

III Beckx C., Torfs R., Arentze T., Int Panis L., Janssens D., Wets G., 2008. Establishing a dynamic exposure assessment with an activity-based modeling approach: methodology and results for the Dutch case study. Epidemiology 19, S378-S379.

IV Beckx C., Int Panis L., Arentze T., Janssens D., Torfs R., Broekx S., Wets G., 2009. A dynamic activity-based population modelling approach to evaluate exposure to air pollution: methods and application to a Dutch urban area. Environmental Impact Assessment Review 23, 179-185.

V Beckx C., Int Panis L., Uljee I., Arentze T., Janssens D., Wets G. Disaggregation of nation-wide dynamic population exposure estimates in The Netherlands: applications of activity-based transport models. Atmospheric Environment, available from: http://dx.doi.org/10.1016/j.atmosenv.2009.07.035

CONTENTS

1 GENERAL INTRODUCTION

1.1 Problem statement

The rapid economic development in most Western countries has led to a quasi linear growth in the yearly number of vehicle miles travelled since the 1970's (European Commission, 2001). Personal mobility, which increased from 17 km a day in 1970 to 35 km in 1998, is now more or less seen as an acquired right. For passenger transport, the determining factor in this rise is the spectacular growth in car ownership. The number of cars has tripled in the last 30 years. Although the level of car ownership is likely to stabilize in most countries of the European Union, this will not be the case in the developing countries. The claim about the increasing demand for mobility is also supported by research, based on predictions about world trade, national income and urbanization, which demonstrate that the demand for mobility in Europe is expected to rise considerably in the years to come (United Nations Economic and Social Council, 2001; European Commission, 2001).

Transport has both positive and negative effects on health. On the one hand, transport connections help people to reach services, maintain contacts and interactions. On the other hand transport causes annually hundreds of thousands of premature deaths in Europe. For example every year about 45 000 people die in traffic accidents and 1.5 million people are injured in the European Union. Further, transport related gaseous and particulate emissions are one of the main sources of air pollution. Air pollution is estimated to cause around 370 000 premature deaths a year in the European Union and an average estimated reduction of life expectancy of around 8,7 months per EU citizen (EU, 2006). Traffic air pollutants that raise most health concerns are fine particles (PM), nitrogen dioxide (NO_2) and ozone (O_3).

Due to the negative effects of transport, one of the key challenges of the modern policy making consists of promoting a sustainable transportation system aiming at the prevention or reduction of the negative effects of the transportation system on health and environment. As indicated in the EU White Paper "European transport policy for 2010: time to decide" (European Commission, 2001) a modern transport system must be sustainable from an economic and social as well as an environmental point of view. It is therefore not surprising that governments today are considering several traffic policy measures to reduce the negative effects of the increasing mobility on the environment.

While formulating policy measures concerning traffic and transportation, a number of considerations with regard to the environment, health, etc. needs to be taken into account enabling as such an evaluation of the strategies producing the best net advantages in an integrated manner. However, often only direct isolated measures have been taken into account in the past by governments to reduce a specific targeted negative effect. Amongst these, one can think for instance of measures against impaired driving for improving road safety. We call these measures direct measures because they are created to contribute directly to solving the problem. Yet, there also exist a number of general mobility-related policy measures, mostly to influence transportation demand, but whose impact on the environment is much less straightforward to determine. In other words, these general road policy measures are expected to have only an indirect effect on road safety and environment. They have a direct influence on the demand for transportation (in fact, this is usually their reason for existence, e.g. to reduce congestion). But since the demand for transportation is the principle driver behind problems regarding traffic air pollution, they hereby also contribute indirectly to the environment and ultimately thus also to human health. Examples of such general policy measures include, for instance, promoting telecommuting activities, stimulating car pooling, changing institutional aspects like shop opening hours, etc. Therefore there is an important challenge in developing a coherent framework in which a variety of inputs can be joined and their effects can be evaluated.

To give more accurate and complete estimates on the impact of (transport) policies on the environment, the use of a modelling framework, taking into account the different causal links between activities, trips, emissions, concentrations and exposure, is preferred. Such an integrated approach to describe and mitigate environmental problems is also present in the DPSIR-chain, developed by the Dutch RIVM (Rijksinstituut voor Volksgezondheid en Milieu) in the late 1980'ties and later adapted by the European Environmental Agency (Jol and Kielland, 1997). The DPSIR is a conceptual model used to describe and analyse environmental problems. Driving forces (D) like transport and industry lead to environmental pressures (P) that degrade the state (S) of the environment that has an impact (I) on human health or the environment which makes society carry out a response (R) through various actions. In Figure 1 the DPSIR concept has been illustrated using the case of air pollution with a focus on transport. This concept can be considered as a leitmotiv throughout this PhD manuscript and the principle motivation for this study can therefore be summarized as: *Providing a framework that enables an assessment of general traffic policy measures on transport, emissions, concentrations and human health*".

Further, besides the motivation out of modelling perspective, another important topic in this research concerns the improvement of the travel demand link in the problem chain. To provide more insight into people's travel behaviour, information is required on travel aspects like: 'why are people travelling', 'who is performing the trips', 'when are trips performed', etc. Also, insights need to be present on the interactions among individual and household travel decisions to be able to give good estimates on the impact of transportation control measures (TCMs) on the travel behaviour. Traditional four-step trip-based models lack in the ability to model these interactions. These trip-based models focus on individual trips, ignoring the spatial and temporal interrelationships between all trips. In this PhD study a different approach for travel demand is therefore adopted: an 'activity-based' approach.

The rich information provided by activity-based transportation models (i.e. information on why, when and where people are travelling) enables a more accurate approach to assess the impact of transport on the environment. The activity-based approach models an individual's daily pattern of activities in its entirety, taking into account his/her role in the household and experiencing various constraints like time availability and coordination with other household members. Further, activity-based models offer a technique to micro-simulate activity patterns of a population with a high resolution in space and time. Due to these advantages, the use of an activity-based approach in the modelling framework should enable a more accurate assessment for air pollution exposure.

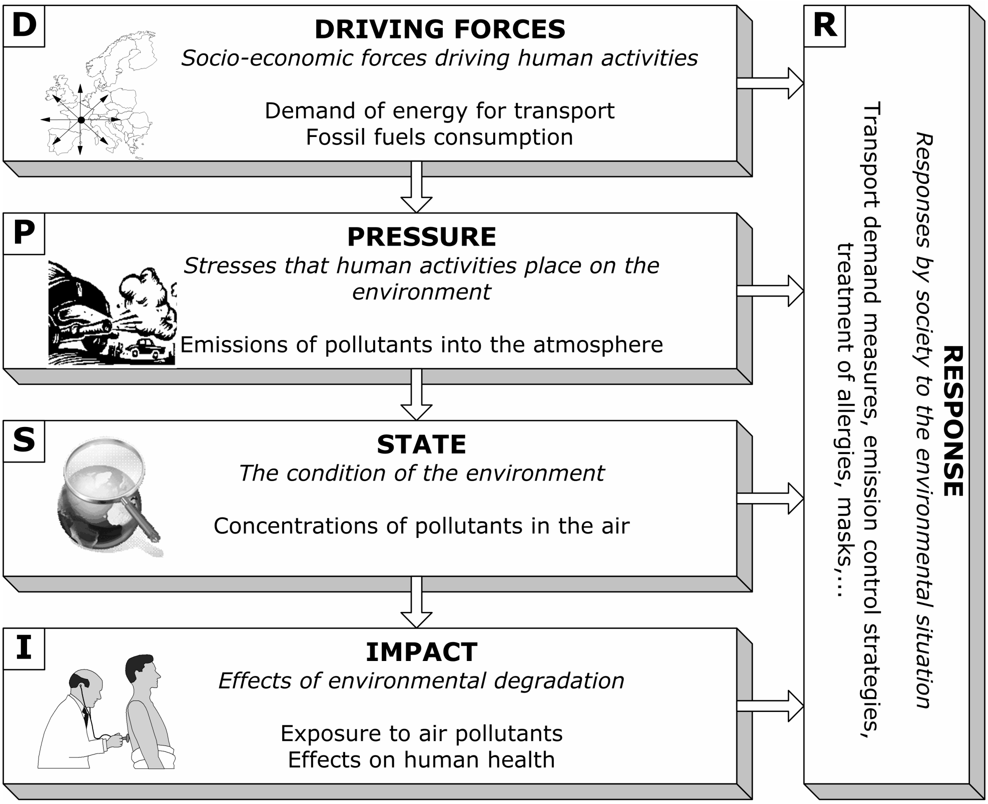

Figure 1. Illustration of the DPSIR concept for transport related air pollution

1.2 Research objectives

The overall objective of this doctoral dissertation work is *"To develop and evaluate an activity-based modelling methodology for the assessment of population exposure to air pollution"*.

This approach should involve all the compartments of the DPSIR-concept, as mentioned in the previous section, to give a complete overview of this environmental problem of air pollution exposure. First the activities and the travel demand of people should be modelled (D), then the emissions resulting from the modelled vehicle trips need to be simulated (P), the concentrations and the exposure of people to these pollutant concentrations should be calculated (S) and the health impact (I) has to be assessed. Finally, this exposure model should allow for evaluating various responses (R) by recalculating all the values in the different compartments for a certain scenario.

The overall objective can by achieved by performing the following three specific tasks.

- Calculate and validate the emissions resulting from passenger car trips by using the trip information from an activity-based model (I) ***(D,P)***
- Calculate and validate the pollutant concentrations by converting the activity-based emissions into ambient pollutant concentrations (II) ***(S)***
- Establish a population exposure model using the time series population information from an activity-based model and detailed air quality data (III, IV, V) ***(I)***

The original articles that tackle each task in detail are listed in parentheses, their link with the components of the DPSIR-chain is also indicated. Each of these specific tasks will be presented in more detail in chapters 3 to 6. Developing new models or applying large adjustments on existing models was not part of this thesis. It was rather recommended to apply and combine existing models from the different domains. Therefore model experts from each domain were involved to achieve the thesis objectives efficiently. Information on the models used for the listed tasks can be found in chapter 2.

1.3 Background on exposure assessment

Exposure assessment involves a description of the population exposed, the pollutants and the duration of the exposure. This section briefly describes the assessment methods used in current exposure studies and lists the projects that apply an integrated exposure analysis.

1.3.1 Exposure assessment methods

Human exposure may be estimated by different methods. Basically, exposure methods can be classified in direct and indirect approaches.

1.3.1.1 Direct methods

Personal monitoring and biological monitoring are direct methods to measure exposure to air pollution. Personal portable samplers can be used in personal monitoring to measure the concentrations a person is exposed to. Biological monitoring is also a personal monitoring method where the concentration of a pollutant or the metabolite of a pollutant is determined in biological material e.g. urine or blood.

Direct exposure methods have the advantage that they give the 'correct' exposure results. Personal samplers e.g. indicate the amount of pollutants in the immediate vicinity of the individuals. By planning large scale experiments with a lot of personal samplers (e.g. in a sensor network) good insights can therefore be provided on the variation in exposure between individuals and locations. Further, by taking into account measures or estimates on parameters like breathing rate, the inhaled dose for specific pollutants can be assessed by using this direct method. Biological monitoring methods immediately measure the amount of pollutants taken in by the individual over a certain period of time (see e.g. Koppen et al. 2008). However, exposure varies a lot between individual receptors and is determined by numerous parameters. The main drawback of using these direct methods is therefore the amount of time and receptors (people) that is necessary to draw general conclusions about the population exposure.

1.3.1.2 Indirect methods

Fixed monitoring stations

Indirect exposure studies determine personal or population exposure indirectly by combining pollutant concentration information with information about the time people spend in specific environments. A crude indirect method is the use of fixed location measurements, e.g. from the ambient air quality monitoring stations, to obtain an indicator for population exposure (Dockery et al. 1993; Pope et al. 2002; Pope et al. 2009). However, fixed monitor stations are generally poor indicators of personal exposure as they represent a single point in space and they are not able to reflect the variety of personal exposures. Monitoring is also extremely costly, so the density of these monitoring networks is often limited. Moreover, by using only residential address information to determine people's location, this method implicitly assumes that people are always at home and often underestimates the 'real' exposure of people (assuming that the exposure at out-of-home locations such as at workplaces and near traffic is generally higher than at home). For epidemiological purposes the residential exposure information is however of much interest since exposure-health functions, developed in the epidemiological research, are mainly based on this kind of exposure information (Dockery et al. 1993; Pope et al. 2002). On the other hand, for policy purposes it would be interesting to obtain more information about where and when the exposure occurs and who is at risk, therefore taking into account people's travel behaviour during the day.

Microenvironment approach

Another indirect method is the microenvironmental approach where air pollution data in different microenvironments are combined with the time people spend in each of these microenvironments. Using the microenvironmental approach the integrated exposure of an individual can be calculated as:

$$E_i = \sum_{j}^{J} c_j * t_j$$

where E_i is the integrated exposure of an individual i who visits J different microenvironments with a concentration C_j in microenvironment j during time period t_j.

Exposure models like NEM, AirPEx and SHAPE are based on an indirect exposure method using this microenvironmental approach (Jenssen, 1999). These models combine air quality data in selected microenvironments with the time-activity patterns of individuals that describe the time that individuals spend in these microenvironments. This method provides better indicators of personal exposure than using fixed monitors but they are usually limited to studies of a small number of subjects.

Time-activity patterns and dispersion models

For many uses, the need is to understand much more about the geographic variation of both pollutants and populations. Combining the results from pollutant dispersion models with information on the location of people, as also used in the current work, defines therefore the last indirect exposure method. This method takes into account the spatial and temporal variation in both the air pollution and the population. This approach involves the use of a geographic information system (GIS) to match the pollutant data exactly with the population data. This method is perhaps the most complete exposure assessment method since people's travel behaviour is also taken into account (instead of using only residential information) to calculate the population exposure. However, due to the fact that accurate information from different sectors is required (both travel behaviour and air quality), this kind of interdisciplinary method is usually less explored compared to studies using the fixed monitor approach.

Examples of this approach can be found in Kousa et al. (2002) and Marshall et al. (2006). In Kousa et al. (2002) the spatial and temporal variation of the average exposure of an urban population was evaluated by combining population data with predicted concentration data. Population data however did not originate from a population simulation procedure, but from combining information on the home/work locations with standard time-activity patterns.

Marshall et al. (2006) examined the distributional characteristics of the exposure and inhalation intake for certain subgroups of the population. As in the doctoral research, this study was restricted to pollutants of outdoor origin, i.e.. it does not incorporate intake in a microenvironment from direct emissions into that microenvironment. The population data, however, were not simulated, but extracted from geocoded activity diaries. By approaching a large number of respondents in this survey, still good insights were provided on the variations in exposure between locations and between people.

In the next section a number of projects are listed that apply an integrated modelling approach to assess both travel and environmental aspects in one general framework.

1.3.2 Integrated exposure analysis

The complexity of today's policy decision making has motivated several research teams to develop policy frameworks aimed at evaluating the impact of transportation policy measures on emissions, concentrations and exposure. This section provides an overview of some important initiatives, mostly carried out as (part of) European projects. At the same time, the most important differences of those projects compared with the current work are addressed.

The HEAVEN project (Healthier Environment through Abatement of Vehicle Emission and Noise) is a European project (HEAVEN, 2003) funded under the Information Society Technology Programme (1998-2002) (Tomassini, 2003). Its main objective was to develop and demonstrate a decision support system (DSS) which can evaluate the environmental effects (air quality and noise quality – both emissions and dispersion forecasting) of Transportation Demand Measures (TDMs) in large urban areas. The project was applied under real-life conditions in the project cities of Berlin, Leicester, Paris, Prague, Rome and Rotterdam. The most important differences of the HEAVEN project compared to this work are:

- The HEAVEN project was set up as a tool to obtain a description and inform professional users and the public in near real-time about the traffic and environmental situation in urban agglomerations. It therefore combines near real-time traffic flow and environmental information into emissions and dispersion models. The approach in this study is rather different. Although the model framework presented here will also provide the ability to estimate effects on a very low level of detail, both in time and space, it is not the objective to create (near) real-time forecasts and feed the model with real-time traffic flow and environmental information to provide online scenario testing. The presented framework in this research should therefore be seen as an off-line model.
- The HEAVEN project does not model the exposure to pollutants. It does model the emission and dispersion of pollutants, but since there is no information available on activity behaviour of individuals, it is not possible to estimate the exposure to pollutants at a particular point in time and space.
- The HEAVEN project deals with TDMs in the field of infrastructure and traffic management and regulation, such as changes in vehicle fleet, access restrictions, speed limits, park-and-ride schemes and changes to the street network. The proposed model in the current work however enables to assess the effects of a wider range of TDMs including also measures like telecommuting, road pricing, flexible working hours, …

The HEARTS project (Health Effects And Risks of Transport Systems) is a European research project carried out under the Fifth Framework Programme (WHO, 2006). The HEARTS project provides a method for estimating the health effects of air pollution, noise and road accidents and an instrument for integrating health impact assessment in the decision-making on and assessment of transport and land-use policies in urban areas. Case studies were carried out in the cities of Leicester, Lille and Florence. The most important differences of the HEARTS project compared to the current research are:

- The HEARTS project models, in detail, over relatively smaller areas of the city across peak and off-peak periods. This is rather different from the current work since the activity-based transportation model enables complete time-segmentation for different time periods during a day and thus enables to create complete time-segmented origin-destination (OD) –information.
- Concerning the traffic modelling, within the three cities running case studies, classical traffic models have been used. These include a typical static 4-step transport model such as EMME/2 (Constantin, 2000) and a typical micro-simulator such as PARAMICS (see paramics-online.com/).
- The HEARTS project also models noise and the effects on health. These aspects are not covered in the current project. However, the necessary information to enable such analyses is available and can be used as input for noise modelling or for health impact studies.

The TRANS-TOOLS project (TOOLS for TRansport forecasting ANd Scenario testing) is a research project co-funded by the European Commission under the 6th Framework Programme for Research and Development (Burgess and Nielsen, 2008). TRANS-TOOLS aims to produce a European transport network model covering both passengers and freight, as well as intermodal transport. The project builds on several existing transport models and networks, such as SCENES, VACLAV, NEAC and SLAM. Some notable differences with this research project are:

- The TRANS-TOOLS project deals with a strategic European-wide transport model and is designed to produce European level transport forecasts, both for freight and passenger transport. The activity-based model used within this study deals with national passenger transport only.
- The TRANS-TOOLS project uses the classical 4-stage transportation approach (trip generation, trip distribution, modal split and assignment), whereas in this project an activity-based approach was adopted. For example, this implies that in the TRANS-TOOLS project trip generation in passenger transport is driven by socio-demographic and economic

variables of the zones, whereas in the presented study trip generation is also driven by the activities that households perform.

- The TRANS-TOOLS project makes forecasts for 3 time periods (peak, off peak and rest of the day) whereas this modelling framework enables continuous time segmentation throughout any user-defined period of the day.

The aim of the ISHTAR project (an Integrated Models Suite for Sustainable Transport Planning) was to build an Integrated Suite of software models to assess the impacts of urban policies on the quality of life, and in particular on traffic congestion, air quality, human health and the conservation of monuments (Agostini et al. 2005) . Differences between ISHTAR and the current study are:

- Concerning the traffic modelling, an analysis of the available transport models was part of the ISHTAR project. Based on this screening, the VISUPOLIS traffic model was described as the best tool to integrate within the suite. However, future users are not obliged to use this model and can link their own traffic model with the ISHTAR suite, indicating that the traffic modelling part was not the main research topic in this project. In the doctoral research, however, this topic is one of the main research themes.
- The suite calculation path goes through the modelling of traffic safety, noise emissions and monuments degradation. These aspects are not covered by the current work although they might be included in future research since necessary data for performing these analyses is available.
- The ISHTAR framework is primarily developed for use within urban areas whereas the study area of the current work is larger and also wants to take into account inter-city issues.

1.4 Study area

To illustrate the feasibility of the integrated exposure framework, this research will involve a case study in one specific study area: The Netherlands. Reasons counting in favour of this choice can be found in the activity-based modelling part since, at the beginning of the research, a fully operational activity-based model was already available for The Netherlands.

The Netherlands cover an area of approximately 42 000 km² with a population of around 16 million people. Some well-known cities in the Netherlands are Amsterdam, The Hague, Rotterdam and Utrecht. Exposure to air pollution is considered a major problem in The Netherlands, as well as in neighbouring regions. A European analysis e.g. estimated that the average life expectancy in The Netherlands was reduced by about one year in 2000 because of exposure to pollutants such as $PM_{2.5}$ (Amann et al. 2005).

Future activity-based model developments however can facilitate their application for other study areas. Recent research projects for example aim at establishing an activity-model for Flanders (Belgium) and specifically focus on the flexibility of the activity-based platform towards 'foreign' data (i.e. data from other years or other regions) (Janssens et al. 2007). Of course, these developments can result in applications in other study areas based on the approach presented in this thesis.

1.5 Outline of the dissertation

This introductory chapter gives a short introduction to the state of the art in exposure analysis as well as a rough description of the problem. It also indicates the need for and the advantages of an exposure modelling framework.

In Chapter 2 more background information is presented on the different models included in the PhD modelling framework. In this work three types of models are interrelated to establish an integrated exposure framework: an activity-based transport model, an emission model and a dispersion model. Chapter 2 presents the general characteristics of these models and describes the specific model used in the modelling framework of the PhD project. For each model the model input and its configuration are described. Changes performed within the scope of the current research are listed separately.

Chapters 3 to 6 deal with the specific steps in the development towards an integrated exposure framework. In chapter 3 the first step, the link between the activity-based transport model and the emission model, is described. This chapter presents the methodology to couple the activity-based model (ALBATROSS) with the emission model (MIMOSA) to calculate the vehicle emissions in the Netherlands. The estimated emission results are compared with reported emissions to validate the applied methodology. Chapter 4 continues on the work described in Chapter 3 and describes the methodology to calculate pollutant concentrations in the Netherlands based on the emission results from the activity-based emission approach. This chapter describes the conversion of the emissions into concentrations by using the dispersion model AURORA. The estimated concentration results are compared with measured concentrations at Dutch measurement stations to validate the applied methodology..

By combining these concentration data with the activity-based population data, the integrated exposure modelling framework was established In Chapters 5 and 6 two applications of the integrated exposure framework are presented. Chapter 5 describes the calculation of population exposure in a Dutch urban area and mainly focuses on differences between the activity-based exposure approach and the traditional static exposure approach assuming that people are always at home. In Chapter 6 the study area is extended to the whole Netherlands and exposure is disaggregated based on information from the activity-based framework.

Chapter 7 summarizes the new information and conclusions resulting from this PhD work. It concludes with some recommendations for future studies.

To clarify the content of the different chapters in this manuscript Figure 2 gives an overview of the developed exposure modelling framework and indicates in which chapter the different components of the framework are further explored. Parts of this figure will be reused in the methodological section from their corresponding chapters to clarify the adopted methodology in this PhD.

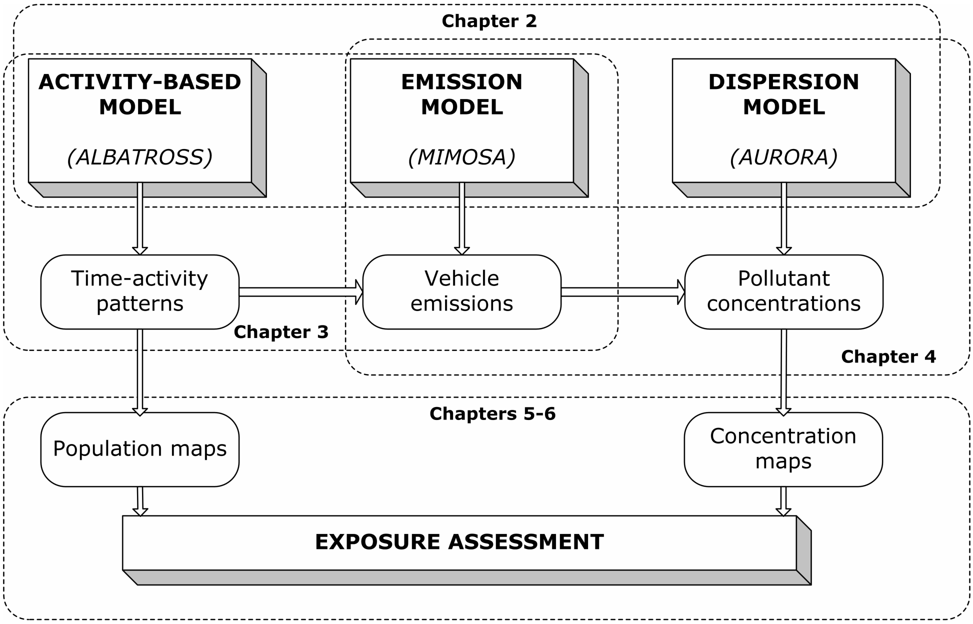

Figure 2. Overview of the exposure modelling framework with references to the relevant chapters in this book.

2 OVERVIEW AND DESCRIPTION OF USED MODELS

2.1 Introduction

The evaluation of population exposure to air pollution requires spatial and temporal information on both air quality and population attributes. In this research an integrated model framework was therefore established including the following models: an activity-based model (to derive information on the population and the travel patterns), an emission model (to convert trips into air emissions) and a dispersion model (to convert the air emissions into concentration levels). As it was not the purpose of this PhD to develop new models, but mainly to combine existing models in an innovative way, modelling experts from the different research institutes (IMOB, VITO, TU/e) were closely involved to perform the modelling steps efficiently.

In this chapter some general information is provided on each model type and a description is given of the specific model that was used in the current research. The model changes performed within the scope of this research are listed separately. A schematic overview of the different models being part of the modelling framework can be found in Figure 2 from the introductory chapter.

2.2 Activity-based modelling

2.2.1 Overview of the activity-based modelling approach

2.2.1.1 The evolution towards an activity-based approach

Modelling traffic patterns has always been a major area of interest in transportation research. Since 1950, due to the rapid increase in car ownership and car use in the US and in Western Europe, several models of transport mode, route choice and destination were used by transportation planners. These models were necessary to predict travel demand on the long run and to support investment decisions in new road infrastructure which originated from this increased level of car use. In these days, travel was assumed to be the result of four subsequent decisions which were modelled separately: trip generation, trip distribution, modal split and trip assignment. Within transportation literature those models are also referred to as Four-Step trip-based models (Ruiter and Ben-Akiva, 1978). Many of these aggregate Four-Step models failed to make accurate predictions. Their major drawback clearly is the focus on individual trips, where the spatial and temporal interrelationships between all trips are ignored. Furthermore, another drawback is the complete negation of travel as a demand derived from activity participation decisions.

From the mid seventies onwards the original Four-Step models were replaced by tour-based models (Daly et al. 1983). In the tour-based model, trips are explicitly connected in chains that start and end at the same home or work base. By means of this property, the spatial interrelationship, which was so apparently lacking in the Four-Step trip based models, is dealt with. Nevertheless in these models, travel still has an isolated existence and the question why people undertake trips is completely neglected. This is why activity-based transportation models came into play.

The contributions of Hägerstrand (1970), Chapin (1977) and Fried et al. (1977) are the undisputed intellectual roots of activity analysis. Hägerstrand suggested the time-geographic approach characterizing a list of constraints on activity participation. Chapin has identified patterns of behaviour across time and space. Fried dealt with the social structure and the question of why people participate in activities. These contributions came together in a study of Jones et al. (1983), where activities and travel behaviour were integrated. This was the first attempt to model complex travel behaviour with an activity-based approach.

The major idea behind activity-based models is that travel demand is derived from the activities that individuals and households need or wish to perform, with travel decisions forming part of the broader activity of scheduling decisions (Ettema and Timmermans, 1997). Travel is merely seen as just one of the attributes. Moreover, decisions with respect to travel are driven by a collection of activities that form an agenda for participation. Travel should therefore be modelled within the context of the entire agenda, or in other words, as a component of an activity scheduling decision.

Activity-based approaches aim at predicting which activities are conducted, where, when, for how long, with whom and the transport mode involved.

McNally (2000) has listed 5 themes which characterize the activity-based modelling framework:

(i) travel is derived from the demand for activity participation;

(ii) sequences or patterns of behaviour, and not individual trips are the relevant unit of analysis;

(iii) household and other social structures influence travel and activity behaviour;

(iv) spatial, temporal, transportation and interpersonal interdependencies constrain activity/travel behaviour;

(v) activity-based approaches reflect the scheduling of activities in time and space.

In the more recent work from Davidson et al. (2007) a synthesis of the first practices of activity-based models for travel demand is provided and the main features of this 'new' generation of regional travel demand models are listed as follows:

(i) an activity-based platform, implying that modelled travel is derived within a general framework of the daily activities undertaken by households and persons;

(ii) a tour-based structure of travel where the tour is used as the basic unit of modelling travel instead of the elemental trip;

(iii) micro-simulation modelling techniques that are applied at the fully-disaggregate level of persons and households.

Over the last years, several research teams have focused on building activity-based models of transport demand. Partial and fully operational activity-based micro simulation systems include the Micro-analytic Integrated Demographic Accounting System (MIDAS) (Goulias and Kitamura, 1996), CEMDAP (Bhat et al. 2004), Prism Constrained Activity-Travel Simulator (PCATS) (Kitamura and Fujii, 1998), SIMAP (Kulkarni and McNally, 2000), ALBATROSS (Arentze and Timmermans, 2000; 2004; 2005), Florida's Activity Mobility Simulator (FAMOS) (Pendyala et al. 2005), the Travel Activity Scheduler for Household agents (TASHA) (Miller and Roorda, 2003), the FEATHERS framework (Janssens et al. 2007) and other systems using a nested-logit framework (Bowman and Ben Akiva, 2001). Other AB models currently in use are present in New York City (Vovsha et al. 2002), Columbus (Vovsha and Bradley, 2004) and San Francisco County (Bradley et al. 2001).

2.2.1.2 Advantages for air quality purposes

Although the activity-based model was originally developed to gain more insights into people's travel behaviour, the activity-based approach for transport modelling also offers advantages for other sectors. In this section the main benefits of using an activity-based approach for air quality purposes are presented.

Transportation information

The accuracy of air emissions and air quality estimates can be no better than the underlying transportation information (Int Panis et al. 2001; 2004). Due to the richer set of concepts which are involved in activity-based transportation models the estimate of some important transportation variables can be improved by using an activity-based approach (Shiftan, 2000). E.g. vehicle energy use and emissions depend not only on distance and the driving speed, but also on the number of trips, the time between them, and whether the engine was hot or cold when started (Recker and Parimi, 1999). The activity-based prediction of trips as parts of a tour can identify whether a trip is a cold or a hot start.

Furthermore, an activity-based model, by predicting which activities are conducted, where, when, for how long, with whom and the transport mode involved, gives in addition information about important transportation variables such as vehicle miles travelled (VMT), travel mode and occupancy rates for auto modes, travel by time of day and time/location of starts. These variables all are relevant and important for vehicle emission analysis.

Temporal travel and emission analysis

In most traffic air pollution studies aiming at a temporal differentiation of traffic emissions, either hourly traffic counts are used (e.g. Ghenu et al. 2008) or the emission model applies normalised distribution factors expressing the time dependency of traffic with respect to peak values (e.g. Schrooten et al. 2006). As a consequence of this time factor approach, similar variations in traffic flows are assumed over the entire region and local characteristics are usually not taken into account. An activity-based approach, however, does not work with traffic counts nor peak hour predictions, but simulates entire activity-travel schedules covering a complete day and taking into account local and temporal variations in travel behaviour. Extraction of the simulated travel information, can therefore provide temporal travel and emission values more accurately.

Activity-based policy measures

Since the demand for transportation is the principle driver behind the environmental problem of traffic air pollution, governments are considering several TDMs to reduce the negative impact of the increasing mobility on the environment. However, for a number of TDMs such as congestion pricing, promoting telecommuting and stimulating car pooling, the impact on the environment is not straightforward to determine. Current transportation forecasting models use the "trip" (usually a vehicular trip) as the basic unit of analysis and prediction. Consequently, by starting with the trip, these transportation models are less accurate in addressing issues related to activities (e.g. telecommuting, teleshopping, trip chaining behaviour,…). Activity-based models on the other hand are able to evaluate the impact of these measures on travelers' responses, and due to this, the impact on travel behaviour and air quality can be better assessed.

Secondary effects

One of the main advantages of the activity-based modelling system is its ability to consider the secondary effects of TCMs (Shiftan and Suhrbier, 2002). Secondary effects are adjustments to the activity pattern that have to be made in response to the primary effect. For instance, a public transport subsidy may make a commuter change his or her mode from drive alone to public transport; this is the primary effect of the TCM. However, because the person no longer drives to work, there can be no stop on the way back to do the shopping. Therefore, upon returning home, the person takes the car and drives to a nearby store. This is the secondary effect. In such cases, the environmental advantages of this TCM may be limited, and the reduction of the work auto trip is partially offset by a new shopping auto trip. Due to the considered constraints and household interactions, an activity-based approach is most suited to deal with these secondary effects (Shiftan, 2000).

Exposure assessment

Conventional exposure studies take into account variations of the emission sources, but typically assume static receptor conditions (Pope et al. 1995; Pope et al. 2009; Walker et al. 1999). According to this approach the receptors (i.e. the people) are considered to be always at home and, therefore, only exposed to pollutants at their home address. Attempts for assessing dynamic exposure are very rare and often focus on long time scales (e.g. De Ridder et al. 2008a; 2008b). However, when temporal information is available on both the sources (i.e. the emissions) and the receptors of the air pollution, a dynamic exposure procedure can be established. An activity-based approach takes into account that people move during the day and therefore this approach can account for the exposure to pollutants at different locations and different moments. Further, by taking advantage of information on 'which activity is performed' or 'who is performing the activity', the activity-based procedure allows for a disaggregated exposure analysis according to different subgroups. This information can for example give more insights into the subgroups most at risk.

2.2.1.3 *Applications of activity-based models for environmental purposes*

Although the advantages of an activity-based approach for air-quality purposes are well-known (see section 2.2.1.2), models that have been developed along these lines are still scarce. Perhaps the most ambitious project in this field of research is TRANSIMS (Rickert and Nagel, 2001). TRANSIMS, the TRansportation ANalysis and SIMulation System, was developed at the Los Alamos National Laboratory as part of the multi-track Travel Model Improvement Program (TMIP). The TRANSIMS project is a major effort to develop new integrated transportation and air quality forecasting procedures to satisfy the Clean Air Act Amendments (CAAA) and the Intermodal Surface Transportation Efficiency Act (ISTEA). The detailed simulation in TRANSIMS, in comparison with simplistic and unrealistic aggregate link cost functions used in conventional models, provides increased accuracy in prediction of environmental impacts (e.g. emissions) and travel times. An important disadvantage of this micro simulation approach is the large amount of data required to make accurate predictions on this detailed time-space level. Considering the fact that a lot of policy questions do not require such a time-consuming microscopic analysis and that detailed analyses are not suited for very large study areas, less detailed emission estimations are desirable. Moreover, TRANSIMS is somewhat limited regarding the prediction of activity patterns. Activity schedules of simulated individuals are drawn from activity data sets and hence the model, on that level, is insensitive to changed space-time conditions that may be involved in applications.

Another application of activity-based models for air quality can be found in Recker and Parimi (1999). They developed a microscopic activity-based framework to analyze the potential impacts of TCMs on vehicle emissions. Although this approach is very useful in estimating upper bounds of certain policy measures in reducing vehicle emissions, their framework falls short of actually forecasting changes in travel behaviour.

In Shiftan (2000) the first application of a real activity-based model in the US was examined, evaluating the advantages of the Portland activity-based model for emissions and air quality analyses against the use of a traditional four-step model. Only qualitative comparisons were made. Afterwards, this research was further explored, evaluating the transportation and air-quality impacts of four travel demand strategies with the Portland activity-based model (Shiftan and Suhrbier, 2002). The following strategies were evaluated: pricing of automobile travel, telecommuting incentives, transit improvements and a combination of the three measures. By predicting a wider range of impacts and taking indirect effects into consideration, the activity-based approach proved to be very useful in determining some important variables for emission estimation.

The most recent accomplishment in this line of research concerns the integration of the Canadian version of the MOBILE6.2 emission model with the travel demand modelling capabilities of the Travel Activity Scheduler for Household Agents (TASHA) (Hatzopoulou et al. 2007). This study provided an initial attempt at quantifying vehicle emissions in the Greater Toronto Area with an activity-based transport model. By exploiting travel information from the TASHA model, travel activity inputs (for light-duty gasoline vehicles) were provided for the MOBILE6.2 emission model and emissions were calculated more accurately compared to the default version by taking into account region specific information on activities and vehicles (on hourly basis). In a next phase, Hatzopoulou also calculated pollutant concentrations by applying the CALPUFF model (Hatzopoulou, 2008).

Unfortunately, both the Portland and the Canadian study demonstrate the advantages of the activity-based approach for the analysis of environmental topics, but do not carry out an independent benchmark based on external information of the predicted emissions or concentrations. Further, the Portland study has not looked beyond emissions.

2.2.2 ALBATROSS

For use within the exposure modelling framework, the activity-based model ALBATROSS, developed at the Eindhoven University of Technology (TU/e), was selected. The version of the Albatross model used in this study is version 2.0, which was the latest one at the time of this study. Prof. dr. Theo Arentze from the TU/e is kindly acknowledged for his support with the ALBATROSS modelling procedures.

The activity-based model ALBATROSS, A Learning-Based Transportation Oriented Simulation System, was developed for the Dutch Ministry of Transportation, Public Works and Water Management as a transport demand model for policy impact analysis. The model is able to predict which activities are conducted, when, where, for how long, with whom, and the transport mode involved. Albatross is unique in that 'decision rules' as opposed to 'principles of utility maximization' underlie the scheduling decisions. Furthermore, the rather detailed classification of activities and inclusion of a full set of space-time and scheduling constraints are distinctive features of the model compared with most other models.

2.2.2.1 Model input

ALBATROSS is a computational process model that relies on a set of decision rules, which are extracted from observed activity diary data, and dynamic constraints on scheduling decisions, to predict activity-travel patterns (Arentze and Timmermans, 2000; 2005; Arentze et al. 2003). To simulate activity-travel patterns for a whole population, information on both the population characteristics and their activity-travel patterns is required. Other necessary input data include physical information about the study area.

Population data

In the Dutch case study presented in this dissertation, ALBATROSS was used to simulate activity schedules for the individuals within the Dutch population. The model was estimated by Arentze and Timmermans (2005) on approximately 10,000 person-day activity-diaries collected in the period of 1997-2001 in a selection of regions and neighbourhoods in the Netherlands. In a sub application of the model, a synthetic population was created with iterative proportional fitting (IPF) methods, using demographic and socio-economic geographical data from the Dutch population and attribute data of a sample of households originating from a national survey including approximately 67,000 households. IPF is used to generate a sample consistent with known statistics of the target population. In IPF the sample defines an initial frequency cross table of all attributes involved. Demographic data are used to define constraints on marginal distributions of the tables. IPF is applied to find cell proportions that are consistent with given marginals.

Attributes of households/individuals that Albatross considers as potential predictors of choice behaviour include (see also Arentze and Timmermans, 2000; 2005):

- Household type: single non-worker, single worker, double non-workers, double one-worker, double two workers
- Age of the oldest member of household: younger than 25 years, 25-44, 45-64, 65 or older
- Age of the youngest child: no children, younger than 6 years, 6-11 years, 12 or older
- Socio-economic class: very low household income, low, average, high
- Cars: number of cars in household
- Gender of person
- Availability of car for person (capable of driving)
- Number of weekly working hours of person

The first five attributes are measured at the household level, whereas the last three attributes relate to individuals within households. In the Netherlands several nationwide surveys exist that are updated on a regular basis and can provide these attribute data at household/individual level. For the ALBATROSS model development, data were used from the Dutch national travel survey (NTS) ('Onderzoek Verplaatsingsgedrag' or 'OVG' in Dutch), which is used by the Dutch Ministry of Transportation for travel demand analysis and forecasting. The Dutch NTS records trips of persons of 12 years or older of households that participated in the survey. Although it is a trip-based database, the complete list of household and individual attributes is included in every recorded trip. Therefore, household and individual information about all persons that participated in the survey can be derived from the trip data.

Activity-travel data

The empirical derivation of the model is based on several pooled activity diary sets that were collected specifically for various research projects. These include the following:

(i) the Zwijndrecht/Hendrik-Ido-Ambacht data collected for Albatross 1.0;

(ii) the Voorhout data set collected for investigating the impact of a new railway station ;

(iii) a data set of nationwide random neighborhoods collected for investigating the impact of urban form on activity-travel patterns

(iv) the Amsterdam/Utrecht/Almere data set collected for the Amadeus research program.

Except for the last data set, the diary formats used in the different surveys were the same. They all used an open format, a precoded activity scheme, and similar classifications of activities and attributes. The Amadeus diary differed in that travel data were reported at the more detailed trip-stage level and the activity classification was less detailed.

Information on the classifications of activities and choice facets used in ALBATROSS can be found in Appendix A and in Arentze and Timmermans (2000, 2005). The distinction between fixed and flexible hereby refers to activities that supposedly belong to the schedule skeleton (fixed) and those that supposedly are scheduled on a daily basis (flexible). The duration and start time of fixed activities are predicted on a continuous time scale, whereas in the case of flexible activities these facets are treated as a choice between pre-defined discrete alternatives.

Physical information

The 4-position postcode area (4PCA) was chosen as the spatial unit for the ALBATROSS database and model. The Netherlands counts a total of approximately 4000 4PCA's. Given a population of roughly 16 million people, the average number of individuals per 4PCA is approximately 4000 people. The average size is approximately 880 ha and area size is inversely related to urban density. For the highest level of urban density measured on a 5-point scale the average size is 109 ha and for the lowest level (i.e. rural areas) average size is 14 210 ha. Therefore, we should keep in mind that the identification of location is more precise in urbanized areas than in non-urbanized areas.

Distance data between locations for car and slow modes (walking, cycling) are derived from an existing national transport network data file called 'Basisnetwerk'. This file describes the nationwide road network down to the level of neighborhood roads. Each record describes a network link in terms of begin and end node, average speed by car, length, and type. Car distance data derived from the Basisnetwerk are based on fastest routes, whereas slow mode data are based on shortest routes. In the Basisnetwerk file, link speed represents an average flow speed on the link concerned throughout the day at the level of individual links for main roads. To estimate time-dependent travel times, free-floating, morning-peak, and evening-peak travel time data are used, which are available through the current national model system. Time-of-day-dependent travel time adjustment coefficients for each pair of PCA's were derived from these data. Besides information on car trips and slow modes, public-transport-system data and land-use data are also included in the database.

Additional information on the data sources used to construct the physical database for ALBATROSS is listed in appendix A. More detailed information can be found in Arentze and Timmermans (2000; 2005).

2.2.2.2 Model configuration

The activity scheduling agent of ALBATROSS is the core of the system which controls the scheduling processes. The scheduling model of ALBATROSS 2.0 and higher, which generates a schedule for each individual and each day, consists of four major components as displayed in Figure 3 (adapted from Anggraini et al. 2007). The first model component generates a work activity pattern consisting of one or two work episodes, their exact start time, the duration of each episode, and their location. It also predicts the transport mode to the work activity. The second component determines the part of the schedule related to secondary fixed activities such as bring/get activities, business and others. It determines which types of activities are conducted that day, the number of episodes of each activity that occurs, their start time and duration. Furthermore, it also identifies possible trip-linkage to the work activity and predicts the location of each episode. The third component concerns the scheduling of flexible activities. Almost similar to the previous component, it predicts activity types, the number of episodes of each activity type, the start time and duration of each episode as well as the location of each episode. The additional prediction of sequence of activities and possible trip-chaining links between activities are also part of this stage. Finally the last model component predicts the transport mode used for each tour (except for the work activity where transport mode is known as the outcome of an earlier decision). These main components assume a sequential decision process in which key choices are made and predefined rules delineate choice sets and implement choices made in the current schedule. Interactions between individuals within households are to some extent taken into account by developing the scheduling processes simultaneously and alternating decisions between the persons involved. ALBATROSS does not represent activity schedules of children explicitly. More information about the detailed working of this model and other computational process models can be found in Arentze and Timmermans (2005) and Anggraini et al. (2007). Validation studies of the scheduling process of ALBATROSS are described in Arentze et al. (2003) and Arentze and Timmermans (2004).

Concerning the computer runtime, total time required to simulate activity-travel schedules for a synthetic population of 30% (i.e. approximately 2 million household days), amounts 73 hours. Part of this runtime is used for the simulation of the synthetic population (+/- 5 hours), the rest is applied for assigning the individual schedules. Computer runs were simulated on a Dual Core Intel 7500 2.20 GHz processor with 2.00 GB RAM. The size of the final schedule file amounts approximately 2 GB.

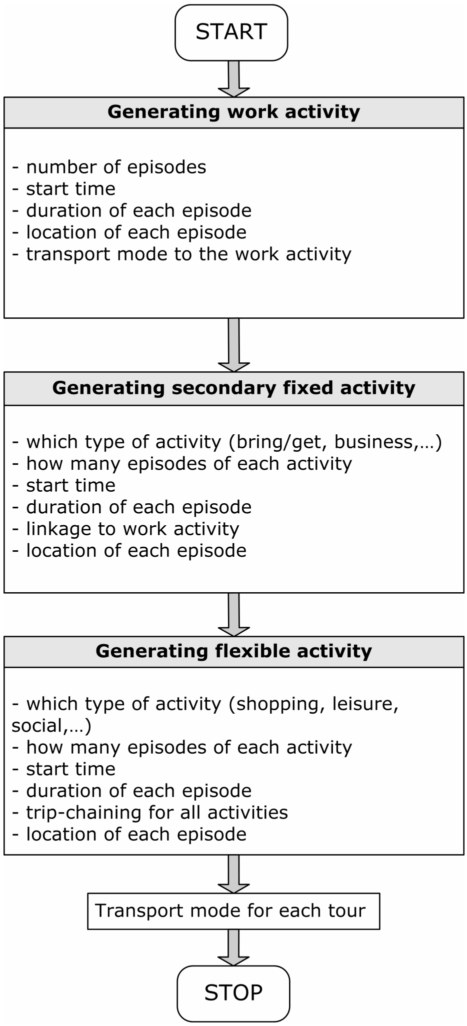

Figure 3. Schematic representation of the main steps of the ALBATROSS process model. Source: Anggraini et al. (2007)

2.2.2.3 Model adjustments for this research

Since the ALBATROSS model was already developed for simulation of activity-travel patterns for the Dutch population, no considerable changes were introduced in the ALBATROSS scheduler nor were the model input data from this model version altered. However, since the current work requires a more detailed spatial and temporal resolution compared with previous ALBATROSS applications, the analysis module from the model was somewhat modified and also a larger synthetic population was simulated compared with previous applications. The following adjustments or additional analyses can be listed:

- A synthetic population of 30% was simulated instead of using the smaller synthetic populations used for previous ALBATROSS projects. A synthetic population of 30% was, at that time, the maximum population size that could be synthesized and yields results that are virtually identical to a simulation of the whole population.
- Whereas previous model applications only worked with the synthetic population results to make conclusions, the current work finally deals with the total Dutch population (approximately 11 million adult inhabitants). Information about the 30% synthetic population was therefore extrapolated to represent the entire Dutch adult population.
- Based on the scheduled activity-travel patterns, the ALBATROSS model enables to extract origin-destination (O/D) matrices to represent the number of trips from one location to another. Instead of working only with O/D matrices for an average weekday, the current work applied more detailed O/D 's, extracted for different time periods per day and for three different days (weekday, Saturday and Sunday).
- To obtain information about the number of vehicles per traffic link (required for the emission assessment) the simulated O/D matrices were assigned to a road network (Basisnetwerk). An 'all-or-nothing' traffic assignment algorithm from the TRANSCAD software program (Caliper, 2004) was therefore applied to convert the matrices into traffic flows. 'TransCAD' is a GIS platform designed specifically for transportation purposes (Caliper, 2004). The 'all-or-nothing' algorithm from this programme assumes that all traffic from zone A to zone B occurs on the same route and it therefore does not take into

account that people will adapt their route when traffic volumes reach road capacity.

- Information from the national travel survey (NTS or 'OVG' in Dutch) (SWOV, 2000) was used to reorganize the periodical, mainly two-hourly traffic flows into hourly traffic flows. As a result of this procedure hourly traffic flows were available for every link in the Dutch road network.

The model adjustments mentioned in this section are further clarified in chapter 3 where the use of the ALBATROSS model for emission assessment in The Netherlands is described.

2.3 Emission modelling

2.3.1 Overview of the emission modelling approach

Vehicle emission modelling is a necessary step to quantify the impact of traffic flows on air quality. Depending on the purpose of the emission model, distinction can be made between macroscopic and microscopic modelling.

On a microscopic scale emissions are calculated on instantaneous (second-by-second) vehicle parameters like speed and acceleration. A microscopic emission modelling approach is therefore able to assess the impact of changes in driving behaviour. Examples of these microscopic models are the MODEM emission model (Joumard et al. 1995) and the VeTESS computer program (Pelkmans et al. 2004; Beckx et al. 2007a) where emission calculations are based on previously performed measurements on engine test benches. Input data for these emission models often originate from microscopic traffic models and can be limited to 'speed' and 'acceleration' profiles. However, the generation of these data is very time consuming and input (e.g. acceleration) is often not validated (Int Panis et al. 2006). An approach to use microscopic emission models on a larger scale includes the use of GPS based travel data instead of micro simulation traffic models. In Jackson et al. (2005) the ability of GPS receivers to measure real-world operating mode for emissions research is already demonstrated. Beckx et al. (2006; 2007b) applied a similar approach to convert real-time travel data into emissions by using the PARROTS data collection tool developed by Kochan et al. (2005). In addition driving behaviour and parameters like revolutions per minute, engine temperature and fuel consumption can also be monitored by using CAN information data as demonstrated by Beusen et al. (2009). These types of microscopic emission modelling are useful to gain more insights into the relationship between travel, driving behaviour and emissions, but not appropriate for assessing the impact of transportation measures taking place at a larger scale.

Vehicle emission modelling inventories in Europe are usually performed with macroscopic emission software tools like COPERT (Computer Programme to calculate Emissions from Road Transport) (Ntziachristos and Samaras, 2000). With this macroscopic approach total emissions are calculated on a medium and large scale as a product of activity data (number of kilometres on the road) and speed-dependent emission factors (expressed in g/km), assuming an average trip speed. Input data like the average trip length and the number of vehicle kilometres travelled per year usually originate from both travel data and traffic counts. Other emission models operating with a similar methodology are the US Environmental Protection Agency (EPA) Mobile model (current version is Mobile6) (US EPA, 2009) and California's EMFAC model (California Air Resources Board, 2007). Since the emission factors in these models are based on an average driving situation, the macroscopic model is not sensitive to vehicle's operating modes such as idling, accelerating, cruising and decelerating and therefore changes in driving behaviour can not be taken into account. However, this macroscopic approach does have the advantage of being simple and easy to apply in emission estimations for larger areas. Further, it allows to quantify the effect of scenarios on technological enhancements or changes in the vehicle fleet, and it can estimate the large scale impact of TDMs by taking into account the changes in vehicle activity data. Considering the scope of the current research and the size of the study area, a macroscopic emission modelling approach was preferred in this research.

2.3.2 MIMOSA

The emission model that was selected for the current work, is the macroscopic MIMOSA emission model, applying mainly the COPERT emission functions, as mentioned in the previous section. The first MIMOSA emission model was developed by Mensink et al. (2000) for the city of Antwerp. Later the model was further extended and improved by Lewyckyj et al. (2004) to calculate emissions and emission reduction scenarios for larger study areas (e.g. Schrooten et al. 2006). Mr. Jean Vankerkom from VITO is kindly acknowledged for his assistance with the MIMOSA modelling procedures.

2.3.2.1 Model input

In order to calculate the vehicle emissions, MIMOSA requires input information on the road network and the traffic situation. Emission factors are used to convert the vehicle distances into emissions. In this section an overview of the required input data is provided.

Road network data

MIMOSA not only aims at calculating total emission evaluations, but also calculates geographically distributed emissions. Therefore, the geographic location of the different traffic links in the study area is required. For every link in the road network the xy coordinates of the start point and endpoint are necessary. Further, information on the road type (highway, national road, main road outside the city, main road inside the city, secondary road) is also required to take into account the variations in the vehicle fleets on different road types.

Traffic flows

One of the most important pieces of information for the modelling of emissions is of course the amount of vehicles passing on each traffic link. This information usually originates from a traffic model, but it can also be obtained through traffic counts. At least the total amount of vehicles passing during traffic peaks is required to calculate the emissions for larger time periods (by using time factors to simulate the traffic flows at off peak periods), but hourly traffic flows can also be used by the model. In order to take into account the impact of speed on the emissions of pollutants, the average driving speed per traffic link should be available.

Emission factors

The MIMOSA road traffic emission model uses a ‘static’ emission approach, i.e. hourly average speeds of the different vehicles instead of short-term fluctuations in speed (accelerations and decelerations) are used. The emission factors (g/km) used within the MIMOSA model were partially extracted from experimental data collected by on-road measurements (Lenaers et al. 2003) as well as from the COPERT-III report (Ntziachristos and Samaras, 2000). For missing data (some specific pollutants e.g. PM emissions), emission functions from MEET (1999) were applied. Within the basic model four major vehicle categories can be distinguished (Passenger Cars, Light-Duty Vehicles (LDV), Heavy-Duty Vehicles (HDV), Motorcycles and Mopeds) with further sub-categories depending on the age of the vehicle and its cylinder capacity for the passenger cars. In this study, however, only the emissions from passenger cars are modelled explicitly. Furthermore, a distinction can be made between four fuel types (gasoline, diesel, LPG and 2-stroke gasoline), with lead and sulphur contents depending on the year of the simulation. More detailed information on the used emission factors in this research are provided in Appendix B.

2.3.2.2 Model configuration

MIMOSA belongs to the ‘average speed macroscopic emission models’, expressing emission and fuel consumption rates for each trip as functions of average speed.

The basic version of MIMOSA calculates geographically distributed hourly traffic emissions for Flanders based on peak-hour (17h–18h) mobility data from a Flemish road traffic model (the ‘multimodal modal Flanders’). The time dependency of the traffic flows/emissions is simulated using normalized distribution factors expressing the fluctuations of the traffic flow as a function of the hour of the day, the day of the week and the month of the year. By using this approach a uniform traffic flow variation is therefore assumed in the entire study area.

Concerning the emission calculation, the model uses a ‘static’ macroscopic approach, i.e. hourly average speeds per road segment are combined with emission factors to calculate the emissions per road segment and per hour.

By combining hourly traffic volumes computed per road segment with fleet statistics and the corresponding emission factors, the MIMOSA model can calculate temporally and geographically distributed traffic emissions. These emissions include hot, cold and evaporative emissions. Cold start emissions can be calculated based on information on the trip length and the ambient temperature. Short trips, carried out with cold engines, will result in higher emissions. Evaporative emissions are only obtained for the running losses, i.e. vapour losses generated in gasoline tanks during vehicle operation which are significant at high temperatures. Ambient temperature data are therefore used to calculate these evaporative emissions.

Since the COPERT approach was originally developed for emission estimation of entire trips (not traffic links), one should be careful when reporting the MIMOSA emissions on a very detailed link level. A presentation of the emission results at larger scales should therefore be preferred. Previous studies (e.g. Lewyckyj et al. 2002) already reported on comparisons between the emission results from MIMOSA with results from the COPERT-III model, the European reference model in scientific emission research. Using the same data as input, both models provided similar emission results. However, in comparison with the COPERT-III model, MIMOSA adds three important advantages:

- MIMOSA model simulations can be performed for every requested time period (going from one hour up to several years). This is not possible with the COPERT-III model.
- MIMOSA model calculations are made separately for every traffic link in the study area, allowing for a geographic distribution of emissions. The COPERT approach is designed for aggregated emission estimates, allowing general emission estimates for an entire study area.

- MIMOSA emissions can be calculated on the basis of speeds from a traffic flow model, resulting in more realistic estimates than the use of only generic vehicle speeds as done in COPERT-III

Concerning computer runtime, the MIMOSA modelling procedure to calculate emissions for the predicted traffic flows in this research, took approximately 4-6 hours on a Dual Core Intel 7500 2.20 GHz processor with 2.00 GB RAM.

2.3.2.3 Model adjustments for this research

In order to calculate the vehicle emissions for passenger car trips in the Netherlands, as aimed at in this study, the basic, Flemish, MIMOSA model was adjusted with information regarding the Dutch vehicle fleet and road conditions. Further, the settings within the model were altered to benefit maximally from the information provided by the activity-based approach. Summarizing, the following adjustments can be mentioned:

- The MIMOSA model was originally developed for applications within the Flemish region of Belgium. To be able to calculate the emissions for the Dutch study area, as aimed at in this dissertation, the input data were adjusted to the Dutch situation. Information on the Dutch road network was therefore added to the MIMOSA input data. The Dutch road network, 'Basisnetwerk', used in this research includes information on the geographic coordinates of each traffic link and on the type of road. Information on the Dutch vehicle fleet was obtained by statistical information from the Dutch statistical agency (CBS, 2001). Appendix B provides more information on the characteristics of the used vehicle fleet.
- For each traffic link information on number of vehicles per hour and the traffic speed was provided. This information did not result immediately from the activity-based model, but was provided by an intermediary calculation with a traffic flow model that assigned the simulated activity-based trips to a road network (as stated in section 2.2.2.3). Further, based on statistical information on the Dutch vehicle fleet (including data from traffic counts and vehicle registration actions) the MIMOSA vehicle fleet composition was determined per road type (CBS, 2001, see also Appendix B).

- Because the activity-based approach used in this study only focuses on personal travel behaviour, only the characteristics of the passenger cars were taken into account for the emission analysis. Emission results for freight transport were therefore not calculated nor reported separately. As explained in section 2.4.2.3 on the concentration modelling, information on the emissions from freight transport was obtained from other sources.
- The basic version of MIMOSA calculates geographically distributed hourly traffic emissions based on peak-hour (17h–18h) mobility data. However, by using an activity-based approach instead of this peak-hour approach, hourly traffic flow information was provided for all considered road segments. In this study the uniform traffic flow method from the basic MIMOSA model was therefore replaced with an advanced traffic simulation procedure, allowing geographic and temporal differences in traffic flows and emissions (e.g. simulation of emissions per hour and per km²).
- Link-specific traffic speeds were not provided from a traffic model, but are derived from the activity-based estimates on the travel time between different locations. These link-specific traffic speeds refer to an average speed over the course of a day and were estimated for the Dutch road network according to expert assessment at the level of individual links and they are applied in ALBATROSS to estimate network distances and travel times by mode between different activity locations (Arentze and Timmermans, 2005).

The model adjustments mentioned in this section are further clarified in chapter 3 where the combined use of MIMOSA and ALBATROSS to calculate emissions for the Netherlands is described.

2.4 Dispersion modelling

2.4.1 Overview of dispersion modelling

Calculating emissions is useful for environmental policy, but it is not sufficient to study human exposure to air pollution. Dispersion models are needed to convert the emissions into concentrations at which the population is exposed. Over the past decade several modelling tools were developed to assess air quality at various scales, ranging from the local scale to the continental scale (Mensink et al. 2008).

Local-scale dispersion models quantify the concentration levels of pollutants that can cause adverse health effects at a very detailed spatial level. These local-scale models are able to allow for the structure of the atmospheric boundary layer and the various local-scale effects, such as the influence of buildings and obstacles. Examples of such models include the Computational Fluid Dynamics (CFD) models and the Gaussian plume models. Both are widely accepted as tools for local air-quality assessment. They are used in assessing the environmental impact of certain private or public initiatives. Unfortunately, without information on boundary conditions, the modelling domain of these local-scale models is rather small. CFD models for example generally work with study domains of approximately 500 by 500 meters. In Flanders, the Gaussian IFDM (Immission Frequency Distribution Model) is often used for regulatory purposes and environmental impact studies (Cosemans et al. 1997). This model applies a receptor-based concentration calculation approach allowing for concentration modelling in an irregular receptor grid.

In order to calculate pollutant concentrations at larger scales, regional and global atmospheric models are used. Examples of such models include BelEuros and AURORA. BelEuros is based on the EUROS (European Operational Smog) model and calculates the foreign contributions to local pollutant concentrations (Deutsch et al. 2008). It was originally developed for Belgium, but can also used for other countries if the necessary input data are available. The AURORA (Air quality modelling in Urban Regions using an Optimal Resolution Approach) model (Mensink et al. 2001, De Ridder et al. 2008a) can be applied from a regional down to an urban scale to calculate pollutant concentrations.

2.4.2 AURORA

For application within the current modelling framework, the AURORA large scale dispersion model was used. Dr. Karen Van de Vel and dr. Wouter Lefebvre from VITO are kindly acknowledged for performing the AURORA modelling steps required for this doctoral research.

AURORA, Air quality modelling in Urban Regions using an Optimal Resolution Approach, is a 3-dimensional model of the atmosphere (Mensink et al. 2003; De Ridder et al. 2008a). The model assesses how, after being emitted from a source, air pollutants are transported and mixed in the air, undergo chemical reactions, generate secondary pollutants, etc. Both air pollutants in the gaseous and the particulate phase are taken into account. The model's outcome are 3-dimensional concentration fields, giving an overall assessment of the air quality for the region of interest, and this from the ground up to approximately 20 km altitude.

AURORA provides concentration fields on an hourly basis, allowing for the assessment of the hourly and daily variation in air pollution levels. In the following sections the input data for the AURORA model are presented and all modules that are needed to run the AURORA model are discussed as well as the way the different elements are coupled to each other into an integrated system.

2.4.2.1 Model input

In order to calculate pollutant concentrations, AURORA requires information about the meteorological conditions, the amount and location of emitted pollutants and the physical situation of the study area (land use, vegetation cover,…).

Meteorology

AURORA requires the specification of 3-D fields of relevant meteorological parameters, including wind vector components, temperature, humidity, precipitation, radiation, cloud properties, and turbulent diffusion coefficients, among others. The meteorological fields were simulated using the Advanced Regional Prediction System (ARPS), a non-hydrostatic meso-scale atmospheric model developed at the University of Oklahoma. More information about ARPS can be found in Xue et al. (2000; 2001).

Emissions

The emissions input required by the AURORA model consists of gridded two-dimensional emissions maps on an hourly basis. AURORA contains routines in order to combine emission data from different sources. Emission sources are broken down over 11 SNAP categories: 10 anthropogenic source sectors and one natural sector (biogenic emissions), whereby SNAP stands for 'Selected Nomenclature for sources of Air Pollution' (European Environmental Agency, 2007). AURORA distinguishes between the following emission classes :

1. combustion in energy and transformation industries;
2. non-industrial combustion plants;
3. combustion in manufacturing industry;
4. production processes;
5. extraction and distribution of fossil fuels and geothermal energy;
6. solvents and other product use;
7. road transport;
8. other mobile sources and machinery;
9. waste treatment and disposal;
10. agriculture;
11. nature.

For the anthropogenic emissions of sectors 1-6 and 8-10 as well as for the road transport emissions outside the Netherlands, the E-MAP GIS tool was applied. E-MAP performs a spatial disaggregation of CORINEAIR/EMEP emission inventories by using spatial surrogate data (Maes et al. 2009). CORINAIR (Core Inventory of Air Emissions) is a project performed since 1995 by the European Topic Centre on Air Emissions, with the aim to collect, maintain, manage and publish information on emissions into the air, by means of a European air emission inventory and database system (European Environmental Agency, 2007). EMEP is the scientific programme of the Convention on Long-range Transboundary Air Pollution. The spatial variables include the CORINE land cover data, EPER database, TREMOVE data, EUROSTAT statistics together with ESRI data and maps. A good description of these auxiliary data sets can be found in Maes et al. (2009).

The annual emissions are distributed temporally according to monthly (January – December), daily (Monday – Sunday) and hourly (0h – 23h) correction factors. These factors are specific to each pollutant and emission sector, and hence reflect the different energy-use patterns as a function of time. Apart from the above-mentioned anthropogenic emissions, biogenic emissions from forests were also taken into account. Geographically distributed maps were calculated on an hourly basis, using the hourly temperature and shortwave radiation values simulated by the meteorological model ARPS and the land cover data.

Other input data

Below a brief overview is provided on the external data required to run the meteorological, emission and air quality calculations. These data consist of both European and international databases, as well as satellite-derived data :

- Land use parameters were specified from CORINE land use data, covering Europe at a resolution of 250m (Heymann et al. 1994);
- Vegetation cover fractions were derived from SPOT-VEGETATION imagery containing the Normalized Difference Vegetation Index (NDVI). The vegetation cover fraction was used to estimate the fractional green vegetation cover of each model grid cell at the surface;

- Terrain height was interpolated from the Global 30 Arc-second Elevation Data Set distributed by the U.S. Geological Survey;
- Sea surface temperature was derived from the MODIS instrument onboard the TERRA/AQUA satellites;
- Lateral boundary conditions (see section 2.4.2.2).

2.4.2.2 Model configuration

The AURORA air quality modelling system consists of different parts allowing for:

1. meteorological calculations to derive the relevant meteorological parameters (a.o. air temperature, wind speed and direction, humidity, …);
2. the generation of two-dimensional emission fields for air pollutants;
3. the release, chemical transformation, the transport and the deposition of air pollutants.

The first two issues, meteorology and emissions, are discussed in a previous section (2.4.2.1). The actual "heart" of the AURORA model is a number of routines dealing with the transport (advection, diffusion and deposition) and chemical transformation of the air pollutants. They are all indicated in Figure 4. In order to drive these modules AURORA needs meteorological data, emission data and background concentrations.

By using the AURORA dispersion model one aims at producing high-resolution air quality maps for one specific region or country. However the air quality at one country is not only determined by emissions taking place in its territory, but also by air pollutants that are being emitted in the neighbouring countries. These air pollutants are taken into account through applying the following method. The AURORA calculations are initiated covering a large domain (at coarse resolution) and gradually move to the region of interest at ever higher resolutions. The lateral boundary conditions of the model domain are always specified from the previous run (or from external data in the case of the outer domain). This method can also be referred to as the nesting principle.

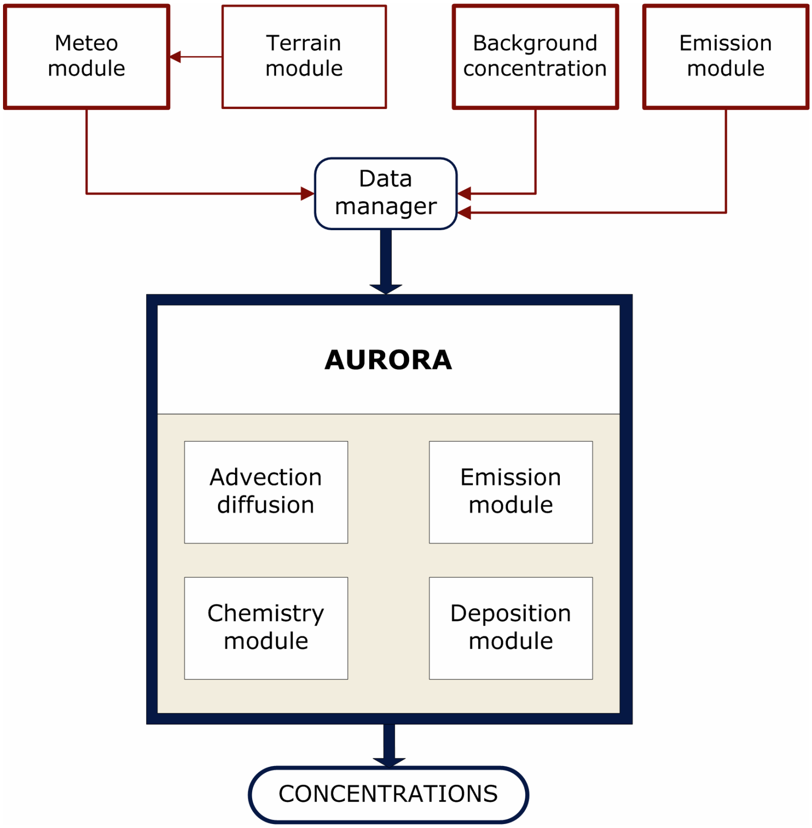

Figure 4. Lay-out of the AURORA modelling system

The same principle of nesting also applies to the ARPS meteorological calculations, allowing large-scale atmospheric features to enter the domain through the lateral boundaries. In order to specify the lateral boundary conditions for the ARPS model archived output data from Final Analysis data from the US National Centre for Environmental Prediction was used. These data are provided at a six-hourly time step and at a resolution of 1° (approximately 100km), they were interpolated to the AURORA model grid (De Ridder et al. 2008).

More detailed information on the model configuration, the chemical transformation of air pollutants and other input data (land use parameters, vegetation cover,…) can be found in (De Ridder et al. 2008a). The AURORA model is also registered in the Model Documentation System of EIONET (http://air-climate.eionet.europa.eu/databases/MDS/index_html) and the "Model Inventory" database of COST 728 (http://www.mi.uni-hamburg.de/List-classification-and-detail-view-of-modelentr.567.0.html?&user_cost728_pi2[showUid]=101).

Concerning the computational performance, modelling hourly pollutant concentrations for 6 calendar months on a 3 by 3 km grid takes approximately 14 days. This runtime includes the meteorological modelling by ARPS (+/- 10 days) and the concentration modelling by AURORA (+/- 4 days). Hereby a Quad-Core Xeon E5335 2GHz processor with 4 GB RAM was applied and processors were used in parallel. For each hour, a 75 MB file was generated by AURORA.

2.4.2.3 Model adjustments for this research

As already stated in section 1.2, the objectives of this dissertation did not include large scale adaptations on existing models, but rather focused on the combination of existing models into a new modelling framework. The main modifications in the AURORA model for this study therefore mostly concern the adaptations to the study area. Other specifications within this project that can be mentioned involve the size and resolution of the model grid, and the calculation period. These specifications were altered by the AURORA modelling experts from VITO. The following issues can be mentioned:

- Concerning the spatial resolution, three different resolution steps were used for the AURORA modelling, starting with a domain at 30km resolution (2400 km x 1500 km) through 10km down to 3km resolution. This 3 by 3 km resolution defines the 'AURORA grid'. The AURORA model (run at 30km) was driven by the BelEUROS model (Deutsch et al. 2007; 2008). This model calculates air quality above the whole of Europe at a resolution of 60km. Hourly BelEUROS data were interpolated to the AURORA model grid. Within this domain, a smaller domain was nested with a spatial extension of 700 km and a resolution of 10 km. Within the latter a still smaller domain covering an area of 360 by 270 km was modelled with a resolution of 3-km centred on the Netherlands and the Northern part of Belgium. Only results from the 3-km resolution model domain will be discussed in this research. Studies on a smaller, more precise grid size can be performed in future research.

- Concerning the emission input in the current work, the share from Dutch car traffic (tailpipe only) emissions (sector 7 from section 2.4.2.1) was calculated by means of the MIMOSA emission model on an hourly basis. The MIMOSA results were therefore interpolated to the AURORA grid (see section 2.4.2.2 for grid details). The remainder of the emissions from this sector (car non-tailpipe as well as heavy duty vehicles, motorbikes, ….) for the Netherlands were taken from the national Dutch emission inventory (PBL, 2008), which distinguishes between the various types of road transport. The Dutch emission inventory is available on a yearly basis, and at a geographical resolution of 5x5km². Bi-lineair interpolation techniques were employed to transfer the data to the AURORA grid.
- Hourly pollutant concentrations were calculated for the following six months: March, April, May and September, October, November, all in the year 2005. Calculating hourly pollutant concentrations for 6 months was sufficient to validate the results from the dispersion model. Often much less data are used for such a validation analysis (see also the characteristics of other validation studies in chapter 4).

The model adjustments mentioned in this section are further clarified in chapter 4 where the combined use of AURORA, MIMOSA and ALBATROSS to calculate concentrations for the Netherlands is described.

3 ACTIVITY-BASED MODELLING OF EMISSIONS: LINKING ALBATROSS WITH MIMOSA

<ins>Adapted from</ins>: Beckx C., Arentze T., Int Panis L., Janssens D. Vankerkom J., Wets G., 2009. An integrated activity-based modelling framework to assess vehicle emissions: approach and application. Environment and Planning B: Planning and Design. In press.

3.1 Introduction

Advances in technology (e.g., the European directives 91/441/EEC, 94/12/EC and 98/69/EC) have played and will continue to play a role in managing the emissions associated with vehicular transport. However, the report of the European Environmental Agency (2006) "Transport and the Environment: facing a dilemma" highlights how the technological improvements which have led to reductions in vehicle emissions are being offset by the growth of transport volumes. Due to this, one of the key challenges of modern policy making consists of promoting a sustainable transportation system aiming primarily at the prevention of the negative effects of the transportation system on environment and health. Many transportation control measures (TCMs), including transportation demand management (TDM) strategies specifically focusing on the driving forces of the problem, have therefore been defined. Their main purpose is to counter the rise in vehicle emissions and energy consumption due to increased travel. A good overview of potential TDMs can be found in the TDMs encyclopedia of the Victoria Transport Institute (2009).

In the US, the Clean Air Act Amendments (CAAA) and the Intermodal Surface Transportation Efficiency Act of 1991 (ISTEA) have, in combination, defined a broad range of TCMs and established procedures and requirements for integrating such TCMs as flexible work hours, congestion and parking charges, ridesharing, signal prioritization and expansion of public transport into transportation and environmental planning (Recker and Parimi, 1999). Also in Europe, similar initiatives are established to examine the potential impact of policy measures such as telecommuting, congestion pricing and no-drive days on travel demand and air quality (e.g. Emmerink et al. 1995; Priemus, 1995). However, because of the limited data available to predict the travel effects of combined (or even individual) TCM strategies and the inadequacy of conventional trip-based models to forecast changes in travel behaviour, the impact of these TCMs is often uncertain.

The lack of interactions among individual and household travel decisions in response to TCMs lay at the heart of the failings of conventional trip-based models to provide adequate measures of their potential impact. These trip-based models focus on individual trips where the spatial and temporal interrelationships between all trips are ignored. Further, these conventional approaches tend to focus on peak hour values whereas the impact of certain policy measures can take place at other moments, either direct or indirect. These kinds of issues limit the possibilities for the use of these trip-based models for policy impact analysis.

In the early nineties, the US Department of Transportation supported four projects to examine how transportation planning models could and should be improved to properly address both the impacts of new transportation technologies and the need for real policy sensitivity, particularly relative to air quality considerations (Spear, 1996). Three of the four proposals recommended that the former trip-based methodologies be replaced by activity-based approaches. The activity-based model framework is based on the premise that travel is derived from the need to perform various personal or household activities (Ettema and Timmermans, 1997). Under this premise, an individual's daily pattern of activities is modelled in its entirety, as a function of his/her role in the household, and influenced by various constraints including time availability, access to alternative travel modes, coordination with other household members, etc.. By assuming the 'activity', instead of the 'trip', as the basic unit for transportation analysis and prediction, and incorporating such constraints as interpersonal dependencies among household members this activity-based approach is a better representation of the actual decision making process. However, although the potential advantages of an activity-based approach for air quality purposes have been recognized from the beginning (e.g., Spear, 1996) and have been re-iterated more recently (e.g. Beckx et al. 2005; Shiftan, 2000; see also section 2.2.1.2) - to the best of our knowledge - models that have been developed along these lines are still scarce (see section 2.2.1.3 for a brief overview).

The aim of this study is to make a contribution to this line of research by proposing a comprehensive activity-based emission modelling framework. For this purpose, the activity-based model ALBATROSS (see section 2.2.2) was applied to micro-simulate activity patterns for the Dutch population. By using the simulated vehicle trips as input for the MIMOSA emission model (see section 2.3.2), the vehicle emissions for base year conditions in the Netherlands can be evaluated. Furthermore, by converting the predicted activity-based trips into emissions, temporal emission estimates instead of aggregated daily or yearly emission values can be assessed. The model's ability to replicate base year travel behaviour and emission assessment with good accuracy and precision was verified in this study by comparing the travel and emission results with officially reported Dutch emission values.

3.2 Methodology

To illustrate the activity-based approach for emission evaluation, the activity-based model ALBATROSS was combined with the MIMOSA emission model to assess the vehicle emissions in the Netherlands. This section briefly presents the adopted methodology and describes the data that were used to validate the model results. A detailed description of the used models with a list of the model adjustments that were necessary for this research is provided in Chapter 2.

3.2.1 General approach

This study comprehends the first step of the modelling framework to assess a dynamic population exposure to air pollution.

Figure 5 schematically presents the methodology applied in this first modelling step. Basically, in this first step, the activity-based model ALBATROSS was combined with the MIMOSA emission model. As indicated in Figure 5 the time-activity patterns, predicted by the ALBATROSS model, were converted into vehicle emissions by the MIMOSA emission model. In this section a brief description is present on how the time-activity patterns were obtained and how they were converted into emissions.

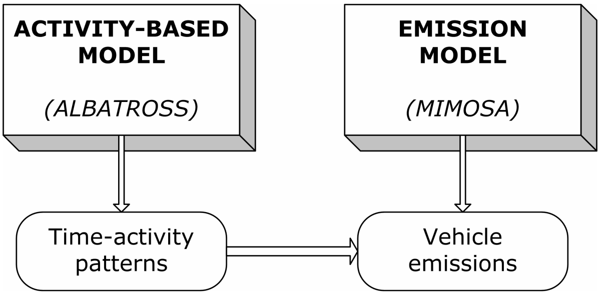

Figure 5. Schematic presentation of the emission modelling methodology

To obtain the necessary time-activity patterns, the ALBATROSS model was used to simulate the activity-patterns for a synthetic population representing 30% of the Dutch population (see section 2.2.2 for more information on the ALBATROSS model configuration and specifications). Based on the predicted patterns, origin-destination (O/D) matrices for the synthetic population were extracted from the activity schedules. The O/D information was based on a subdivision of the Netherlands in 1308 zones (the so-called 'LMS subzones'). As the focus in this study is on passenger car trips, the O/D-matrices only provided information on car trips. Furthermore, trip matrices were analyzed for different time periods, to account for intra-day and intra-week differences in travel behaviour.

After multiplying the matrices from the synthetic population by the inverted sample fraction, the trip matrices, representing the travel behaviour of the whole Dutch population, were assigned to the Dutch road network (the 'Basisnetwerk'). By using a standard 'all-or-nothing' traffic assignment algorithm from the software package 'TransCAD' (see section 2.2.2.3) the conversion of O/D-matrices into traffic flows was performed. After this traffic assignment procedure, detailed traffic information, taking into account intra-day and intra-week differences in traffic flow, was available for all the car passenger trips in the Netherlands. Traffic flow information was available on hourly basis per traffic link.

In a final step, the simulated hourly traffic flows were converted into emissions by applying the emission factor approach from the macroscopic MIMOSA emission model (see section 2.3.2 for more information on the MIMOSA model configuration and model specifications). Besides information on the traffic flows (i.e. amount of vehicles per traffic link per hour) information on the average speed is also required to calculate the emissions with the COPERT-like emission functions. Hereby we assumed that the average speed remained constant during the day and equalled the speeds used as input for the ALBATROSS model to calculate travel times between different zones (Arentze and Timmermans, 2005). By using this approach emissions for The Netherlands could be estimated for hourly and yearly time periods as well as for different geographic locations.

3.2.2 Validation data

The (activity) travel values and emissions from the activity-based approach were compared with reported values originating from other (independent) travel surveys to examine the accuracy of this innovative activity-based emissions approach. In this study data from the Dutch National Travel Survey (NTS) and the Dutch Scientific Statistical Agency (CBS) were used to perform a validation test.

Although the Dutch NTS uses trip diaries (as opposed to activity diaries), this travel survey has very similar survey characteristics as the activity-based survey (no holiday trips, no freight trips, no vehicle kilometres in other countries, no vehicle kilometres of foreigners), and is executed yearly to gain more insights into the travel behaviour of the Dutch population. The travel results from the year 2000 survey were used for comparison. This survey includes trip diaries of more than 100,000 persons and results were reweighed to compensate for the under– and over-representation of certain groups, e.g. degree of urbanization, age, journeys,… More information about the NTS in the Netherlands can be found in Van Evert and Moritz (2000) and on the Dutch Road Safety Website (SWOV, 2000).

The emission results from the activity-based emission modelling approach were compared with reported emission values provided by the CBS. These emission results are published yearly by this statistical agency since 1990 and provide good insights into the emissions of passenger cars. These values are obtained in cooperation with other environmental and traffic institutes by multiplying gathered activity data (vehicle kilometres and fuel consumption) with corresponding vehicle fleet emission factors. The emission results from the year 2000, including hot emissions, cold emissions and evaporative emissions were used for comparison (CBS, 2000). Non-exhaust emissions, e.g. PM emissions caused by abrasion or resuspension, were not included in the figures used for the validation of the emission estimates.

3.3 Results & discussion

In this section the results of the activity-based modelling approach for base year conditions in the Netherlands are presented and the model outcome is validated against travel and emission results from other studies.

3.3.1 Model outcome

3.3.1.1 Synthetic population data

Using IPF methods, a synthetic population procedure was first established to simulate a population representing 30% of the Dutch population in the base year. The individual and household characteristics of this synthetic population are presented in Table 1, Table 2 and Table 3. In total the synthetic population consists of approximately 3 million individuals or 2 million households. Each individual is characterized by its gender and work status, whereas each household is characterized by the household composition, the age of the youngest child (if present) and the age of the oldest person of the household.

Table 1. Characteristics of the synthetic population at the individual level

	Gender		Work status		
Total	Male	Female	No work	Part-time	Full-time
3,121,667	1,544,367	1,577,300	1,719,059	333,418	1,069,190

Table 2 Household characterization by composition of the household

	Household composition*				
Total	S-0W	S-1W	D-0W	D-1W	D-2W
1,938,224	363,335	391,446	446,383	462,958	274,102

*S-0W: Single No Work; S-1W: Single One Work; D-0W: Double No Work; D-1W: Double One Work; D-2W: Double Two Work

Table 3. Household characterization by age of the household members. The values indicate the number of households.

Age of youngest child			
No	< 6	6-12	> 12
1,396,129	262,383	154,292	125,420
Age of household head			
< 25	25-44	44-64	>64
65,155	868,378	569,958	434,733

3.3.1.2 Trip analysis

The ALBATROSS model simulated activity schedules for every individual within the synthetic population. These activity schedules include information on both activities and trips (if two consecutive activities occur at different locations). Next in the modelling procedure, the predicted trips were extracted from the activity database and extrapolated for the whole population. Further, matrices for the whole population were assigned to a Dutch road network (Basisnetwork) using standard traffic assignment algorithms from the software package TransCAD.

By means of example Figure 6 presents the road network file with the resulting traffic flows for an average weekday. This figure gives more insights into the study area and the geographic location of zones with high traffic intensities. The higher traffic intensities (up to 150,000 vehicles per traffic link) near the larger cities such as Amsterdam, Rotterdam and Utrecht can be easily distinguished from the map. The peripheral roads tend to have smaller traffic loads .

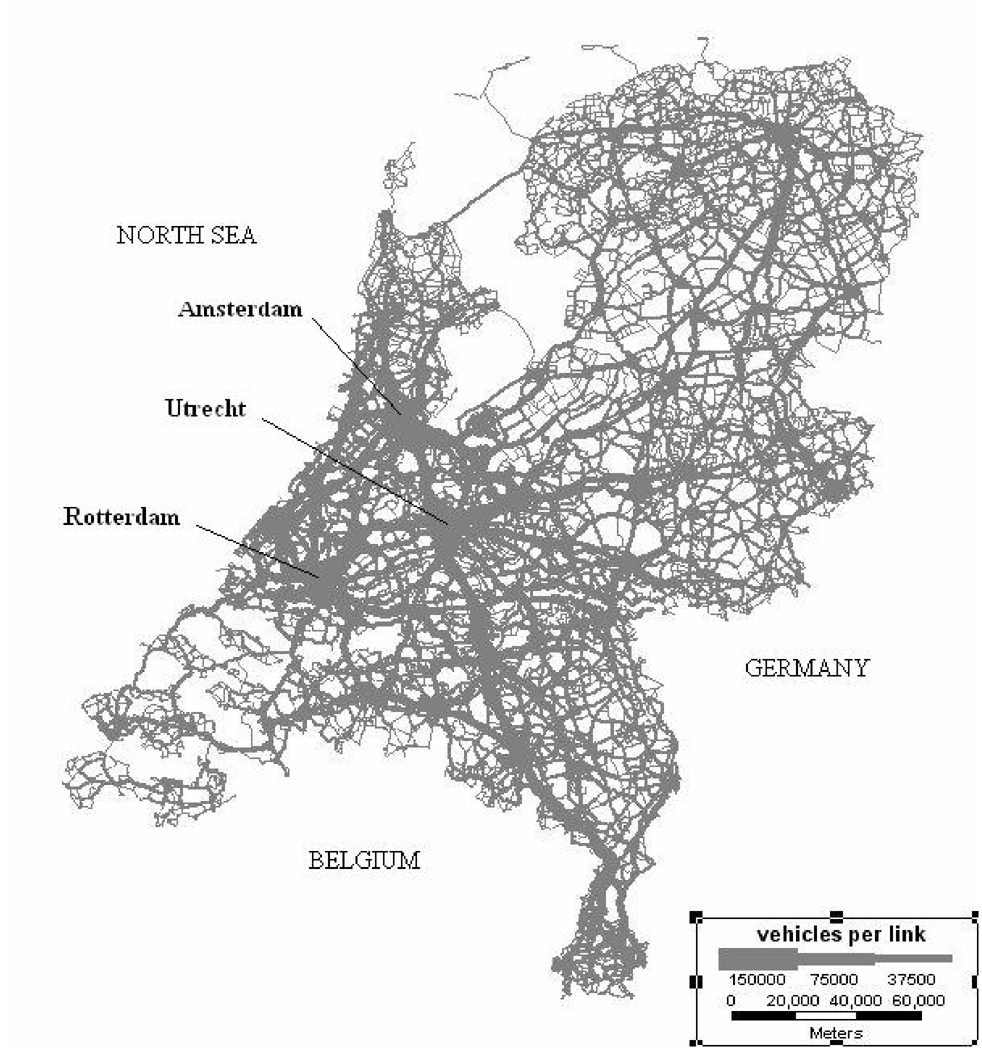

Figure 6. Geographic map of the study area (the Netherlands) with the simulated traffic flows per traffic link for an average weekday in the base year.

3.3.2 Model validation

In this section the simulated traffic flows and emission estimates are compared with reported values to validate the accuracy of the integrated model results.

3.3.2.1 Validation of the vehicle trips

In Figure 7 and Figure 8 the hourly distances travelled are presented for weekdays and weekend days respectively. Both the predicted values from the activity-based modelling procedure (bars) as the reported values from the NTS (line) are presented.

In Figure 7 the morning and evening traffic peaks can be easily distinguished from both curves. Both approaches have similar predictions for the morning peak, simulating a traffic peak around 7 a.m., but differ in their predictions for the evening peak. According to the activity-based approach the evening peak occurs at 6 p.m. whereas the NTS largest peak occurs one hour earlier.

In Figure 8 the variation in travelled distances during the weekend days in the year 2000 is presented. According to the activity-based prediction distances travelled during the daytime remain rather constant with the exception of one small traffic peak at 9 a.m. The NTS curve shows a higher amount of travelled distances during the day, but did not reproduce the small morning peak at 9 a.m. A possible explanation for this small peak might be visits to the church (Arentze, personal communication 2009). The predicted travelled distances during the early morning and the late evening seem to correspond well with the NTS values.

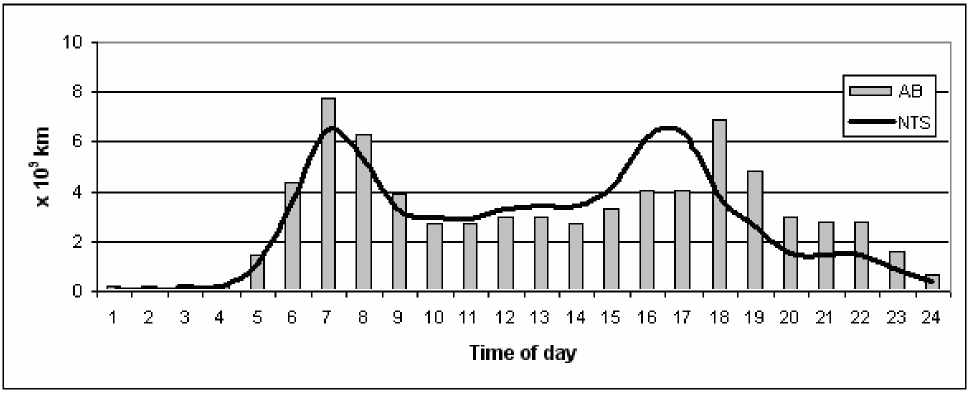

Figure 7. Hourly distances travelled on weekdays in the year 2000: predicted activity-based (AB) values versus reported NTS values (SWOV, 2000)

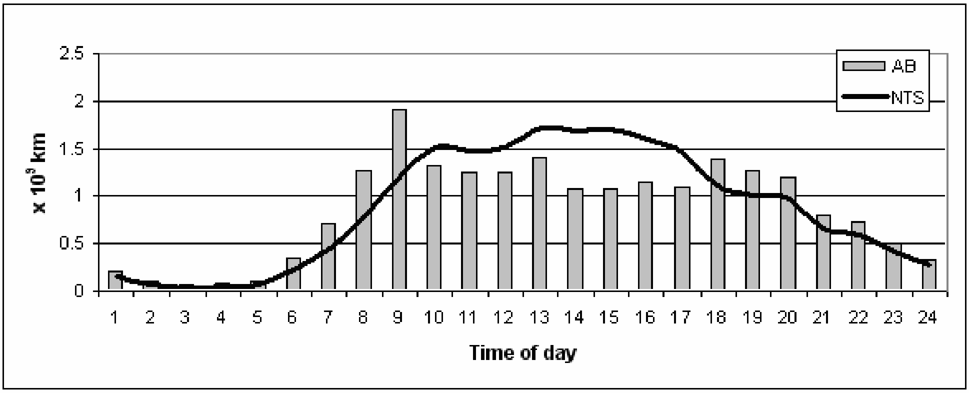

Figure 8. Hourly distances travelled on weekend days in the year 2000: predicted activity-based (AB) values versus reported NTS values (SWOV, 2000)

By aggregating the results from the traffic assignment procedure and extrapolating the values for a whole year, the total travelled distance during a whole year was calculated. In Table 4 the calculated value is presented next to the reported travelled distance value from the NTS, representing the total number of travelled kilometres by passenger cars during the base year. The relative difference between both values is less than 10%. This small overestimate by the activity-based model can be attributed to the characteristics of the survey. The activity-based survey uses activity diaries to gather activity and travel data in a very comprehensive way. Respondents are asked to report every performed activity, together with information about the time, the location, travel mode, etc.. The NTS survey, on the other hand, works with travel diaries where respondents only need to fill in information about their travel behaviour. Previous research already indicated that the trip-diary method often slightly underestimates the amount of trips (SWOV, 2000). Small, short trips are frequently under-reported by the respondents in the NTS method while these trips are much better reported in the activity diary method. This underreporting in the NTS method can explain (part of) the difference with the activity-based results.

Table 4. Total travelled distance by passenger cars in the Netherlands in the year 2000 ([a]SWOV, 2000)

	Travelled distance (x 10^9 km)
Modelled travelled distance	93.3
Reported travelled distance[a]	85.9
Relative difference (%)	8.6 %

3.3.2.2 Validation of the vehicle emissions

Based on the modelled traffic flows, the emission model MIMOSA calculated traffic emissions produced by the predicted vehicle trips. The results for five major air pollutants: carbon dioxide (CO_2), nitrogen oxide (NO_x), volatile organic compounds (VOCs), sulphur dioxide (SO_2) and particulate matter (PM) are presented in Table 5. Since hourly emission values or location-specific emissions could not be validated against reported values, only the aggregated emission values are presented here.

In Table 5 the differences between predicted and reported total emission values for the base year are presented. Relative differences vary between 3 and 26 % for PM and SO_2 respectively. Given that the SO_2 emissions are based on a fixed ratio of sulphur in the fuel, the result for SO_2 indicates that the emission model overestimated the sulphur content in the fuel. The sulphur content of the fuel is subject to national standards, changing every few years, so this can be an acceptable explanation of this difference. Since the CO_2 emissions are highly related to the number of kilometres travelled, a small overestimate in the amount of CO_2 emissions can be expected. The CO_2 predictions differ by approximately 11 % from the reported CBS emission values, NO_x emissions are overestimated by 17 % and the VOCs are overestimated by 9 %.

Table 5. Total vehicle emissions for the year 2000: predicted versus reported values ([a]CBS, 2000)

Emissions ($x10^6$ kg)	***CO_2***	***NO_x***	***VOC***	***SO_2***	***PM***
Modelled results	19292.25	70.21	43.97	1.59	2.97
Reported results[a]	17346.00	60.10	40.35	1.26	2.88
Relative difference (%)	11.22	16.71	8.98	26.30	3.21

3.3.2.3 Discussion

Of course, there are some qualifications to the presented results that need to be discussed. First of all the 'static' emission factor approach used in this study can be a subject of discussion. This static approach assumes hourly stable traffic conditions and, at first sight, ignores the local dynamics in driving patterns and street characteristics which influence emissions (De Vlieger, 1997; De Vlieger et al, 2000). However, the average speed emission factors do take into account the characteristics of the underlying driving patterns depending on the estimated average speed and the location of the specific road (urban, rural or highway) (Ntziachristos and Samaras, 2000). This emission factor based approach is widely used in modelling traffic-related emissions (e.g. Salles et al. 1996; Jenssen, 1999) with its accuracy of course depending mostly on the reliability of traffic data (traffic volume and velocity, their temporal and spatial variations, on road vehicle composition etc.) and the choice of emission factors.

Another issue in the discussion can be the use of an all-or-nothing traffic assignment to distribute the traffic over the network. This kind of assignment is a simplification of the real traffic patterns since it does not take into account redistributions at peak hour situations unlike the more advanced, equilibrium assignment. However, since this study does not include information on freight traffic and only focuses on passenger cars, using the more advanced procedure would not improve the model outcome and an all-or-nothing procedure is therefore justified. If hourly freight data is available together with link-specific capacity information, future research can include the emission assessment of all road traffic based on a more advanced traffic assignment procedure (see also section 7.2.1.1 on the potential improvements for traffic flow prediction).

Finally, one can argue the validation method in itself. The predicted results from the activity-based emission modelling approach were compared with travel and emission values from the Dutch Scientific Statistical Agency whose data originates from other model simulations. A good agreement between both values does not automatically indicate a good representation of the real situation, and only states the similarity between both models. Moreover, uncertainties in both simulated and reported data were not looked at. Ideally, a validation method should comprise the use of measurements instead of simulation values, but the procedure of comparison with other models provides useful cross-validation (e.g. Int Panis et al. 2006; Schrooten et al. 2008). Since travel and emission measurements were not available on a national level (only concentration measurements are executed), the values from the Dutch Scientific Statistical Agency were therefore considered as an acceptable alternative for the validation of travel and emission data. In a next step of this modelling framework, pollutant concentrations (based on the emissions presented here) will be used for validation purposes by comparing the model results with air quality measurements (see Chapter 4).

3.4 Conclusion

In this study the use of an activity-based model for the assessment of mobile source emissions was described and illustrated. For this purpose the activity-based model ALBATROSS was combined with the emission model MIMOSA to assess the total amount of vehicle emissions produced by passenger cars in the Netherlands and the distribution of emissions across space and time. By converting the predicted travel behaviour into emissions and comparing the results with values from the Dutch Scientific Statistical Agency, the model's ability to replicate base year travel behaviour and emission assessment with good accuracy was verified.

Regarding the temporal variation in travel behaviour, the activity-based predictions corresponded well with the reported NTS results. Both the timing and the magnitude of the morning traffic peak were predicted with good accuracy by the activity-based model. The prediction for the evening peak on weekdays slightly differed from the NTS values, but the overall picture of the temporal variation turned out very well. The feasibility to model the temporal variation in travelled distance instead of using only peak-hour information is an important improvement compared to most other travel studies (e.g. Schrooten et al. 2006) who often work with time factors to derive hourly information from one peak-hour value. When the traffic flows fluctuate differently throughout the study area, this activity-based approach will certainly be a better option.

Concerning the total distance travelled, the activity-based approach overestimated the total travelled distance by approximately 8% compared to the NTS values. The results of the emission assessments varied between pollutants. For the CO_2 emissions the estimated value differed approximately 11% from the reported value. The SO2 emissions differed 26% from the published value. The predictions for NOx, VOC and PM differed from their reported counter values for 16%, 9% and 3% respectively. Considering the overestimation of vehicle kilometres compared to the NTS values, these relative differences are quite small and probably the amount of PM emissions is still underestimated.

The validation test in this study is an essential first step: if a model is unable to replicate its base year behaviour, it has little hope of forecasting the future adequately. Based on the results presented in this chapter we can conclude that the activity-based modelling approach is able to reproduce base year travel and emissions with sufficient accuracy and that the resulting emissions can be used as input for dispersion modelling.

4 ACTIVITY-BASED TRANSPORT MODELS AND AIR QUALITY MODELLING: ESTABLISHING THE LINK WITH THE AURORA DISPERSION MODEL

Adapted from: Beckx C., Int Panis L., Van De Vel K., Arentze T., Janssens D., Wets G., 2009. The contribution of activity-based transport models to air quality modelling: a validation of the ALBATROSS - AURORA model chain. Science of the Total Environment 407, 3814-3822.

4.1 Introduction

Activity-based approaches aim at predicting which activities are conducted, where, when, for how long, with whom and, if travel is involved, the transport mode used. Using an activity-based approach will provide more accurate estimates of the emissions produced in a certain study area due to the richer set of concepts which are involved in activity-based modelling (information on travel by time of day and location, vehicle miles travelled,…). In the previous chapter the integration of the MIMOSA emission model with the travel demand modelling capabilities of the Dutch ALBATROSS model was already described. The fact that this activity-based emission approach is based on hourly travel and emission values, instead of using aggregated results or peak hour values, a common practice with other traditional models, is an important added value.

Validation results from this latter study indicated that the total amount of emissions predicted by the ALBATROSS-MIMOSA model chain corresponded well with reported emission values from the Dutch statistical agency. However, that validation analysis only compared the results from two different emission 'models' without evaluating the situation on the spot, and only aggregated emission results were evaluated. By converting these emissions into concentrations, a more accurate validation analysis can be performed using the actual measurements in the study area and examining also the temporal and spatial variation of the predictions. Taking into account that the activity-based approach provides more detailed information on pollutant emissions, one can expect the activity-based approach to also contribute to more accurate concentration modelling results.

The aim of this study is to present and validate an integrated activity-based air quality modelling framework where calculated pollutant concentrations are compared with measured concentrations at Dutch monitoring stations.

4.2 Methodology

To illustrate the activity-based approach for air quality modelling, the emission information from a previous application of the activity-based model ALBATROSS (see Chapter 3) was used as an input for the AURORA dispersion model to calculate pollutant concentrations in the Netherlands. This section briefly presents the applied methodology to develop the activity-based air quality modelling chain and also describes the data that were used to validate the model results.

4.2.1 General approach

This study comprehends a second step in the modelling framework to assess a dynamic population exposure to air pollution. It continues on the work previously performed to link the activity-based model with the emission model (see Chapter 3) and focuses on the conversion of the emissions into concentrations. Figure 9 schematically presents the applied methodology.

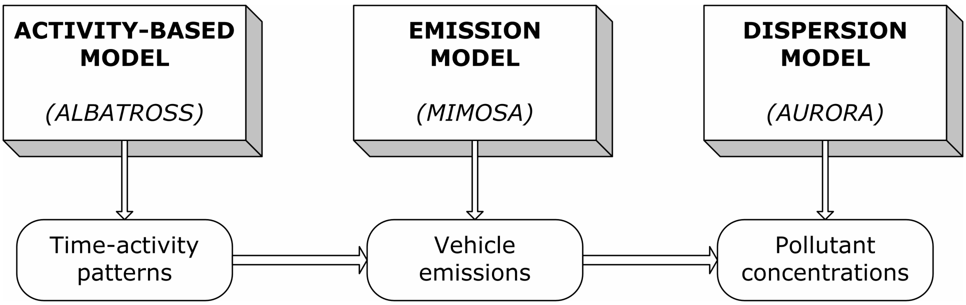

Figure 9. Schematic presentation of the adopted methodology

In a previous study, the application of ALBATROSS for the simulation of traffic flows and emissions for the Netherlands was already examined (see chapter 3). In that study, the activity-based model ALBATROSS was first used to simulate the travel behaviour for the individuals in the Dutch population (results from a 30% simulation run were extrapolated to the whole population). Next, hourly O/D trip matrices were composed for all the motorized trips in the activity schedules and these matrices were assigned to a traffic network to simulate hourly traffic flows. In combination with the MIMOSA emission model, the resulting hourly traffic flows and traffic speeds were converted into geographically and temporally distributed traffic emissions. Using this hourly emission information as input for an air quality model will result in temporally and geographically distributed concentration fields. For this purpose, the AURORA dispersion model was applied (see section 2.4.2 for more information on the AURORA model configuration and specifications).

In the AURORA dispersion model the MIMOSA emissions were combined with emission data from other sources (household, industry,…) and meteorological data (temperature, wind speed, wind direction,…) to calculate the pollutant concentrations on a 3 by 3 km grid. The model hereby assesses how, after being emitted from a source, air pollutants are transported and mixed in the air, undergo chemical reactions, generate secondary pollutants, etc. AURORA calculations were performed on hourly basis for six months (March, April, May, September, October and November) for the year 2005 and the following pollutants were considered: NO_2, O_3 and PM_{10}.

4.2.2 Validation data

To validate the results from the AURORA model, predicted concentrations were compared with measured concentrations from monitoring stations. There are around 100 stations in the Netherlands that monitor air quality within the European environment information and observation network (Eionet). The Eionet database was accessed and hourly pollutant concentrations for a six month period in the year 2005 were extracted (Airbase, 2008). The concentrations for three 'spring'-months (March, April and May) and three 'fall'-months (September, October and November) were analyzed for the following pollutants: NO_2, O_3 and PM_{10}. Since not all the Eionet monitoring stations measured (one of) these pollutants (continuously), different subsets of the monitoring stations per pollutant were made. NO_2 concentrations were observed by the largest number of stations (37), followed by O_3 (33) and PM_{10} (31).

Table 6 presents an overview of the number of stations that have continuously monitored PM_{10}, O_3 and NO_2 over that period. The stations were classified in zones according to their spatial characteristics. The zone is called urban, when the station is located in a city. Residential areas outside a main city represent the suburban zone. When a station is located outside a city, far from city sources of air pollution, the type of zone is called rural. Further, a distinction can be made regarding the specific type of location of the station. When a station is located such that its pollution level is determined predominantly by the emissions from nearby traffic, the type of station is called traffic station. When the pollution level is not determined significantly by any single source or street, but by the integrated contribution from all sources upwind of the station, the station is said to be located in a background area. All of these types of stations can be located in urban, suburban as well as rural zones. Most stations in the study have been classified as rural. Concerning the location, most stations were classified as background locations, but a significant number are referred to as traffic stations, meaning their location was specifically chosen to reflect the contribution of important local traffic sources.

Table 6: Number of Dutch air quality monitoring stations for which the data are used in the validation of the ALBATROSS - AURORA modelling results. Classification by type and area. See Figure 10 for the locations of these stations.

		Area		
Pollutant	**Type**	**Urban**	**Suburban**	**Rural**
NO_2	Background	5	2	20
	Traffic	9	0	1
O_3	Background	5	2	20
	Traffic	6	0	1
PM_{10}	Background	4	1	16
	Traffic	9	0	1

In Figure 10 the locations of the air quality monitoring stations that were used in this study are presented. The network consists of 37 monitoring stations in total, distributed over the entire study area. Each of the stations measures concentrations of NO_2 on an hourly basis and most of them also register hourly concentrations of O_3 and PM_{10}. Each pollutant is monitored by at least 31 monitoring stations and the dataset for each monitoring station consists of ~4000 hourly observations for each pollutant in the selected time period. Most other validation studies work with significantly fewer stations, shorter time periods or larger time resolutions (see also the characteristics of other validation studies listed in Table 8). The comprehensive and elaborated dataset used in this validation study can therefore be considered as quite uncommon.

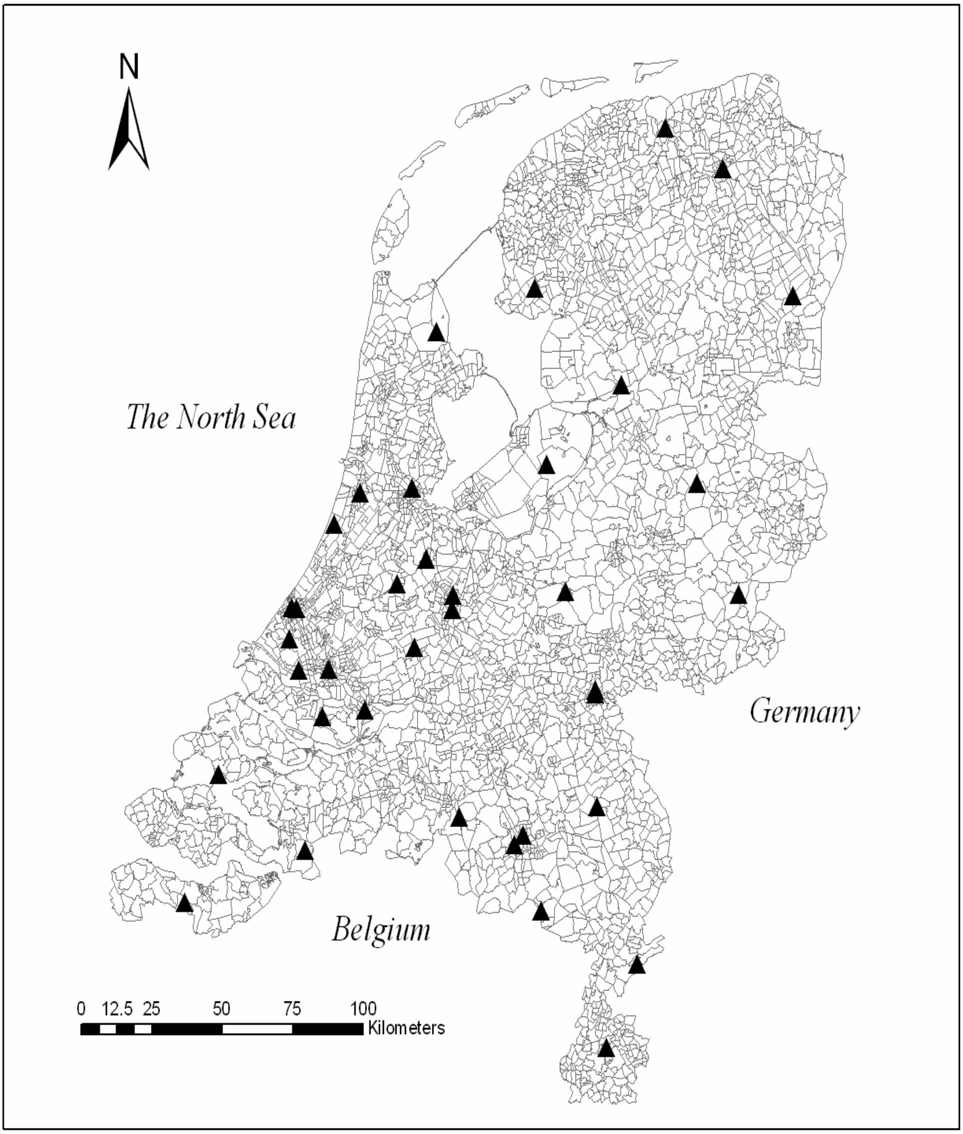

Figure 10. The air quality monitoring network in the Netherlands in the year 2005. The triangles represent the 37 measurement stations that were used in this study (see table 2 for more details)

4.3 Results & discussion

The agreement of model predictions with observations from the measurement stations was evaluated using a statistical analysis on the hourly concentration data. In this section the statistical parameters are first described and then the validation results of the activity-based air quality model in the Netherlands are presented.

4.3.1 The statistical parameters

To evaluate the performance of the activity-based air quality model chain a statistical analysis was carried out on the predicted and measured hourly concentration values. The statistical analysis includes the calculation of four statistical parameters: the index of agreement (*IA*), the correlation coefficient (*r*), the normalised mean square error (*NMSE*) and the fractional bias (*FB*). Although no single set of evaluation techniques is universally recommended for the validation of an air quality model, the statistical measures used here have been widely used in regional air quality and meteorological model evaluations (Kousa et al. 2001; Choi and Fernando, 2007; Karppinen et al. 2000; Kauhaniemi et al. 2008) and have also been discussed previously by Willmott (1981).

The parameters *r, IA,* and *NMSE* are measures of the correlation of the predicted and observed time series of concentrations, while *FB* is a measure of the agreement of the mean concentrations. The four statistical parameters can be defined as follows:

$$r = \overline{\left[\frac{\left(C_o - \overline{C_o}\right)\left(C_p - \overline{C_p}\right)}{\sigma_o \sigma_p} \right]}$$

$$IA = 1 - \frac{\overline{(C_p - C_o)^2}}{\overline{\left[\left|C_p - \overline{C_o}\right| + \left|C_o - \overline{C_o}\right|\right]^2}}$$

$$NMSE = \frac{\overline{\left(C_p - C_o\right)^2}}{\overline{C_p}^2}$$

$$FB = \frac{\overline{C_p} - \overline{C_o}}{0.5\left(\overline{C_p} + \overline{C_o}\right)}$$

C_p and C_o are the predicted and observed concentrations respectively, and σ_o and σ_p are the standard deviations of observations and predictions respectively. The over-bar refers to the average over the hourly values. For each parameter the sum over all the observed/predicted values needs to be taken.

The correlation coefficient *r* has received much criticism (Comrie, 1997; EPA, 1999) because it is not related to the differences between predicted and observed values. It only reflects the linear relationship between two variables and is thus insensitive to either an additive or a multiplicative factor (Chang and Hanna, 2004). Therefore, the index of agreement *IA*, which is based on the squared differences, is used complementarily (Chaloulakou et al. 2003). The index *IA* allows for sensitivity towards differences in observed and predicted values as well as proportionality changes (Borrego et al. 2008). The *IA* varies from 0.0 (theoretical minimum) to 1.0 (perfect agreement between the observed and predicted concentrations) and determines the degree to which magnitudes and signs of the observed value about mean observed value are related to the predicted deviation about mean predicted value. An *IA* value of 0.5 or more represents an acceptable model performance (Park and Seok, 2007; Zawar-Reza et al. 2005). Of course, the applied time resolution will have an impact on this value since annual mean model data will normally agree better with annual averaged measurements than hourly concentration data. *FB* is a measure of mean relative bias and indicates only systematic errors, whereas *NMSE* is a measure of mean relative scatter and reflects both systematic and unsystematic (random) errors. *FB* ranges from -2.0 to +2.0 in cases of extreme under- and over-prediction respectively. Values of *FB* that are equal to -0.67 and +0.67 are equivalent to under- and over-prediction by a factor of two respectively.

A perfect model would have *IA* = 1.0; *r* = 1.0; *NMSE* = 0.0 and *FB* = 0.0. Of course, because of the influence of random atmospheric processes, there is no such thing as a perfect model in air quality modelling. However, calculated values can be used to evaluate model performance and to compare different air quality models.

4.3.2 Results from the statistical analysis

4.3.2.1 Overall statistical values

Table 7 presents the mean concentration values for both the predicted and the observed time series of concentrations, together with the results from the statistical analysis. In this analysis all the concentration values that were monitored and predicted for the entire six month period at all the monitoring stations were taken into account.

Table 7: Results of the statistical analysis of the observed and the predicted hourly time series concentrations of NO_2, O_3 and PM_{10} in the year 2005.

	$\overline{C_o}$	$\overline{C_p}$	***IA***	***r***	***NMSE***	***FB***
NO_2	30	38	0.64	0.43	0.44	0.25
O_3	39	32	0.75	0.58	0.70	-0.20
PM_{10}	33	27	0.57	0.33	0.78	-0.19

Notation: $\overline{C_o}$ = mean observed concentration (in µg/m^3), $\overline{C_p}$ = mean predicted concentration (in µg/m^3), *IA* = index of agreement, *r* = correlation coefficient, *NMSE* = normalised mean square error and *FB* = fractional bias.

Considering the comparison of the averages, the model apparently overestimates the concentrations of NO_2, but slightly underestimates the concentrations of O_3 and PM_{10}. An analysis of the calculated statistical parameters indicates that the model performs best for O_3 with an IA equal to 0.75 and a very small bias. Second best are the model results for NO_2 with an IA value of 0.64 and a FB of 0.25. The lowest IA is found in the evaluation of PM_{10}

concentrations, indicating that it is more difficult to predict the short-term temporal variations of the PM_{10} concentrations compared to NO_2 and O_3. Due to the difficulties to reliably model the temporal variations of the emissions of non-exhaust particulate matter, this weaker performance for PM_{10} is not surprising (Kauhaniemi et al. 2008). However, the overall IA value for PM_{10} evaluation is still above 0.5, indicating that the overall ability of the model to predict concentrations of PM_{10} is still acceptable (Park and Seok, 2007; Zawar-Reza et al. 2005).

4.3.2.2 Comparison with findings from other validation studies

The value of *IA* is a measure of the degree to which the model predictions are error free. Moreover, it is a standardized measure that makes it possible to perform a cross-comparison of its magnitudes for a variety of models, regardless of units (Gokhale and Raokhande, 2008). In Table 8 the *IA* values and study designs from different recent dispersion model validation studies are listed. For each pollutant a number of studies are listed chronologically and, if available, a range of *IA* values calculated for different measurement stations is presented. The purpose here is not to present a complete review of the literature and discuss every study in detail (Table 8 is biased to include more recent studies and air quality models), but it does give a fair overview of the typical accuracy that is achieved by air quality models. The last study mentioned for each pollutant in Table 8 presents the results from the current study of the ALBATROSS - AURORA chain in the Netherlands. The ranges of *IA* values, calculated by ALBATROSS – AURORA, were judged against the ranges calculated for other model applications.

Table 8. Comparison of *IA* values from dispersion model validation studies.

Poll.	Site	N°	Duration	Temp. Resol.	*IA* (Range[a])	Reference[b]
NO_2	Oslo, Norway	1	2 months	Hour	0.78	Walker et al. 1999
	Helsinki, Finland	4	1 year	Hour	0.69 – 0.79	Karppinen et al. 2000
	Helsinki, Finland	7	2 years	Hour	0.65 – 0.82	Kousa et al. 2001
	Helsinki, Finland	1	2 months	Hour	0.70	Kukkonen et al. 2003
	Auckland, New Zealand	4	1 year	Hour	0.50 – 0.80	Scoggins et al. 2004
	Southeast of England, UK	6	5 days	Hour	0.75	Yu et al. 2008
	The Netherlands	37	6 months	Hour	0.40 – 0.70	This study
O_3	Helsinki, Finland	1	2 months	Hour	0.62	Kukkonen et al. 2003
	London, UK	9	10 days	Hour	0.69 – 0.70	Sokhi et al. 2006
	Southeast of England, UK	6	5 days	Hour	0.79	Yu et al. 2008
	The Netherlands	33	6 months	Hour	0.69 – 0.80	This study
PM_{10}	Christchurch, New Zealand	4	6 days	Hour	0.67 – 0.87	Barna and Gimson, 2002
	Christchurch, New Zealand	11	2 months	Day	0.40 -0.70	Wilson and Zawar-Reza, 2006
	Milan, Italy	14	1 week	Hour	0.45 – 0.75	Silibello et al. 2008
	Guwahati, India	1	4 months	Day	0.50 – 0.60	[c]Gokhale and Roakhande, 2008
	The Netherlands	31	6 months	Hour	0.48 – 0.64	This study

[a]If available, a range of *IA*_values over the different measurement stations is shown, otherwise the overall *IA* value is reported. [b]None of these studies reported the use of activity-based transport models. Most have used a traditional approach to traffic modelling based on peak hour values but not all authors are explicit about the methodologies that were used. [c]In this study the results from three different models at one monitoring station were presented.

When comparing the range of calculated IA values for NO_2 with the ranges from the other validation studies in Table 8, the general model performance of the ALBATROSS-AURORA application appeared to be slightly weaker. However, large differences were present between the monitoring stations. The lowest *IA* values in the study approach 0.4, indicating only a moderate model performance. The highest *IA* values approach 0.7, indicating a very good agreement between predictions and measurements. A geographical analysis demonstrated that the stations with an *IA* value of less than 0.5 were all located near the country border, probably indicating a worse prediction of the contribution of 'foreign' emissions to the local NO_2 concentrations in these areas. Hence these lower *IA* values cannot be attributed to the performance of the activity-based approach. Moreover, further analysis demonstrated that these 'inferior' stations did not include any traffic station indicating that the prediction of NO_2 concentrations at traffic stations was better.

For O_3, the results from the ALBATROSS - AURORA chain seem very successful. The AURORA model performance (IA = 0.69 – 0.80) scores even better than the performance results from the other studies in Table 8 who report IA values between 0.62 and 0.79. Since all the stations in the study report IA values of more than 0.69 we can conclude that the ALBATROSS - AURORA model system predicts the hourly O_3 concentrations with sufficient accuracy at all locations.

Concerning the results for PM_{10}, the IA values are comparable with the ranges from the other studies mentioned in Table 8. Given the generally lower agreement values for this pollutant, it is clearly more difficult to simulate the temporal and spatial variations in PM_{10} concentrations. A more detailed analysis on the inferior stations yielded similar conclusions for PM_{10} as for NO_2, namely that the location of the station has an influence on the model performance. Stations located near the border of the country provided the worst validation results.

A lower model performance can also be attributed to the stations exact location. As the model provides predictions for mean concentration values for the grid cells with a resolution of 3 x 3 km and not for specific receptor points within the cells, a monitoring station that is located near the border of a grid cell can be less representative for the concentrations within this cell. Part of the 'inferior' stations for NO_2 and PM_{10} were indeed located near the grid border, indicating that the lower model performance at some stations can be explained by their specific location. For monitoring stations located within a street canyon, a street canyon dispersion model should be used in predicting the concentrations at this station. But, as far as the authors are aware off, no street canyon monitoring stations were present in the Eionet database used in the current study.

Given the study design from the current study and the results from the statistical analysis, the validation results presented in Table 8 are very promising for all three pollutants. The other studies mentioned included 'only' 14 monitoring stations or less while the validation study took into account the hourly concentration results of more than 30 monitoring stations distributed over the entire Dutch study area during a period of six months. Obviously, the larger the study area and the larger the number of monitoring stations, the more difficult it is to predict the concentrations at all the different locations accurately. Still, the ranges reported in Table 8 indicate that the model performance is acceptable at most locations and comparable with the performance results from other studies, except for a limited number of peripheral stations in the NO_2 and PM_{10} modelling.

4.3.2.3 Temporal and spatial analysis

Besides a statistical analysis taking into account all the concentration values of the monitoring stations, also a more detailed analysis was performed on different subsets of the monitoring data to gain more insight into the model performance. Statistical analyses, involving the calculation of statistical parameters as described in section 4.3.1 were performed on both a spatial and a temporal subset of the monitoring data. For the spatial classification the concentration data were classified by the type (background versus traffic) and by area (rural, suburban or urban) of the monitoring station. For the temporal classification a statistical analysis was separately performed on the daytime (8h – 20h) and the nighttime values; and on the weekend versus the weekday concentration values.

Only for the analysis of NO_2 a classification of the concentration data yielded different statistical results. The statistical parameters for PM_{10} and O_3 did not significantly change by using subsets of the concentration data (although O_3 predictions performed slightly worse during nighttime). Given the fact that only NO_2 is considered to be a typical traffic pollutant, this definitely makes sense. This may indicate that the air quality model can make good predictions for all three pollutants, but that the results from the activity-based transport model do not significantly change the prediction of O_3 and PM_{10}.

Concerning PM_{10}, in general both the spatial and temporal differences are small because the West European concentrations are mainly dominated by background concentrations from a multitude of sources and they are affected by local traffic emissions only in a very limited way. The indices for PM_{10} in Table 7 are therefore primarily an indication of how well AURORA has incorporated biogenic and (non-transport) anthropogenic emissions as well as boundary conditions and meteorology.

Concerning the detailed statistical analysis for O_3, statistical results were also very similar across all subsets of monitoring stations which makes sense for a secondary pollutant (i.e. the reactions take some time and the pollutant is formed at some distance away from the source yielding a more average concentration field). The presence of slightly worse results for O_3 during night time has been reported previously (e.g. by Sokhi et al. 2006). There are various possible factors which could cause these discrepancies, but they can often be explained by errors in the meteorological parameters (especially wind speeds) during the night (Int Panis and Beckx, 2007). Since the results for O_3 and PM_{10} did not significantly change across different subsets of monitoring data, only the spatial and temporal results for NO_2 will be discussed further. In Table 9 and Table 10 the results for NO_2 are presented for the spatial classification and the temporal classification respectively.

Table 9. Spatial disaggregation of the statistical analysis for NO_2 concentrations by type or by area of the measurement station

Classification	**Monitoring stations**	$\overline{C_o}$	$\overline{C_p}$	***IA***	***r***	***NMSE***	***FB***
Type	Background	24	37	0.59	0.43	0.47	0.41
	Traffic	46	44	0.62	0.37	0.36	-0.04
Area	Rural	22	35	0.55	0.38	0.53	0.47
	Suburban	29	38	0.60	0.39	0.46	0.29
	Urban	43	44	0.64	0.40	0.33	0.04

Notation: $\overline{C_o}$ = mean observed concentration (in μg/m^3), $\overline{C_p}$ = mean predicted concentration (in μg/m^3), *IA* = index of agreement, *r* = correlation coefficient, *NMSE* = normalised mean square error and *FB* = fractional bias.

Table 10. Temporal disaggregation of the statistical analysis for NO_2 concentrations by day/night or by week/weekend.

Classification	**Monitoring data**	$\overline{C_o}$	$\overline{C_p}$	***IA***	***r***	***NMSE***	***FB***
Day/night	Daytime	31	37	0.67	0.46	0.44	0.18
	Night	28	41	0.59	0.39	0.43	0.37
Week/weekend	Week	32	40	0.62	0.43	0.41	0.21
	Weekend	24	35	0.58	0.39	0.51	0.39

Notation: $\overline{C_o}$ = mean observed concentration (in µg/m^3), $\overline{C_p}$ = mean predicted concentration (in µg/m^3), *IA* = index of agreement, *r* = correlation coefficient, *NMSE* = normalised mean square error and *FB* = fractional bias.

The results presented in Table 9 indicate that AURORA predictions match actual measurements better in grid cells with traffic stations in comparison with grid cells containing background stations: slightly higher IA ($p < 0.05$ for unpaired one-sided t-test), much lower error estimates and better agreement of average values. Due to the resolution used in this study (3 by 3 km) the impact of traffic sources to the mean grid cell concentrations will of course be not very clear. However, one can assume that the contribution of traffic sources will be more explicit in grid cells with traffic stations compared to the background cells. The statistical analysis therefore indicates that the spatio-temporal variations in NO_2 emissions of traffic sources have been estimated better than the NO_2 emissions from other sources. Since the traffic sources originated from the activity-based model ALBATROSS, these validation results demonstrate that the ALBATROSS model was able to simulate the traffic sources that contribute to local concentrations with good accuracy.

Concerning the classification by area, the urban stations presented the best model results for the statistical parameters compared to the suburban or rural stations ($p < 0.05$ for unpaired one-sided t-test on IA values). Given the fact that the traffic modelling that preceded this study occurred more accurately in the urban areas (the size of the ALBATROSS traffic zones is inversely related to the population density, see section 2.2.2.1 on the physical information), this result also makes sense. Since these urban areas will attract a lot of people and concentration values will often approach the concentration limit values in urban areas, the reliable model evaluation in these populated areas is positive news with an eye on future studies on exposure and health.

In Table 10 the results of the temporal classification are presented. Clearly, the model's ability to predict pollutant concentrations is much better during the day than in the night. The results in Chapter 3 already demonstrated that the activity-based traffic flows during the day were simulated much better than the nightly traffic flows. This can be an explanation of the observed differences between the day and the night concentration results. The same assumption can be made for weekly and weekend traffic flows since that study also indicated a much better simulation for week trips than for weekend trips. Again, this result is very important for further studies on the exposure analysis. Since most trips and activities occur during the day, a good estimate of the daytime concentrations is very important to conduct realistic exposure analyses in a next phase.

Further, Table 10 presents mean model NO_2 concentrations that are higher at night than during the day, whereas the opposite is observed in reality at the measurement stations. This can be explained by two main reasons. First of all, as already mentioned, nightly traffic flows (and the resulting vehicle emissions) were slightly overestimated by the ALBATROSS model. Secondly, at night, there is more stability in the atmosphere than during the day, when the sun creates instabilities due to diurnal heating. This is observed in reality, but is also represented in the AURORA model by means of a lower boundary layer height. As a result of this boundary layer, the local emissions are not dispersed as easily which increases surface concentrations. As can be seen in Table 5 this physical effect is overestimated in the AURORA model.

4.4 Conclusion

In this chapter the use of an activity-based model for the assessment of air quality was presented. Therefore, the ALBATROSS-MIMOSA link was combined with the AURORA air quality model to estimate concentrations of PM_{10}, O_3 and NO_2 across space and time. By comparing the predicted hourly concentrations with actual measurements the ability of the ALBATROSS - AURORA model chain to replicate base year concentration profiles in different areas and time periods was evaluated.

The results of the statistical analysis demonstrate that the modelling framework is able to predict hourly concentration values for NO_2, PM_{10} and O_3 with sufficient accuracy (IA values > 0.5). The best agreement between modelled and observed concentrations was calculated for O_3 (overall IA of 0.75) while the overall agreement for PM_{10} was weaker (IA of 0.57). The statistical results for NO_2, a traffic related air pollutant, are the most important in this study, considering the fact that this research wants to evaluate the use of an alternative transport model to give good estimates of the contribution of traffic sources to ambient pollutant concentration levels. Overall statistics for NO_2 were satisfying with an overall IA value of 0.64. Poor results were reported in border stations indicating a possible wrong assessment of the contribution of foreign traffic. In comparison with other model validation studies this validation study included an extended dataset with hourly concentration data from more than 30 measurement stations distributed throughout the Netherlands. The agreement of predicted and measured concentrations of the modelling system was very similar to the statistical results presented in the other papers, indicating that the ALBATROSS - AURORA system is definitely able to simulate both temporal and geographical variations of concentrations with sufficient accuracy.

A more thorough analysis of the NO_2 results demonstrated that better model results were calculated for the traffic stations than for the background stations indicating a positive contribution of the activity-based transport model. Further, better agreement results were reported in urban areas compared to rural areas. Concerning the temporal analysis of the concentrations, the model performed better during the day and on weekdays. A similar conclusion was made in the Chapter 3 involving the calculation of traffic flows and emissions with the ALBATROSS. By comparing the predicted traffic flows with reported traffic values, the analysis in this chapter also concluded that the ability of the activity-based model to simulate traffic flows during the day and on weekdays is better than the simulation of (nightly) traffic flows during the weekend. In general, one can conclude that the ALBATROSS-AURORA model chain performs well (given the results from the validation analyses presented here), but improvements on the nightly traffic flows (and resulting emissions) and on the boundary layer specifications will possibly produce even better agreement results.

The results presented in this chapter demonstrate the ability of the AURORA model to simulate hourly concentrations of NO_2, PM_{10} and O_3 and show that an activity-based model can be used to predict the contribution of traffic sources to local air pollution with sufficient accuracy. This result confirms the usefulness of activity-based transport models for air quality purposes, and demonstrates their application in pollutant concentration modelling for the first time.

5 STATIC VERSUS DYNAMIC EXPOSURE ESTIMATES

Adapted from: Beckx C., Torfs R., Arentze T., Int Panis L., Janssens D., Wets G., 2008. Establishing a dynamic exposure assessment with an activity-based modeling approach: methodology and results for the Dutch case study. Epidemiology 19, S378-S379.

And: Beckx C., Int Panis L., Arentze T., Janssens D., Torfs R., Broekx S., Wets G., 2009. A dynamic activity-based population modelling approach to evaluate exposure to air pollution: methods and application to a Dutch urban area. Environmental Impact Assessment Review 23, 179-185.

5.1 Introduction

The study described in the previous chapter demonstrated that important differences in pollutant concentrations can occur over the day and between different locations. At the same time however, the location of individuals also varies over space and time causing a large geographical and temporal variation in the number of people present at any location during the day. Traditional exposure studies that link concentrations with population data however do not always take into account the temporal and spatial variations in both concentrations and population density, often because temporally resolved data are simply not available (Hertel et al. 2001).

Epidemiological studies have consistently indicated a link between current levels of air pollution and public health. Ozone and PM are thought to be the key drivers although knowledge on the causal links between exposure to an air pollution mixture and resulting health effects remains imprecise. However, studies throughout the world have shown that any short term 10 µg/m³ increase in PM_{10} levels increases the mortality rate on the next day by 0.6% (Nawrot et al. 2007) and long term exposure to PM is considered to be responsible for a significant fraction of cardiovascular mortality and lung cancers among non-smokers (Pope and Dockery, 2006). Several studies have tried to demonstrate that vehicle exhaust related air pollution is more harmful than PM_{10} in general and that proximity to busy roads is linked to health impacts (e.g. Beelen et al. 2008; Brugge et al. 2007). These new insights have made policy makers aware of the fact that it is exposure of people that should be reduced in order to reduce health effects. The latest European directive on air quality (2008/50/EC) has therefore introduced new standards, mentioning for the first time a reduction of the exposure to air pollution. On one hand there is a specific ECO ('Exposure Concentration Obligation') of 20 µg $PM_{2.5}$/m³ in urban areas (where most people live) to be reached by 2015. On the other hand the average exposure of people in urban areas to $PM_{2.5}$ should be reduced by up to 20% between 2010 and 2020 depending on the current level of exposure.

Since previous air quality directives (e.g. 1999/30/EC; 96/62/EC) only focused on the reduction of concentration limit values, the recent focus on exposure means that new scientific methodologies to estimate exposure more accurately should be devised. Exposure has traditionally been calculated by multiplying population densities with concentrations at different geographical scales (Kousa et al. 2002). While concentration data from models is often available at high temporal and spatial resolution, the population data is usually based on static administrative address data. According to this static exposure approach the receptors (i.e. the people) are only exposed to pollutants at their home address. Important policy related studies have likewise adopted this approach to exposure modelling to derive external costs of traffic (Friedrich and Bickel, 2001). This approach is only sufficient for rough assessments at the national level. Any assessment focusing at urban or suburban scales (consistent with the new European legislation) should take into account that people are often exposed to air pollution at different sites, other than their home address, during the day. To establish such an improved assessment of human exposure, however, it is necessary to model the activity-travel behaviour of individuals during the day. A micro-simulation model of activity-travel behaviour is able to simulate temporal population maps of people present in a study area during all stages of the day and does not just assume a limited number of microenvironments. By combining these simulated population data with pollution data, a dynamic exposure procedure can be established.

In this chapter the methodology is presented to estimate exposure to air pollution using population data from an activity-based transport model combined with air quality data from a dispersion model. The differences between this 'dynamic' approach and the traditional 'static' approach, that assumes all people stay at their residential address during the day, are presented. The validity of the methodology is demonstrated by applying it to the city of Utrecht in The Netherlands as a case study.

5.2 Methodology

In this section the applied methods and necessary data for establishing an dynamic activity-based exposure framework in The Netherlands are described.

5.2.1 General approach

The activity-based model 'ALBATROSS' was applied to provide the temporal variations in population distribution during the day. For this purpose, consecutive hourly cross sections on the locations of the modelled ALBATROSS population were performed on the schedules data. The resulting dynamic population information was used, together with air quality data from the ALBATROSS-MIMOSA-AURORA chain (see chapters 3 and 4) to assess a dynamic population exposure. On the other hand, static exposure estimates were calculated based on a similar approach but involving only residential population information (extracted from the synthetic population in ALBATROSS). In Figure 11 a schematic overview of the applied methodology is presented. The static and dynamic exposure assessment method is explained in more detail in the next section.

The concentration information for both the static and the dynamic approach is provided by a previous study involving the dispersion model AURORA (see chapter 4). Hourly concentration maps were developed with grid cell sizes of 3 by 3 kilometre. In this study the concentration data for PM_{10} and $PM_{2.5}$ for the month of April 2005 were used for analysis. Results for other pollutants and other time periods can be obtained by adopting a similar approach.

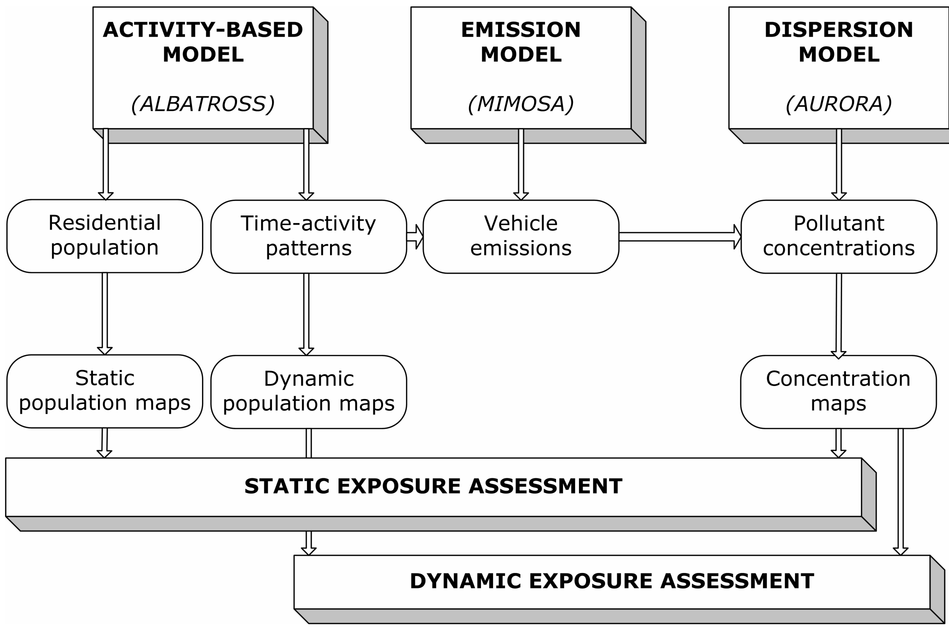

Figure 11. Schematic overview of the applied methodology

5.2.2 Static and dynamic exposure assessment

A synthetic population representing the residential information for 30% of the households in the study area was created with the ALBATROSS model. This population was extrapolated (multiplied with the inverted sample fraction) to represent the total Dutch residential information and considered as the 'static population' for further exposure analyses. In a next step, activity schedules for all the individuals within this Dutch population were generated using the scheduling process in ALBATROSS as described in section 2.2.2. The dynamic population was generated by extracting population location information from these simulated activity schedules. Consecutive cross sections of this modelled population result in a representation of a dynamic population. As in the traditional ALBATROSS approach, the 4-position postcode area (PCA) was chosen as the spatial unit for the database and time steps of one hour were chosen as the appropriate time unit.

By combining the population data with air quality data from the AURORA dispersion model two different exposure assessments can be established (see also Figure 11): a static and a dynamic exposure assessment.
On the one hand, by combining the static (synthetic) population with the hourly concentration information, static hourly exposure estimates can be made. In this traditional static method, applied by most conventional exposure studies, people are considered to be only exposed to concentrations at their home address.
On the other hand, the combination of the dynamic population maps, provided by the scheduling process in ALBATROSS, with the concentration information will result in dynamic hourly exposure assessments. In this case, people's travel behaviour is taken into account and therefore they will be also exposed to concentrations at out-of-home locations.
Both the static and the dynamic exposure assessment are performed in a GIS environment since population information as well as concentration information is available on a similar geographic level. Static and dynamic exposure estimates can be finally compared to examine the impact of using a different methodological approach on exposure evaluations. Observed differences are only due to differences in the population modelling approach since modelled concentration data have been kept identical for both approaches.

5.2.3 The study area

Activity-travel schedules were generated with ALBATROSS for all the individuals belonging to the Dutch adult population. However, to examine and present the population (and exposure) results more accurately, only the results for one specific location in the Netherlands will be analyzed in this chapter. The Dutch population information from the ALBATROSS model was therefore reduced to represent only the population present at one specific urban location: the city centre of Utrecht. The selection for this location out of all the Dutch urban areas was made arbitrary.

The Utrecht city centre is an urban area in the centre of The Netherlands. It is the fourth largest city of The Netherlands with a population of over 0.25 million. It is an attractive city to live, work, shop, or recreate which causes a large inflow of people during the day. This is enhanced by the fact that the old historical centre and the cities central location tends to attract people from a large area for these purposes. The city centre of Utrecht (the inner part of the city) counts 9 PCA's with areas varying from 46 ha to 115 ha and covering a total area of approximately 800 ha.

5.3 Results & discussion

5.3.1 Dynamic population results

Hourly cross-sections of the population present in the Utrecht city centre were first made to examine the in –and outflow of people in this region. Figure 12 presents the variation in population during an average Monday for the Utrecht area. Results for other weekdays yield similar results. Population dynamics in the weekend differ from the travel behaviour on weekdays due to the larger amount of flexible (non-work) activities compared to weekdays. At 4 a.m. the dynamic estimate approaches the residential population. During the day (at 10 a.m., 12 p.m. and 16 p.m.) more people tend to travel to Utrecht, resulting in an increase of the population during the day.

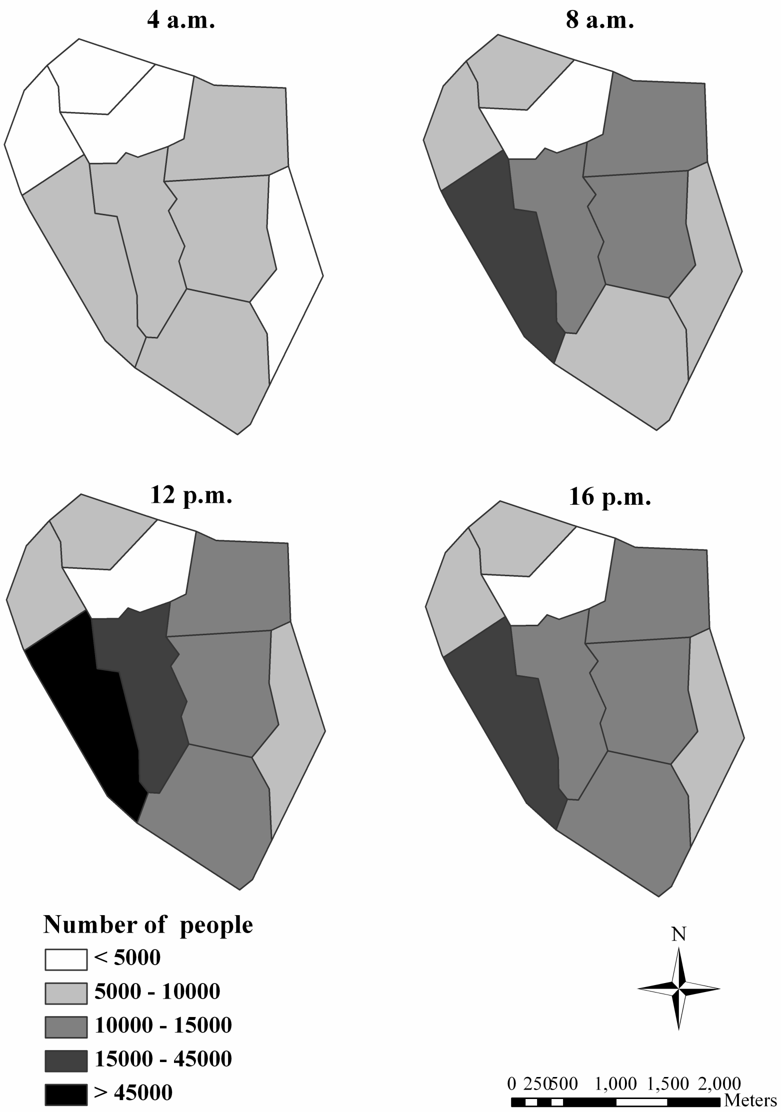

Figure 12. Geographic presentation of the number of people present in the Utrecht city centre on an average Monday at four different points in time: 4 a.m., 8 a.m., 12 p.m. and 16 p.m.

5.3.2 Air pollution

As a result of the AURORA dispersion modelling, hourly concentration maps for PM_{10} and $PM_{2.5}$ were available for the Netherlands for the month of April in 2005. In a GIS environment the 3 by 3 km concentration grid cells were analyzed for the study area: the Utrecht city centre. Considering the variation in concentrations between the different locations, concentration differences of more than 50 µg/m^3 were reported for both PM_{10} and $PM_{2.5}$.

5.3.3 Exposure assessment

As explained in section 5.2.2 and illustrated in Figure 11 static and dynamic exposure estimates were calculated by combining population data and concentration information. For the Utrecht area, two kinds of exposure analyses were made on the static and dynamic population data: a calculation of the total exposure in the study area and an analysis of the exposure hours (i.e. the total number of hours spent in or above a certain concentration).

The first exposure analysis in the Utrecht area concerned the calculation of total hourly exposure estimates by multiplying, for each hour, the number of people in each PCA with the corresponding concentration level. By summing all the exposure values per hour, a total exposure for the Utrecht city centre was calculated both for the static and the dynamic exposure approach. The relative difference in total exposure on weekdays between the static and the dynamic approach is presented in Figure 13. This figure is similar for all pollutants since it actually represents the relative population difference for the two approaches. Hence, Figure 13 also represents the relative in –or outflow in the Utrecht PCA's during an average weekday, compared to the static population. Between 9 a.m. and 16 p.m. the relative difference between static and dynamic estimates amounts more than 100%, meaning that the Utrecht population more than doubles during a weekday compared to the (static) residential information. At night, the number of people estimated by the dynamic exposure method approaches the number of residents used in the static method. Consequently differences between the total exposure estimates are smallest at night.

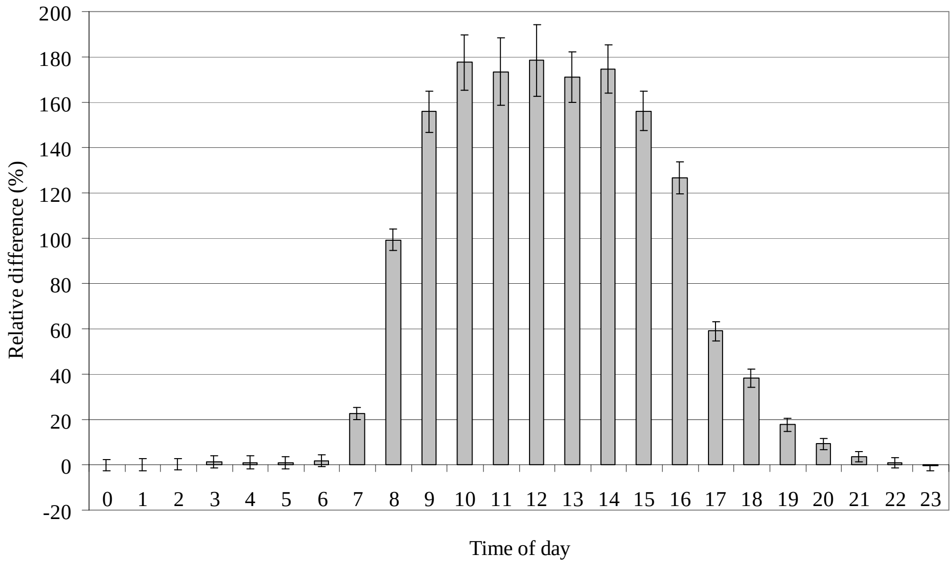

Figure 13. Relative difference between static and dynamic total exposure estimates on weekdays for the city of Utrecht.

The second analysis concerns the amount of hours that people are exposed to/above certain concentrations. For this analysis, the number of people exposed each hour to a concentration was calculated for both the static and the dynamic approach. Each hour spent by a person at a certain concentration, was expressed as a 'personhour'. In Figure 14 and Figure 15 the cumulative number of personhours spent above a certain concentration of PM_{10} or $PM_{2.5}$ respectively is expressed for both the static and the dynamic approach. Both graphs represent exposure assessments for the month of April.

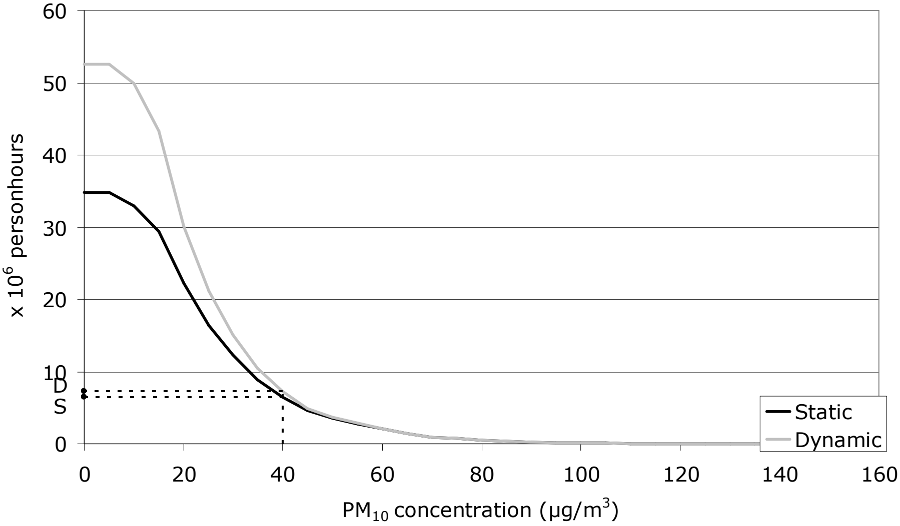

Figure 14. Personhours spent above a certain PM_{10} concentration level in the Utrecht city centre in April 2005 (S-static= 6.50 million personhours and D-dynamic = 7.34 million personhours for PM_{10} concentrations ≥ 40 µg/m3).

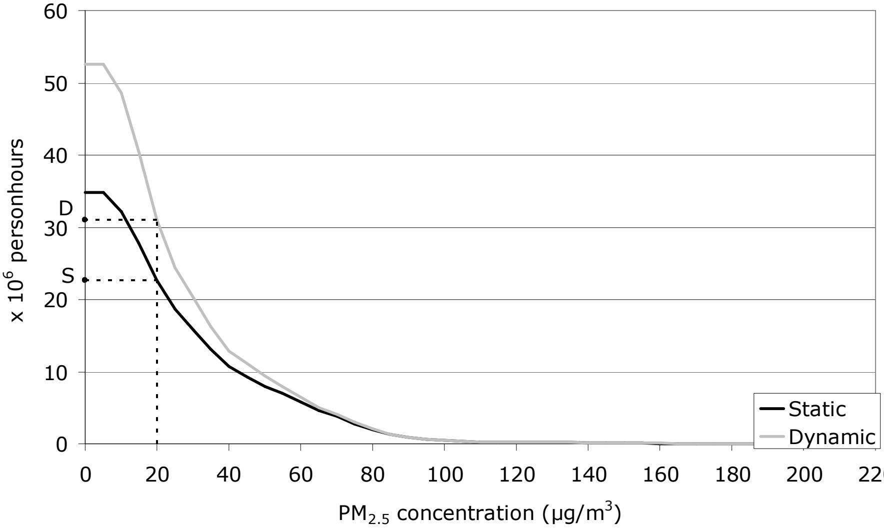

Figure 15. Personhours spent above a certain $PM_{2.5}$ concentration level in the Utrecht city centre in April 2005 (S-static = 22.60 million personhours and D-dynamic = 30.99 million personhours for $PM_{2.5}$ concentrations ≥ 20 µg/m3).

On both figures one can clearly see that the total number of hours spent in the Utrecht area is higher for the dynamic approach than for the static approach. According to the static approach approximately 35 million hours are spent in the Utrecht city centre in the month of April. The dynamic approach, on the other hand, simulates approximately 52 million hours spent in the Utrecht city centre. Apparently, the dynamic approach simulates an increase of the population in the study area during the day, confirming the result presented in Figure 13.

Further, the difference between static and dynamic exposure estimates was also examined for certain concentration threshold values. Concerning PM_{10}, the hours spent at concentrations higher than 40 μg/m^3 were analyzed. This limit value was chosen because it is applied in the European Union as a threshold value for annual average PM_{10} concentrations. As illustrated in Figure 14 approximately 6.5 million hours in the month of April were spent at concentrations above this limit value according to the static approach, whereas the dynamic approach simulated more than 7 million hours spent above 40 μg/m^3, a difference of more than 10%. In Figure 15 the exposure to $PM_{2.5}$ was examined in a similar way. According to the new EU air quality directive (2008/50/EC), EU member states are also obliged to bring $PM_{2.5}$ exposure levels below 20 μg/m^3 by 2015 in urban areas. Therefore, the exposure to concentrations above 20 μg $PM_{2.5}$/m^3 was also examined. The static exposure approach predicted roughly 22 million hours spent at concentrations above this limit value. Using the dynamic approach on the other hand, more than 30 million hours are estimated to be spent at concentrations above 20 μg $PM_{2.5}$ /m^3.

5.3.4 Discussion

One can argue the analysis method in this study and especially the threshold values chosen in this study (40 µg/m^3 for PM_{10} and 20µg/m^3 for $PM_{2.5}$). Official PM_{10} threshold values only exist on daily or yearly basis whereas $PM_{2.5}$ thresholds are only imposed on annual averaged concentrations. However, this kind of approach is also used and approved in other exposure studies (e.g. Borrego et al. 2006b) where the exposure to PM_{10} is evaluated by examining hourly exposure estimates. In the study presented here, it is not the intention to draw direct conclusions on the health impacts of the exposure estimates but only to indicate the large systematic error that is associated with the traditional static exposure approach. Since the results of the dynamic exposure analysis in the Utrecht area revealed significant differences on an hourly time scale, large differences can also be expected on larger time scales.

5.4 Conclusions

In this chapter the use of an activity-based model for the assessment of population exposure to urban air pollution is reported. Hourly population information from the activity-based model ALBATROSS was combined with hourly concentration data from the AURORA dispersion model to calculate the dynamic exposure of people living in an urban area in the Netherlands. This dynamic approach opposes the traditional, static exposure approach where people are implicitly assumed to be always at their residential address. Dynamic exposure estimates for the month of April 2005 were compared with static exposure results to gain insights into to the impact of performing a dynamic population modelling approach on the exposure analysis in an urban area. Results demonstrated large differences between static and dynamic exposure estimates, especially during the day. According to the dynamic approach a large number of people tend to travel to the urban area during the day whereas the static approach works with a constant number of people during the day, explaining the lower exposure estimates for the static approach.

Regarding the analysis on PM concentration thresholds, both approaches (static and dynamic) simulate the exceeding of these values in the month of April. The PM_{10} threshold of 40 $\mu g/m^3$ was exceeded with 6.50 and 7.34 million personhours by the static and dynamic approach respectively. This means that, according to the dynamic approach, more than 7 million hours in April were spent at a PM_{10} concentration above 40$\mu g/m^3$. For $PM_{2.5}$ approximately 22 and 31 million hours were spent above the concentration limit of 20 $\mu g/m^3$ for the static and dynamic approach respectively. The results of these analyses are very important for policy purposes since the real exposure of people to air pollution (and hence also the impact of the exposure) tends to be different than based on traditional analyses. Under the New EU Air Quality Directive (2008/50/EC) EU Member States are required to reduce exposure to $PM_{2.5}$ in urban areas by an average of 20% by 2020 based on 2010 levels. Good exposure assessments, taking into account the exposure of people at locations different than their home address, are necessary to ensure a realistic impact analysis of this measure. In this study the relative difference of the hours spent at $PM_{2.5}$ concentrations above 20 $\mu g/m^3$ differed already more than 20% between the static and dynamic approach.

Based on the results of this chapter we can conclude that the activity-based modelling approach offers the opportunity to perform a detailed, dynamic analysis of exposure to urban air pollution. Considering the fact that these dynamic exposure assessments take the real activity-travel behaviour into account, this accomplishment can lead to a much more sensitive policy impact analysis than previously performed studies (based on static exposure estimates).

6 DISAGGREGATING DYNAMIC POPULATION EXPOSURE ESTIMATES

Adapted from: Beckx C., Int Panis L., Uljee I., Arentze T., Janssens D., Wets G. Disaggregation of nation-wide dynamic population exposure estimates in The Netherlands: applications of activity-based transport models. Atmospheric Environment, available online from: doi:10.1016/j.atmosenv.2009.07.035

6.1 Introduction

To establish an improved exposure modelling framework that takes into account people's travel behaviour, first of all one has to take into account variations in both pollutant concentrations and population. However, concerning the pollutant concentration data, most epidemiological research has focused on relating health endpoints in entire populations to pollutant concentration data from a small number of fixed site monitoring stations (e.g. Wang et al. 2008, Wu et al. 2009). Unfortunately, the measurement data from these fixed stations do not necessarily represent areas beyond their immediate vicinity. For example, Alm et al. (1998) report that only a minor fraction of the variations in personal NO_2 exposure of children was explained by concentration data obtained from stationary monitoring stations. In evaluating the exposure of the population to air pollution, the use of atmospheric dispersion models or widespread sensor networks should therefore be preferred above the use of these fixed stations (Stein et al. 2007). Validated atmospheric dispersion models can provide more detailed information on the spatial distribution of the pollutant concentrations, allowing for more realistic exposure assessments.

Concerning the location of the people, traditional exposure analyses often rely on official address data only, implicitly assuming that people are always at home and, therefore, only exposed to pollution at their place of residence (Hertel et al. 2001). In chapter 5 was concluded that, to establish an improved assessment of exposure, it is necessary to take into account that people move during the day and are therefore exposed to pollutant concentrations other than at their home address (i.e. a dynamic exposure assessment).

Understanding exposure variations among activities and subpopulations further advances the current state-of-the-art and might be even more important for risk management. In addition to this, a more detailed exposure analysis in terms of activities that are performed during the day (working, shopping, leisure,…) or concerning different subgroups (gender, socio-economic status,…) would provide more useful insights into the total exposure. Unfortunately, only few attempts (e.g. Kousa et al. 2002, Marshall et al. 2006, De Ridder et al. 2008b) have been made to perform such a detailed dynamic exposure assessment. Kousa et al. (2002) compared exposure distributions for different activities based on observed time-activity data for 435 adults in the Helsinki Metropolitan Area. They concluded that the average exposure to NO_2 at home and in the workplace was substantially more important than in "other" activities. Marshall et al. (2006) examined exposure differences between population subgroups and reported differences in exposure concentration between whites and non-whites in the California's South Coast Air Basin by examining geocoded activity diaries. Part of these differences were explained by the home location, but a significant fraction of the variation in exposure concentration was due to differences in travel behaviour and different exposures accumulated during daytime activities performed at other locations. De Ridder et al. (2008b) studied impacts on traffic emissions and exposure to air pollution of long-term changes in population densities and associated travel patterns in the German-Ruhr area. However, none of these studies can provide information on large areas or entire population values because they only covered a restricted (urban) area or only a small (non-representative) sample of the population. Furthermore, these studies do not report exposure values or exposure differences on an hourly basis, while this information can be extremely useful for certain policy purposes.

Further, in order to draw general conclusions on the exposure of the whole population, a sufficiently large dataset needs to be gathered, representing different subpopulations and time periods in a realistic and unbiased way. Examples of exposure analyses that use synthetic population data for exposure analysis are described in Burke et al. (2001), Freijer et al. (1998) and Gulliver and Briggs (2005). In general, these studies use observed activity-travel data from different subgroups at different moments to make predictions about the travel behaviour for the entire population. An interesting approach would be to use an activity-based model for such analyses. Activity-based models are not only a convenient way to derive time-location patterns of people (as demonstrated in chapter 5), but they can also provide detailed information about who is performing which activities, providing details that are usually not available in exposure assessments (e.g. activities, socio-demographic details). In accordance to the work reported in the previous chapter, the study presented here aims to further contribute to this line of research by exploring the use of the new attributes of an activity-based model to create a complete national exposure analysis for The Netherlands. To this end, emissions and air quality results from an activity-based analysis of traffic streams are used and combined with dynamic population information over the entire country. The evaluation of population level exposure to NO_2 at different time-periods, locations, for different subpopulations (gender, socio-economic status) and during different activities (residential, work, transport, shopping) in The Netherlands will be presented to point out the new features of this methodology.

6.2 Methodology

In this section the method to perform a disaggregated exposure analysis with an activity-based exposure modelling framework is explained.

6.2.1 General overview

In previous studies (chapters 3 and 4), the activity-based model ALBATROSS was used to model activities and trips of the entire Dutch population in The Netherlands. Trip data were combined with statistical data on the Dutch fleet of passenger cars to estimate emissions and model air quality. In chapter 5 air quality data were combined with population data to calculate static and dynamic exposure estimates. The analysis was performed for one urban area in The Netherlands. In the study presented in the current chapter, these hourly 'dynamic' exposure analyses were extended to comprise the whole Dutch study area and were further disaggregated by different activity-based variables like characteristics on the performed activity or on the person involved. By applying this disaggregation, multiple hourly population maps could be constructed for each category. Figure 16 schematically presents the different components of this integrated activity-based modelling framework. In the next sections the performed disaggregation and exposure calculation are explained.

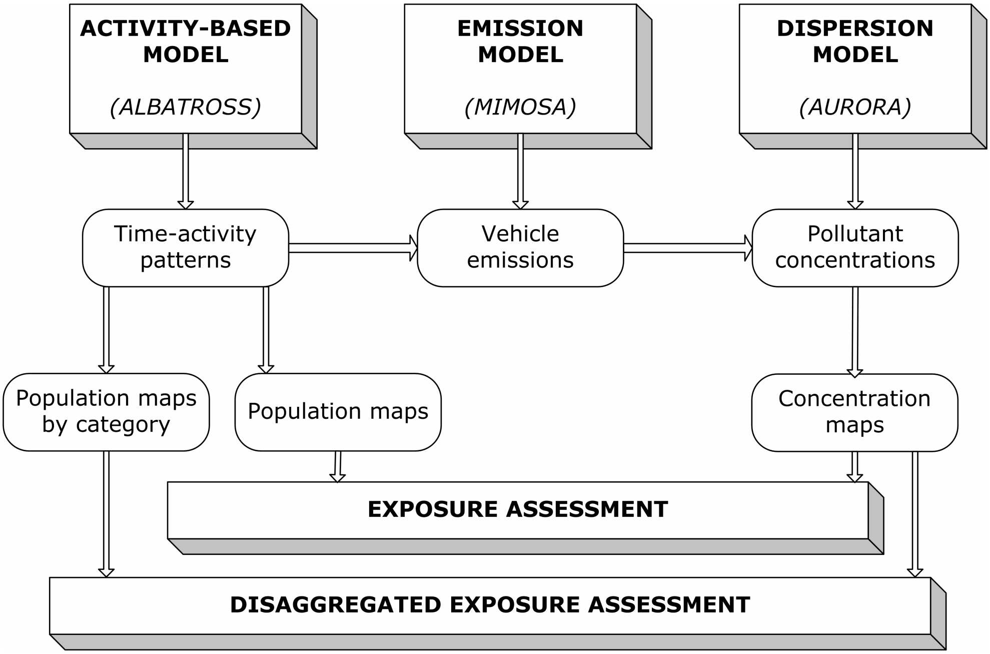

Figure 16. Schematic overview of the integrated activity-based modelling framework

The study area for the components of the integrated modelling approach presented here encompasses the whole territory of The Netherlands. We examined the exposure to NO_2, a pollutant which is typical for transport and is associated with negative health effects. Concerning the time-period for the exposure analysis in this study area, April 2005 was selected due to the availability of the necessary data for both population modelling and air quality modelling. Analyses for other pollutants or other time periods can be performed with a similar approach.

6.2.2 Time-activity data

The ALBATROSS model was used to describe the population distribution over time. As in the previous studies described in this thesis, the 4-digit postal code area (PCA) was chosen as the spatial unit for the location assignment procedure and time steps of one hour were chosen as the appropriate time unit. Information on the performed activity and the person involved was expressed and recorded as 'personhours' performed at a certain location (PCA). Figure 17 presents the distribution of personhours spent on different non-residential activities during an average weekday (Monday-Friday) over the entire study area. Considering the low number of non-residential activities at night in Figure 1, it is clear that most people spend the night at home. However, during the day (between 7 am and 20 pm), non-residential activities account for a proportion of up to 60% of all activities. Performing a paid job outside the house (work) is the most frequent activity. Spending time in traffic between two activities (transport) is the second most time consuming activity before social activities and shopping activities. Considering the high number of personhours spent on non-residential activities, exposure during the day is likely to be significantly influenced by concentration differences between home and workplace and while in transport.

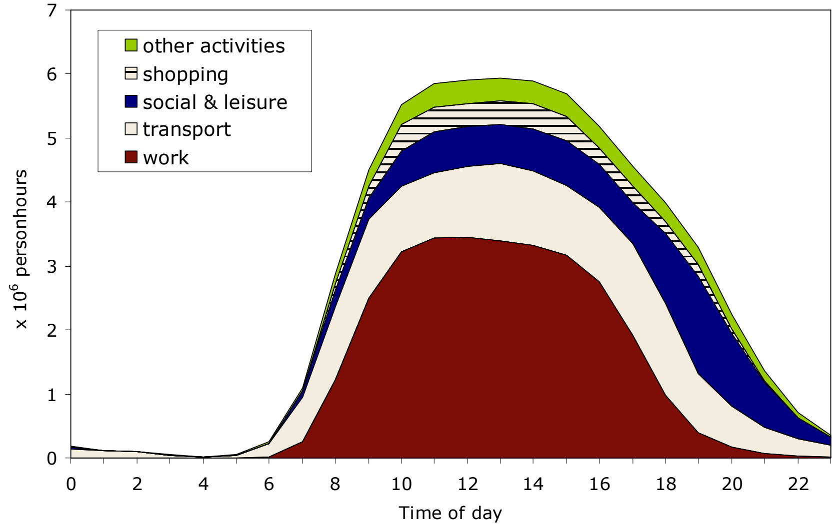

Figure 17. The distribution of non-residential activities performed by the adult population over an average weekday in The Netherlands as simulated by the ALBATROSS model

6.2.3 Exposure modelling

Concentrations to which people are exposed were taken from the gridcel corresponding to the location where the activity was performed (see chapter 4). For this reason the hourly population data were converted to a grid map consistent with the ambient concentration map from the AURORA model. A GIS software tool (ArcGIS) was used to match population data and concentration data on an hourly basis. This approach was adopted for people performing the activities "home", "work" and "shopping". For the activity "in transport" a different approach was adopted since it is more difficult to map this activity onto a set of grid cells. Other authors have circumvented this problem by either ignoring the transport activity (Hertel et al. 2001) or by simply assuming that the trajectory covered a straight line between origin and destination (Marshall, 2006). We have allocated the hourly average NO_2 concentration measured in the Dutch traffic-related monitoring stations to this activity (from the study described in chapter 4). In this way we can attribute specific outdoor concentrations to each activity and exposure can be calculated in a straightforward and transparent way.

For calculating exposure, correction factors to account for specific breathing rates were not used nor did we take into account whether an activity was performed inside or outside. Indoor/outdoor ratios are notoriously inaccurate (Kousa et al. 2002) and exposure in vehicles is even harder to quantify (e.g. Berghmans et al, 2009). We have decided, for clarity and to avoid confounding the main message, to look at ambient outdoor concentrations only in this research.

6.3 Results & discussion

6.3.1 Total exposure evaluation

In order to illustrate the hourly variations in concentrations and population, Figure 18 (a)-(b) and (d)-(e) respectively present concentration and population data for a selected region in the study area (the Amsterdam region) at two different time-periods. Similar geographic illustrations can of course be presented for any other area in The Netherlands, but maps of the entire country would be illegible because of the high resolution and extent of the results. As an example the data values for a night period and an afternoon period are presented for a day that was selected randomly out of the entire dataset. A presentation of random chosen values was preferred above showing average concentration and population values to emphasize that the study takes into account these distinct hourly values for the exposure calculation. The resulting computed exposure values for the selected time-periods are presented in Figure 18(c) and Figure 18(f). The population exposure was calculated by multiplying the concentration value (μg/m³) from the dispersion model and the corresponding population value (personhours).

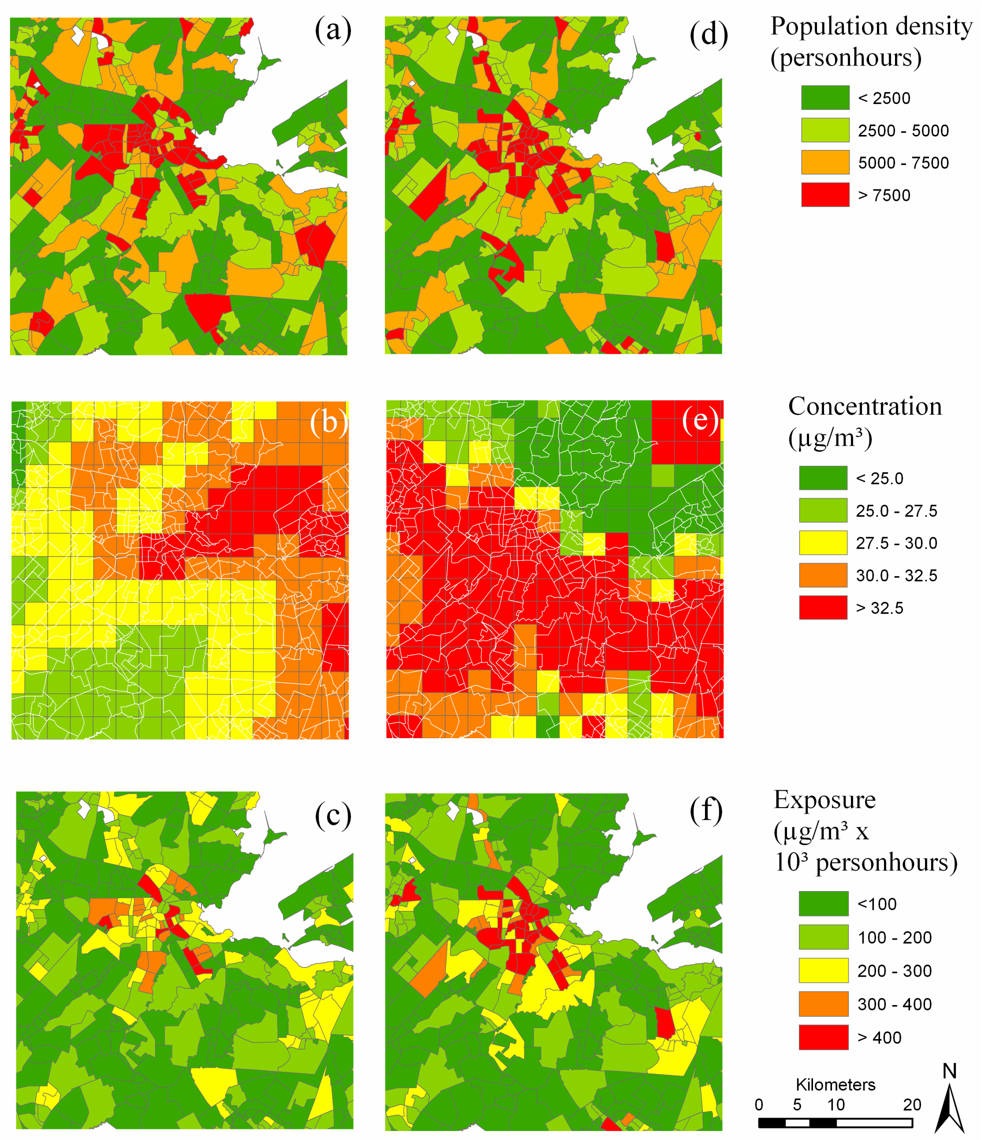

Figure 18 (a)-(f). The predicted density of population (a,d), ambient pollutant concentrations of NO_2 (b,e) and the exposure of the population to NO_2 (c,f), evaluated for two randomly selected moments, both on Tuesday the 19th of April 2005. The maps on the left side (a-c) present values at 2 am while the maps on the right side (d-f) correspond to the values predicted for the 2 pm time-period. The size of the depicted area is 2000 km².

The mean exposure concentrations estimated by this ‘dynamic’ approach for the entire Dutch study area in the month of April 2005 were first compared to results of a traditional ‘static’ approach (departing from residential data only and thus implicitly assuming that people are always at home). The exposure results were examined by time of day (hourly basis) to gain more insight into ‘when’ the largest differences between both approaches occur.
Figure 19 clearly shows that there is no significant difference between the traditional static approach and the new dynamic assessment between 8 pm and 6 am. Since, at night, the dynamic population approximates the residential population this conclusion is quite straightforward. During the day (6 am – 3 pm) the dynamic exposure assessment yields a much higher estimate for the exposure compared to the static mean exposure concentration with aberrations of up to 35 % ($p<0.05$; paired two-sided t-test). At that time, a large part of the dynamic population will be performing out-of-home activities (see Figure 17) and, apparently, these non-residential activities occur at locations with higher NO_2 concentrations. In the early evening (5 pm – 7 pm) however the static mean exposure concentration presents slightly higher exposure values than the dynamic approach, indicating that the NO_2 concentrations near the residential locations are higher than in other areas at that time. In the late evening the differences between both approaches disappear again.

Comparing the weighted daily exposure of the dynamic approach concentration relative to the static exposure concentration results in an overall difference of approximately 4 %. Although relative differences during some hours are much larger, these large differences tend to occur when concentrations are relatively low and vice-versa. Our result implies that, by neglecting people’s activity-travel behaviour the exposure will be underestimated by approximately 4% on average. This is consistent with the results of Marshal et al. (2006) who also concluded that taking into account travel patterns increases estimates of exposure for traffic related pollutants (+5% for benzene and +8% for diesel $PM_{2.5}$). The fact that a dynamic exposure analysis yields a higher estimate of exposure is linked to the fact that workplaces, traffic activities and shopping areas tend to be located in (urban) areas that have, on average, higher concentrations. While the differences may look small at first, we should consider that many national measures and plans to reduce transport related air pollution will only change exposure by a fraction of this amount. Present European policies (EU Directive 2008/50/EC), designed to reduce exposure to air pollution aim for a 5-20% reduction depending on the area. Our assessment shows that traditional exposure assessment methods are probably not accurate enough to develop efficient policies to meet this requirement.

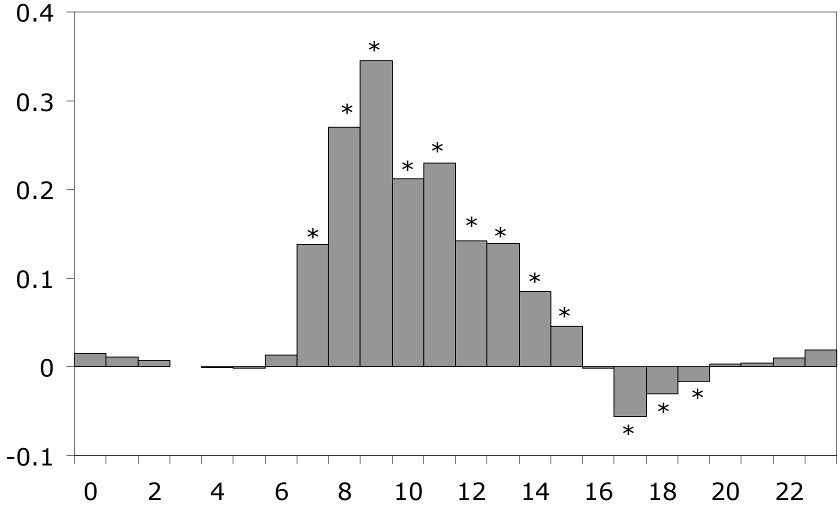

Figure 19. Dynamic exposure estimates relative to exposure concentrations from a static approach. Relative differences for NO2 per time of day for an average weekday in April 2005. The asterisks mark the hours with significant differences between both approaches ($p<0.05$; paired 2-sided t-test).

6.3.2 Disaggregated exposure analysis

In addition to conclusions that have been drawn in the previous sections, the true power of activity-based dynamic exposure modelling lies in identifying subgroups in the population and in activities that are associated with higher pollutant concentrations. To this end, a disaggregation of the exposure concentration by different subcategories is presented in the next section.

6.3.2.1 Exposure by activity

Using activity-based modelling as the basis of exposure assessments enables us to disaggregate exposure for different activities. Because different activities are performed in different areas (postal areas in this case study) each with its own concentration profile (on an hourly basis), different activities can be associated with different average concentrations. This is illustrated in Figure 20 for NO_2 concentrations on an average weekday in April 2005. General modelled concentrations vary between 20 and 80 NO_2 μg/m³ for most locations with a distinct peak in the morning and a protracted peak in the evening. Concentrations associated with work activities are consistently higher than concentrations associated with home-activities. Exposure while shopping only occurs during opening hours and shopping areas are characterized by intermediary NO_2 concentrations when compared to residential areas or workplaces. Average outdoor concentrations of NO_2 encountered while being in transport are often much higher than elsewhere, except in the late afternoon.

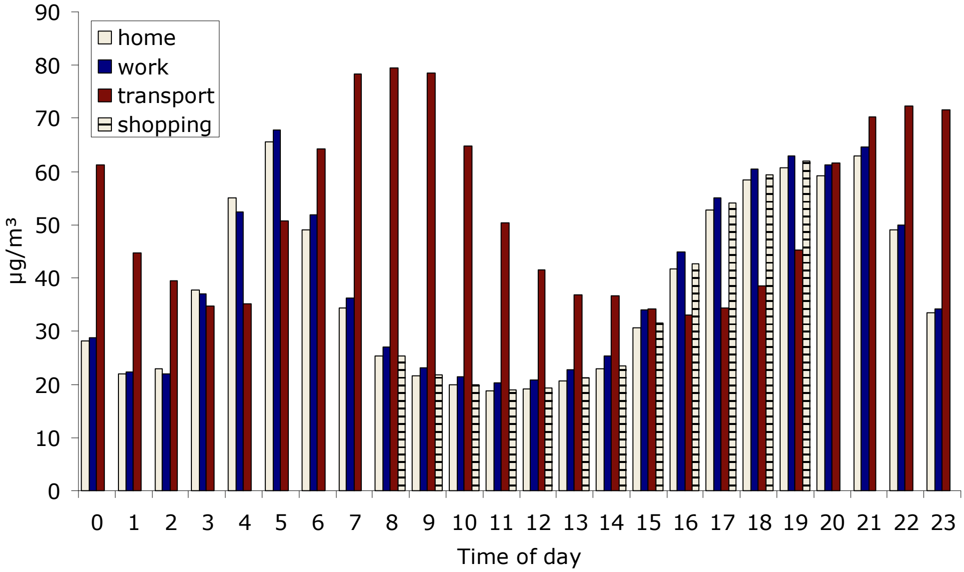

Figure 20. NO_2 exposure concentrations per time of day for different activities on an average weekday in April 2005.

In Figure 21 the estimated exposure concentrations for different activities are presented relative to the dynamic exposure concentrations. The dynamic exposure concentration (expressed relative to the static exposure in Figure 19) can be considered as the weighted average of all the activity-specific exposure concentrations (taking into account the number of personhours spent on each activity). Differences for people working at night are not statistically significant because of low numbers and are therefore not shown. Shopping activities only occur between 8 am and 20 pm. Figure 21 clearly shows that between 6 am and 2 pm the mean exposure concentration at home, at the workplace or in a shopping area is lower than the mean exposure concentration over the entire population. On the other hand, the exposure concentration of people in transport is, on average, much higher than the mean population exposure. In the early evening the analysis yields an opposite observation.

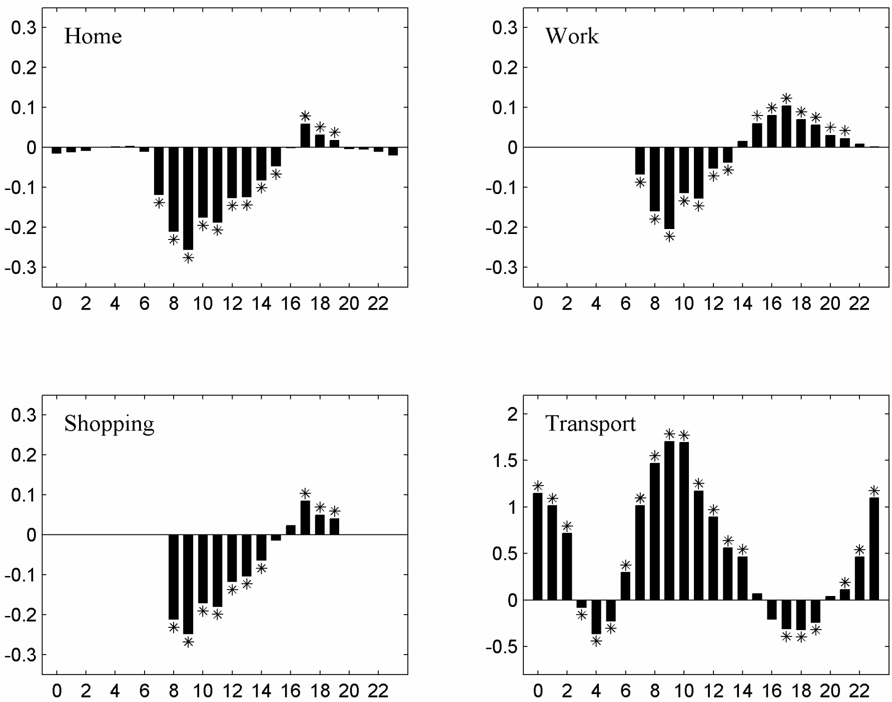

Figure 21. Estimated mean exposure concentration for each subgroup (activity) relative to the overall mean (dynamic) population exposure concentration. Values are presented per hour for the exposure to NO_2 on an average weekday in April 2005. The horizontal axis presents the time of day per hour. Note that a different ordinate scale was used for the transport activity. The asterisks mark the hours with significant differences between both approaches ($p<0.05$; paired 2-sided ttest).

6.3.2.2 Exposure by subpopulation

Another interesting feature of activity-based models is their ability to retain demographic and socio-economic data of the people making trips and performing activities. In this way the exposure analysis can be disaggregated by different population subgroups. In this paper two examples were shown to illustrate this point: an analysis by gender and by socio-economic classification. In Figure 22 the exposure differences were plotted (relative to the total dynamic exposure concentration) by hour of day. The exposure patterns of the male and the female subpopulation display opposite values. Since the exposure values for men and women contribute almost equally to the total dynamic exposure values (there are only slightly more women in the Dutch population than men), this observation is rational. In the early morning men seem to be exposed to higher NO_2 concentrations compared to the mean population exposure values, conversely women are less exposed at that moment. Exposure differences of up to 12% were recorded in the morning, indicating that, at that time, men perform activities at locations with much higher concentrations than women. Since men appear to travel earlier in the morning than women (travel results not shown here) and morning traffic concentrations appear to be quite high (see Figure 20) the difference in the morning can be explained by a different travel behaviour. Exposure differences between 9-11 am are reversed because at that time more women than men travel, exposing themselves to higher concentrations than those experienced by men (many of whom are then subjected to workplace concentration levels). In the afternoon men experience once again a slightly higher exposure which can be explained by the fact that more men than women have a paid job outside the house especially in the afternoon (more women work part-time jobs) and the workplace exposure concentrations are always slightly higher than at home. The overall (24 hour) difference in exposure between men and women is 1.16 % (i.e. exposure of men relative to women), consistent with the findings from Marshall (2008). Marshall (2008) also reported that these differences in pollutant intake rate will be even more explicit when taking into account gender-specific breathing rates (men: 14.9 $m^3 d^{-1}$; women: 10.5 $m^3 d^{-1}$).

In the second exposure analysis by subpopulation a similar disaggregated exposure analysis was used to distinguish the exposures of people of different socio-economic groups. Within the ALBATROSS model people (households) are categorised into four socio-economic classes (SEC) according to their income. By means of example the exposure concentrations between people from the lowest SEC (income less than average) and people belonging to the highest SEC (income more than double of average) was compared. As can be seen in the bottom graphs from Figure 22 people belonging to the lowest socio economic group appear to be exposed to slightly higher concentrations of NO_2 throughout the day, but there is a large variation within the day. Differences of up to 3% in the early morning/night are statistically significant. This effect is caused by concentration differences in the residential areas of both groups, a phenomenon which was also described by Marshall (2008). It is interesting to see the opposite during the morning rush hour. People belonging to the highest SEC then have a higher exposure, an effect that is caused by the fact that they are more likely to be driving to work, exposing themselves to the higher traffic concentrations. This offsets most of the original difference between both classes and hence the overall (24h) difference between both subgroups is small (0.84 %) and not statistically significant.

It is likely that the true difference in exposure between different socio-economic groups is even larger than the value that was presented here. It is well known that lower income groups tend to live in cheaper houses, including those that lose value because of higher noise levels. Differences in noise levels and important differences in NO_2 concentrations are known to occur over much smaller distances than the resolution of the present model version (3x3 km). It is therefore likely that we have underestimated this difference. On the other hand is it remarkable that we can observe this phenomenon even at the national level.

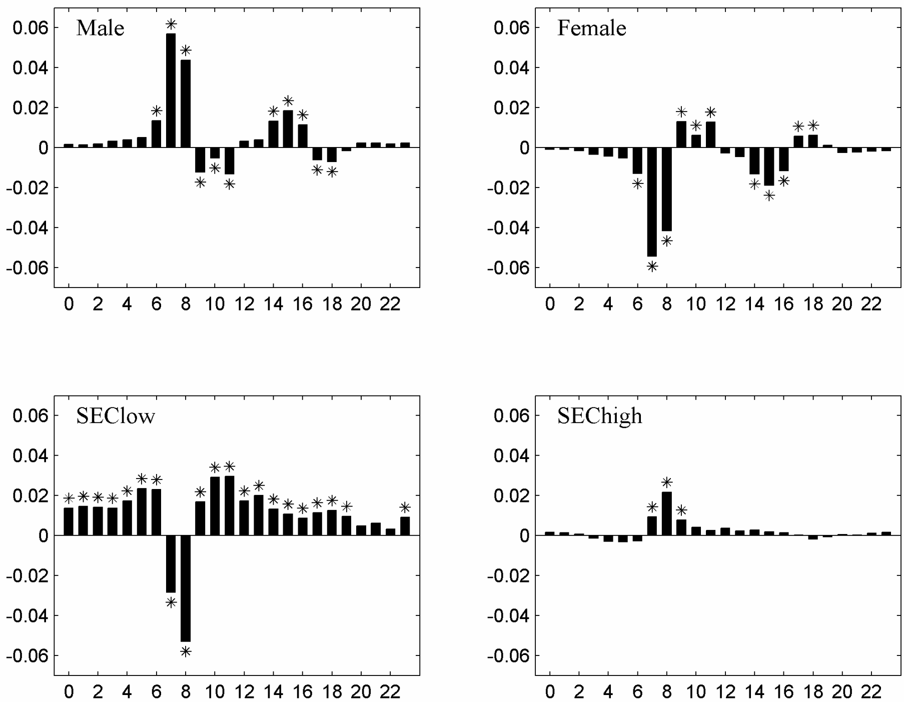

Figure 22. Estimated mean exposure concentration for each subgroup (population) relative to the overall mean (dynamic) population exposure concentration. Values are presented per hour for the exposure to NO_2 on an average weekday in April 2005. The horizontal axis presents the time of day per hour. The asterisks mark the hours with significant differences between both approaches ($p<0.05$; paired 2-sided ttest).

6.4 Conclusion

In this study a model chain is presented to estimate the population exposure to NO_2 based on activities and associated trips. For the first time to our knowledge an activity-based transport model was integrated with concentration data from an air quality model, to perform such a nation-wide dynamic assessment of exposure to air pollution. The dynamic exposure analysis from the activity-based approach yielded higher total exposure estimates than the conventional static assessment that assumes people are always at home. Depending on the perspective taken, differences can either said to be small (approximately 4% over the entire population) or rather important (from an air quality policy perspective).

A disaggregated analysis of the population exposure to NO_2 revealed that exposure may vary significantly between activities and between subpopulations. Concerning the classification by activity, highest exposure concentrations were estimated in-transport, followed by workplaces, shopping areas and home activities. When neglecting the exposure during non-residential activities total exposure values will be underestimated by 4% on average during the day. An analysis on two population classifications was also performed: one by gender and another by socio-economic status. The overall (24h) relative exposure difference between men and women was small but large intra-day differences appeared due to a different activity-travel behaviour (e.g. more men participate in the morning traffic peak). An analysis by SEC revealed that people from the lowest SEC are exposed to slightly higher NO_2 concentrations during the day compared to the mean population exposure except in the early morning. Both the home location (living in more polluted areas) and the travel behaviour (not participating in the morning traffic peak) explain these differences. Such disaggregated population exposure information can be used to refine the health effects resulting from this exposure.

7 GENERAL CONCLUSIONS AND PERSPECTIVES

7.1 General conclusions

This section summarizes the main conclusions that evolved from this research. Research results can be classified under the following topics:

7.1.1 The DPSIR integrated modelling chain

In this dissertation the development of an integrated modelling framework to model the population exposure to air pollution was set as an important goal. In theory, the framework developed in this PhD should comprise al the components of the DPSIR chain, the environmental problem framework, taking into account the different causal links between activities, trips, emissions, concentrations and exposure (see section 1.1). In Figure 23 the DPSIR conceptual model from section 1.1 is presented conform the components discussed in this thesis.

As illustrated in Figure 23, in this thesis the driving forces (D) behind the problem of traffic air pollution (and exposure) are covered by the ALBATROSS model that simulates the activities that people perform. By considering the travel demand as derived from the demand for activities, this model provides insight into reasons for people's travel behaviour. The environmental pressures (P) in the modelling chain are calculated by the MIMOSA emission model. This model determines the amount of pollutants being emitted to the atmosphere. Finally, the state (S) of the environment is modelled by AURORA that converts the emissions into concentrations and the impact (I) of this state on human health is calculated by using the entire exposure assessment framework to calculate the population exposure to air pollution. Hereby the calculation of the real health effects (e.g. the reduction in 'disability adjusted life years') was not part of the scope of this study. On each of these described components (DPSI) the society can carry out a response (R) through various actions to reduce or prevent the negative impacts of traffic air pollution. However, these responses were not evaluated in this research.

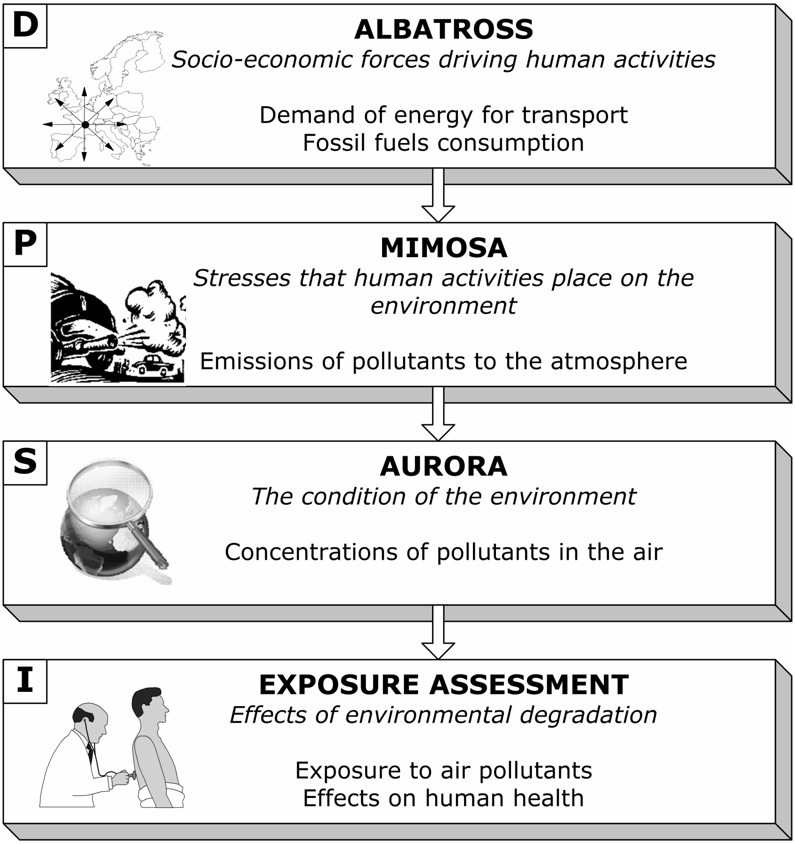

Figure 23. The DPSIR model chain adapted to this dissertation

Except for the 'responses', all components of the DPSIR-chain were covered in this thesis. Each chapter of this manuscript describes one or more steps to develop and evaluate a methodology for the assessment of population exposure to air pollution. Chapter 2 describes the different components of this modelling framework: an activity-based model for modelling the travel-behaviour of people, an emission model to convert vehicle trips into emissions and a dispersion model to convert the emissions into concentrations. Chapters 3 and 4 present two intermediary applications to develop the exposure modelling framework. In chapter 3 the activity-based model ALBATROSS was linked with the MIMOSA emission model (D,P). In chapter 4 this chain was further extended with the AURORA dispersion model to convert the emissions into concentrations (S). In chapters 5 and 6 finally two studies are presented that use the entire activity-based exposure modelling framework to calculate the population exposure to air pollution (I). These latest studies used the activity-based model both for modelling the air quality as for assessing the population exposure. By using this approach, an integrated exposure modelling framework was therefore successfully established.

7.1.2 The activity-based approach for air quality purposes

Activity-based 'transport' models were originally developed to provide more insights into the 'transport' or 'travel' behaviour of people. Recent applications of these models (e.g. Roorda et al. 2008; Timmermans and Zang; 2009) still focus on their advantages for travel behaviour research. However, due to the richer set of concepts which are involved in activity-based modelling (information on travel by time of day, exact time between trips, vehicle miles travelled,…) the advantages for both transportation and air quality purposes are more and more acknowledged. Literature reveals that few authors have described the (theoretical) advantages of activity-based models for air quality purposes, but models that have been developed along these lines are still scarce (e.g. Shiftan, 2000; Hatzopoulou et al. 2007). This is partly due to the lacking of an operational activity-based model. On the other hand this delay can also be attributed to the difficulties arising when trying to setup such a multidisciplinary endeavour.

The applications that were performed as part of this Ph.D. dissertation demonstrate that an activity-based model can definitely be used for air quality purposes. The following three achievements can be mentioned (related to the three 'specific tasks' mentioned in section 1.2):

In a first application the activity-based model ALBATROSS was used to provide **emission** estimates for the Dutch traffic situation. By combining the simulated vehicle trips from ALBATROSS with emission factors from the MIMOSA emission model, vehicle emissions were calculated. A comparison between the modelled emissions and reported emission values demonstrated that both values correspond quite well. CO_2 emissions were overestimated by 11%. Differences between modelled and reported emissions of NOx, Voc, SO2 and PM varied between 3 and 26%. However, the mere replication of approximately the same emission values with a different model is no innovation. In effect this result cannot even be validated because emissions cannot be measured at the national level and hence cannot be compared to model results. Compared to other (technology based) travel or emission studies, this study provides much more detailed temporal and spatial information on passenger car emissions instead of allowing only aggregated (yearly) emission values. Unfortunately the accuracy of spatially disaggregated emissions can also not be validated.

In a second application the activity-based emission approach was further explored by converting the activity-based emissions into pollutant **concentrations**. For this purpose, the AURORA dispersion model was applied to simulate the transport and conversion of the emissions into concentrations. The first important advantage of this air quality modelling step is that it enables to validate the activity-based model predictions by comparing the simulated concentrations with measured concentrations at Dutch monitoring stations. Both temporal and spatial validation analyses were performed. Self evidently this comparison is difficult for PM_{10} which is (in small countries like The Netherlands) largely imported from abroad and formed from other precursors. Results of the statistical analysis demonstrate a very good correspondence between the simulated and measured concentrations of O_3 (IA between 0.69 and 0.80). For NO_2 the IA value varied between 0.40 and 0.70. And for PM_{10}, finally, IA values between 0.48 and 0.64 were calculated. The comparison of concentrations constitutes an end-of-pipe validation of the accuracy of the entire model chain but does not allow a crisp analysis of each models individual performance. We have specifically looked at the results for NO_2 which is a pollutant typical of transport which has both a strong spatial and temporal variation. NO_2 is therefore the pollutant best suited to attempt a validation of the ALBATROSS-MIMOSA-AURORA model chain because its (modelled) concentrations will tend to be sensitive to errors in traffic streams, emission functions as well as atmospheric modelling. This study demonstrated that the activity-based air quality model chain was able to simulate the hourly concentration patterns in the Dutch study area with sufficient accuracy.

The last two applications in this dissertation (see chapters 5 and 6) described the activity-based modelling approach for **exposure** purposes. The predicted hourly concentration fields from the ALBATROSS-MIMOSA-AURORA modelling chain were combined with hourly information on people’s location to calculate the exposure. By using the population information from the activity-based simulation, hourly population maps were simulated and dynamic exposure values could be estimated. As a result of this, a dynamic exposure modelling framework was established. In chapter 5 this framework was applied on a Dutch urban area to demonstrate the importance of taking into account people’s travel behaviour when calculating the exposure. The exposure study in the Dutch urban area demonstrated that large inflows of people occur during the day in the urban areas (the population more than doubled), causing people to be exposed to higher concentration values compared to their residential situation. Traditional exposure studies that link concentration values with residential information therefore often underestimate the exposure values. In chapter 6 these dynamic exposure values were calculated for the entire Dutch study area and further disaggregated according to different activity-based features like the gender of the person or the performed activity. Understanding exposure variations among activities and subpopulations can be very useful for scientific and policy purposes. It can provide information on locations or population groups most at risk, or can indicate where and when the largest exposure values occur.

In summary, this dissertation demonstrated the advantages of an activity-based approach for air quality purposes by presenting three kinds of applications: the calculation of vehicle emissions, the simulation of pollutant concentration patterns and the assessment of the population exposure to air pollution.

7.1.3 Activity-based models for environmental policy making

The kind of integrated modelling approach presented in this thesis, using a transport model for air quality purposes, is not only innovative from a scientific and methodological perspective, but it also offers advantages for policy makers. It enables them to take into account that trips both cause transport related emissions and at the same time change the distribution and attributes of the population which will result in different exposure estimates. The availability of activity-based models for exposure analysis therefore opens up a myriad of possibilities for innovative policies and measures. Policy makers will be able to design measures aimed at reducing the exposure at the most important sites, at the most critical times and for selected population groups. These efforts may partly coincide with currently implemented measures to meet general air quality standards. However, in addition to this, we expect that new policies can especially be made more effective in reducing health impacts. In any case, policies in other domains which nowadays risk to offset environmental policies can be screened on their environmental effects before being implemented. In the past the use of different models and policy schemes has often caused one policy in one domain to offset effects of another policy in a different domain because secondary effects could no be taken into account. Enabling to make the link between policies in different policy domains (e.g. mobility, energy and health) is therefore an important advantage of the integrated modelling chain developed in this research.

Further, by applying an activity-based model for the transport modelling part of this framework, instead of a traditional four-step transport model, the range of measures that can be evaluated will increase. In an activity-based model each individual is represented as an agent belonging to the population of a certain study area. During simulation, the model simulates the full pattern of activity and travel episodes of each agent and each day of the simulated time period. The pattern of activity and travel episodes, i.e. the schedule, is constructed by a scheduling model or scheduler, which takes personal, household, and environmental attributes as well as constraints into account. These constraints can be situational, institutional, household, spatial, timing, and spatial-temporal constraints. The scenarios corresponding to particular policy measures that can be evaluated with such an activity-based model consist of changes in the personal, household, and environmental attributes and/or in the constraints. In this way, the policy measures that are investigated in the scenarios are taken into account by the scheduler, and thus result in potential changes in the scheduling behaviour. The traffic demand is in its turn derived from the schedules of all the agents in the simulation. Examples of measures or scenarios that can be evaluated by such an approach are changing shop opening hours, ageing of the population, teleworking, etc.…

7.2 Recommendations for future research

7.2.1 Methodological challenges

Establishing the link between an activity-based model and an air quality module was an important accomplishment in this PhD research. Applying the developed model chain to a certain region was another important realization. But of course, some challenges still remain to improve this modelling tool even more. For each model in the chain some recommendations are mentioned which can or should be applied to improve the model's outcome. In this section these challenges are briefly described and discussed.

7.2.1.1 Improving the prediction of activity-travel patterns and traffic flows

In this doctoral research the activity-based model ALBATROSS was applied to demonstrate the advantages of activity-based models for air quality purposes. This model was however not originally developed for these environmental purposes but mainly to gain more insights into people's travel behaviour and travel demand. To improve its usefulness for environmental applications, improvements on the following issues can be mentioned:

Limited number of time frames

The ALBATROSS model schedules the fixed activities on a continuous time scale, but flexible activities are allocated to one of the six fixed time periods (<10h, 10h-12h, 12h-14h, 14h-16h, 16h-18h, >18h). To obtain a more detailed temporal analysis in the current research the periodical trips and trip matrices that resulted from the activity-based model were reorganized into hourly values. For this purpose, information from a Dutch travel behaviour research (NTS) was used and derived time adjustment factors were applied. Of course, it would be more precise if the hourly trips were provided immediately from the activity-based model to include the different geographic variations in trip prediction over the study area (the redistribution of the trips per time period was similar for the entire study area).

Stochastic modelling of activity-travel patterns

In this research the activity-based model ALBATROSS was used for the simulation of activity-travel patterns for all the individuals in the Dutch population. After adapting the model according to the specifications presented in section 2.2.2.3 the output of one single model run was used as input in the environmental models. By performing multiple stochastic model runs however, more insights into the model variations can be obtained.

Traffic assignment

Concerning the traffic assignment used in this PhD research, improvements can be made on the following two issues. First of all, after the assignment of the O/D-matrices from ALBATROSS to the traffic network, the activity-based information is lost. Due to technical problems we were not able to keep both the hourly traffic flow information together with the information on the trip performer or on the trip motive when assigning the trips to the road network. This means that the hourly traffic flows cannot be disaggregated by socio-economic groups or by activity, while this information is provided by the activity-based model. An assignment of multidimensional O/D sets to the network should therefore be studied in future research.

Further, the assignment in the current research applied an 'all-or-nothing' assignment algorithm that did not take into account the present traffic volumes when assigning the trips to the road network. This means that we assume that traffic will not be reallocated to alternative routes when traffic volumes reach the maximum capacity of the road. To apply a more realistic, equilibrium assignment, future studies need to include information on the road capacity. Therefore, also information on freight transport flows needs to be available since the presence of freight transport can have a large influence on the remaining road capacity.

7.2.1.2 Improving the calculation of vehicle emissions

Concerning the calculation of vehicle emissions the following improvements can be mentioned.

Hourly average speeds

The activity-based model itself provides no hourly speeds. In this research average link speeds from the 'Basisnetwerk' road network were used, also applied in the ALBATROSS model to estimate travel times between origins and destinations. These average speeds were kept constant during the day. Because average speeds are the single most important input into macroscopic COPERT-like emissions, enabling different average speeds to be modelled on different road segments at different times would greatly improve the power of activity-based models to discriminate between the emissions associated with different time periods and activities. Future research, involving a more advanced traffic modelling procedure that predicts hourly changing speeds per traffic link, can therefore attribute to a more accurate emission assessment. Obviously, one of the previous comments on a more advance traffic assignment procedure is also valid here.

Cold start emissions

Compared to the more traditional four-step transport models, the activity-based models have the advantage that they simulate entire time periods and take into account the interdependency between activities and trips at different moments. Due to this, information on the time between two subsequent trips can be extracted and, therefore, the number of cold starts can be predicted more accurately. In Hatzopoulou et al. (2007) for example this issue was taken into account and engine start emissions were modelled based on the travel patterns of each vehicle in the simulation. However, in the current research this information was not yet taken into account for the emission calculation. Information on the average trip length was used to account for cold start emissions. Future research should bear this issue in mind to improve the emissions assessment.

Disaggregating emissions by activity-based information

A rough analysis of the emissions (after aggregating the trips per activity instead of per hour) was performed by Beckx et al. (2008). In this analysis total yearly emissions were disaggregated according to travel motive to gain more insights into the causes of the emissions. Results from this analysis demonstrated that 47% of the emissions were caused by commuter trips, 17% by social trips, 10% by shopping trips,…. However, as a result of the first limitation mentioned on the traffic assignment (loss of activity-based information after assignment), such a disaggregated analysis could not be performed on the hourly emission values. A more detailed classification, based on socio-economic or activity-related characteristics instead of technological characteristics, could however give regional and local policy makers more information on the sources of this environmental problem per time of day. And since technological issues are regulated at a European level, this information provides them with the tools to manage those aspects of communities, activities and travel that are within their own competences.

7.2.1.3 Improving exposure and health assessment

The final goal of this research was to develop (and apply) an integrated exposure modelling framework that includes an activity-based transport model for both the activity-travel part as for the population exposure. Future research may extend this exposure procedure to include also the following issues.

Indoor exposure modelling

Our analysis was limited to modelling exposure to outdoor pollutant concentrations. A possible future analysis could focus on indoor-outdoor ratios to determine also the indoor concentrations and extend the analysis to the evaluation of indoor exposure. Since these indoor-outdoor ratios are not straightforward to determine, this might require a good thorough research.

Integration of land use information

Another interesting topic for future studies on exposure analysis would be the integration of land use information with population distribution. By taking into account information on the land use, the population can be distributed more accurately within a population zone instead of assuming a homogenous distribution over this location. The activity-based information on the performed activity of each individual can contribute to the assessment of a more precise location, and therefore a more accurate exposure assessment will be achieved. Furthermore, simulations on future land use developments, can provide useful spatial information to the activity-based model when performing long term prognoses on travel behaviour.

Inhaled dose

Besides the use for a more detailed location of the population, the activity-based information can also be taken into account when calculating the inhaled dose for certain pollutants. The distinction between low breathing rates during sleeping activities versus higher breathing rates at work activities for example will allow us to determine the actual inhaled dose during different activities. Further, personal information on the individual (age, gender,…) can also be taken in to account as for example breathing rates of men are higher compared to women (men: 14.9 m^3 d^{-1}; women: 10.5 m^3 d^{-1}; see the study of Marshall 2008).

Individual exposure values

This PhD studies the calculation of exposure at the population level to conclude on differences between different (sub)populations (men versus women, working versus shopping,…) or different approaches (static versus dynamic) population exposure. Another approach would be to focus on the (accumulated) individual exposure level and conclude on differences in total accumulated exposure values during a certain time period (a day, week, year,..). This kind of analysis requires a different computer-technical setup since all the individuals in the population need to be 'followed' during the day. However, it would provide us with more data on the variations in exposure between the individual agents which is very useful for health impact analyses.

Spatial resolution

The more detailed the spatial resolution of both concentrations and individuals, the more accurate the exposure assessment will be. The 3 by 3 km grid used in the current work is therefore not able to capture intrazonal differences in exposure and only provides insights on more general exposure differences that occur on larger distances. A more detailed spatial resolution, for example with a resolution of tens of metres, will provide more detailed exposure analyses. Future research should focus on improving the spatial resolution of the modelling framework. However, the following remarks can already be made. First of all, one should apply a similar detailed resolution on all models involved in the modelling framework, both on the concentration model as on the population model to improve the exposure assessment. This means that the number of zones in the activity-based model and in the emission model have to increase significantly. Also, one should keep in mind that the dispersion modelling step is computationally burdensome, even at a more coarse modelling grid (see details in section 2.4.2.2). Applying a finer spatial resolution will enlarge the computational runtime of this modelling step significantly and can therefore imply that a smaller study area should be looked at to maintain an 'acceptable' runtime.

Health effects

Concerning the health effects of exposure to pollutants such as PM_{10}, $PM_{2.5}$ and NO_2, a lot of studies are already performed. In this study however conclusions on the specific health impacts were not made. Future research can focus on these health effects, but they should take the following issues into account.

Although the link between air pollution and adverse health effects was clearly established 15 years ago (e.g. Dockery et al. 1993) the epidemiological health effect functions that determine the health effects of the exposure are based on static information (residential address data and fixed monitoring stations) and not on a dynamic exposure approach. Several recent epidemiological studies have used the proximity of the home to major roads as a surrogate for exposure and suggested that proximity of people to traffic sources partly explains observed health effects (eg. Beelen et al. 2007). However as demonstrated by Petersen et al. (2004), it is probably the participation of people in traffic that determines risk rather that the location of their home. Exposure analysis could be improved by determining more accurately where people spend their time, because people are only exposed to concentrations occurring in the areas where they are active at that time, which during the day is very often not at their home address. We therefore suggest that exposure modelling takes advantage of the new possibilities offered by activity-based transport models. Besides providing a better total estimate of exposure, activity-based modelling also enables the disaggregation of individual exposure over activities and locations and may therefore serve to reduce exposure misclassification and thus empower epidemiological studies to establish relationships with air quality more precisely. A large challenge for future studies on the health effects therefore concerns the interpretation of dynamic exposure values as effects on human health.

7.2.2 Extending the model chain for scenario analysis

As can be seen in Figure 23, the responses (R) link is missing in the DPSIR-modelling chain. The responses (measures or scenarios) are not discussed in this thesis, but this extension of the modelling chain is definitely possible in future research.

Future research can adopt the new approach presented in this thesis as a policy instrument to study the impact of different societal trends or specific policy measures that have an direct or indirect impact on traffic flows. This will imply setting up a scenario analysis of some kind. Scenarios will typically consist of different parameter settings different from the defaults describing current conditions and referring to a future situation. The fact that we have been able to integrate an activity-based model into the modelling chain will enable us to set-up scenarios of a completely different nature. Environmental analysis is no longer confined within the strict limits of pure technical scenarios. Examples of measures that are currently being studied include the aging of European populations (which impacts on their travel and activity patterns and hence on their exposure) and the impact of institutional constraints like widening of shop opening hours (which tends to shift traffic to the early morning and late evening and hence changes the temporal concentration profile of transport related pollutants). Because one model (the activity-based transport model) is used both for the population modelling as for the travel demand modelling part, the framework enables us to analyze scenarios without overlooking any secondary effects.

Appendix A

This appendix A gives a general overview of the structure of important data files that have been used for the activity-based transport modelling. Data files involve information used by the ALBATROSS model for predicting activity-travel patterns for the Dutch population. We acknowledge the Urban Planning Group from the University of Eindhoven (The Netherlands) for providing us these data and allowing us to simulate activity schedules with the ALBATROSS model.

A.1 Activity classifications

Table A.1 shows the classifications of activities used in ALBATROSS. The distinction between fixed and flexible refers to activities that supposedly belong to the schedule skeleton (fixed) and those that are scheduled on a daily basis (flexible). The duration and start time of fixed activities are predicted on a continuous time scale, whereas the flexible activities are scheduled according to pre-defined discrete time steps.

Table A.1. Activity classifications used in ALBATROSS

Activity	**Description**
Sleep	Sleep activity during the night and morning
Work out of home (long)	Work or school activity longer than 60 minutes
Work out of home (short)	Work or school activity 60 minutes or shorter
Voluntary work	Voluntary work
Bring/get	Bring or get persons or goods
Other fixed	Medical, other non-leisure
Daily shopping	Grocery shopping
Service	Bank, Post office,…
Non-daily shopping	Non-grocery shopping
Social out of home	Social visits family, friends,…
Leisure out of home	Café, restaurant, concert, sport,…
In-home	All in-home activities other than sleep

A.2 Physical data

Arentze and Timmermans (2005) constructed a physical database for ALBATROSS. Table A.2 summarizes the data sources that were used to construct this database.

Concerning the distance and travel time data, information was used from the network file ('Basic Network'). The Basic Network file describes the nationwide road network down to the level of neighbourhood roads. Distance and travel time data for car and slow modes are derived from this file in which car distance data are based on the fastest route (slow mode distance is based on the shortest route) and link specific speeds are used to estimate car travel times. To construct the link specific speeds in the Basic Network file, expert assessment was used to estimate average flow speed on each link throughout the day. However, since it is important to have time-of-day dependent travel times instead of using only daily averages, time-of-day dependent travel time adjustment coefficients were calculated based on information from the national model system (LMS). By applying this approach free-floating, morning-peak and evening-peak travel time data were estimated.

NRM data and LISA data were used to provide useful information on the location. They provide sector-specific employment and population data at the 4PCA level. This information is used in ALBATROSS as indicators of availability and attractiveness of facilities for conducting particular activities (e.g. total employment data indicate the number of work activities, the number of primary school children indicate the number of bring/get activities,…). LMS parking data were collected at the level of subzones. These data describe the number of available parking places for each subzone, subdivided into paid and free parking places and with information on the parking prices.

Table A.2. Physical data sources (see also Arentze and Timmermans, 2005)

Distance/travel time data	
Basic network	Car distance fastest route Car travel time fastest route Slow distance shortest route
LMS car distance/travel time (subzone)	Car travel time fastest route, free floating Car travel time fastest route, morning peak Car travel time fastest route, evening peak
LMS train distance/travel time (subzone)	Distance In-vehicle travel time Access, egress travel time
BTM tariff zones (subzone)	Number of tariff zones passed
NRM data (4PCA)	# of households Total # of employees # of pupils primary schools
LISA employment data (4PCA)	# of employees daily good retailing # of employees non-daily good retailing # of employees banks/post offices # of employees restaurants/cafés
LMS parking data (zone)	# of paid parking places # of free parking places Mean price per hour for long parking times Mean price per hour for short parking times

LMS is the national model system; BTM is bus, tram or metro; NRM is the new regional model; LISA is a national employment database

Appendix B

This appendix B gives a general overview of the structure of important data files that have been used for the emission model MIMOSA. These files involve information on the Dutch vehicle fleet and the COPERT-III emission factors.

B1. Vehicle fleet data

To calculate the emissions for a certain region or country information on the local vehicle fleet is required since the composition of this fleet determines the emission factors that apply to this specific region.

Information on the composition of the Dutch vehicle fleet was obtained from CBS statistical information (CBS, 2001). On the CBS website information was retrieved on the characteristics of the passenger cars in The Netherlands on January 1st 2001. Hereby we assume that the situation on this date reflects the vehicle composition during the past year and can therefore be used to calculate the passenger car emissions for the year 2000. Table B.1 presents the data that were gathered on the Dutch passenger cars. Information on both fuel type and vehicle age (year of construction) were used to construct the composition of the Dutch vehicle fleet. Concerning the fuel type, we did not include the vehicles running on electric energy or on CNG due to the small numbers in the database (58 and 46 for electricity and CNG respectively).

Table B.1. Characteristics of the Dutch vehicle fleet (passenger cars only).

Fuel type	*Age of the vehicle*	*Number of vehicles*
Total	Total	6539040
	<1 year	583333
	1 - 2 year	1105672
	3 - 4 year	887131
	5 - 6 year	808955
	7 - 8 year	794775
	9 - 11 year	1136368
	12 - 14 year	782488
	15 - 19 year	254528
	20 - 24 year	49857
	>24 year	135933
Petrol	Total	5345589
	<1 year	434295
	1 - 2 year	820225
	3 - 4 year	687461
	5 - 6 year	653524
	7 - 8 year	667603
	9 - 11 year	994140
	12 - 14 year	701732
	15 - 19 year	230834
	20 - 24 year	44831
	>24 year	110944
Diesel	Total	870862
	<1 year	132487
	1 - 2 year	238115
	3 - 4 year	140443
	5 - 6 year	99617
	7 - 8 year	79746
	9 - 11 year	92020
	12 - 14 year	61933
	15 - 19 year	19418
	20 - 24 year	3218
	>24 year	3865
LPG	Total	322485
	<1 year	16524
	1 - 2 year	47304
	3 - 4 year	59207
	5 - 6 year	55802
	7 - 8 year	47418
	9 - 11 year	50203
	12 - 14 year	18821
	15 - 19 year	4275
	20 - 24 year	1807
	>24 year	21124

B2. Copert-III emission calculations

Here we briefly describe the methodology and relevant emission factors, incorporated in the computer programme COPERT-III, to calculate emission estimates of road transport. Since the current research only involves passenger cars, information on other vehicle types (light duty trucks, heavy duty trucks,…) will not be discussed here.

COPERT assigns emission factors to vehicles by classifying the vehicles according to information on their fuel type, vehicle size and construction/production year. The production year of the vehicle is hereby used to classify the vehicles according to legislative (ECE, Euro) or technology ('improved conventional', 'open loop') steps. The vehicle categories applied in COPERT are listed in Table B2.1. Besides the vehicle category, also information on the average speed will be applied to determine the appropriate emission factor. Hereby, for some categories or pollutants, different functions will be applied for different speed ranges. A presentation of all COPERT-III emission factors would be to redundant in this manuscript. One example of this approach is given in Table B2.2 on the NO_x emission factor. More detailed information on the applied emission factors can be found in the COPERT-III manual (Ntziachristos and Samaras, 2000).

Table B2.1. Vehicle category split in COPERT (adapted from: Ntziachristos and Samaras, 2000)

Vehicle Class	**Legislation**
Petrol <1.4l	PRE ECE
	ECE 15/00-01
	ECE 15/02
	ECE 15/03
	ECE 15/04
	Improved Conventional
	Open Loop
	Euro I – 97/441/EEC
	Euro II – 94/12/EC
	Euro III – 98/69/EC Stage 2000
	Euro IV – 98/69/EC Stage 2005
Petrol 1.4l-2.0l	PRE ECE

	ECE 15/00-01
	ECE 15/02
	ECE 15/03
	ECE 15/04
	Improved Conventional
	Open Loop
	Euro I – 97/441/EEC
	Euro II – 94/12/EC
	Euro III – 98/69/EC Stage 2000
	Euro IV – 98/69/EC Stage 2005
Petrol >2.0l	PRE ECE
	ECE 15/00-01
	ECE 15/02
	ECE 15/03
	ECE 15/04
	Improved Conventional
	Open Loop
	Euro I – 97/441/EEC
	Euro II – 94/12/EC
	Euro III – 98/69/EC Stage 2000
	Euro IV – 98/69/EC Stage 2005
Diesel <2.0l	Conventional
	Euro I – 97/441/EEC
	Euro II – 94/12/EC
	Euro III – 98/69/EC Stage 2000
	Euro IV – 98/69/EC Stage 2005
Diesel >2.0l	Conventional
	Euro I – 97/441/EEC
	Euro II – 94/12/EC
	Euro III – 98/69/EC Stage 2000
	Euro IV – 98/69/EC Stage 2005
LPG	Conventional
	Euro I – 97/441/EEC
	Euro II – 94/12/EC
	Euro III – 98/69/EC Stage 2000
	Euro IV – 98/69/EC Stage 2005
	Euro IV – 98/69/EC Stage 2005

NO_x emission factors for gasoline cars (adapted from Ntziachristos and Samaras, 2000)

Vehicle Class	**Engine Capacity**	**Speed Range (km/h)**	**NOx Emission Factor (g/km)**
PRE ECE & ECE 15-00/01	cc < 1.4l	10-130	$1,173 + 0,0225V - 0,00014V^2$
	1.4 < cc < 2.0l	10-130	$1,360 + 0,0217V - 0,00004V^2$
	cc > 2.0l	10-130	$1,5 + 0,03V + 0,0001V^2$
ECE 15-02	cc < 1.4l	10-130	$1,479 - 0,0037V + 0,00018V^2$
	1.4 < cc < 2.0l	10-130	$1,663 - 0,0038V + 0,00020V^2$
	cc > 2.0l	10-130	$1,87 - 0,0039V + 0,00022V^2$
ECE 15-03	cc < 1.4l	10-130	$1,616 - 0,0084V + 0,00025V^2$
	1.4 < cc < 2.0l	10-130	$1,29e^{0,0099V}$
	cc > 2.0l	10-130	$2,784 - 0,0112V + 0,000294V^2$
ECE 15-04	cc < 1.4l	10-130	$1,432 + 0,0026V + 0,000097V2$
	1.4 < cc < 2.0l	10-130	$1,484 + 0,013V + 0,000074V^2$
	cc > 2.0l	10-130	$2,427 - 0,014V + 0,000266V^2$
Improved conventional	cc < 1.4l	10-130	$-0,926 + 0,7192\ln(V)$
	1.4 < cc < 2.0l	10-130	$1,387 - 0,0014V + 0,000247V^2$
Open Loop	cc < 1.4l	10-130	$-0,921 + 0,616\ln(V)$
	1.4 < cc < 2.0l	10-130	$-0,761 + 0,515\ln(V)$
EUROI	cc < 1.4l	5-130	$0,5595 - 0,01047V + 10,8E-05V^2$
	1.4 < cc < 2.0l	5-130	$0,526 - 0,0085V + 8,54E-05V^2$
	cc > 2.0l	5-130	$0,666 - 0,009V + 7,55E-05V^2$

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Curriculum vitae

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EDUCATION

2004 – 2009 PhD in Transportation Sciences
(VITO – Hasselt University)

2003 – 2004 Master in Environmental Sciences
(Antwerp University)

1999 - 2003 Master in Biology
(Hasselt University – Antwerp University)

PUBLICATIONS

International publications with peer review

Beckx C., Torfs R., Arentze T., Int Panis L., Janssens D., Wets G. (2008). Establishing a dynamic exposure assessment with an activity-based modeling approach: methodology and results for the Dutch case study. Epidemiology, 19, S378-S379.

Beckx C., Int Panis L., Arentze T., Janssens D., Torfs R., Broekx S., Wets G. (2009). A dynamic activity-based population modelling approach to evaluate exposure to air pollution: methods and application to a Dutch urban area. Environmental Impact Assessment Review, 23, 179-185.

Beckx C., Int Panis L., Van De Vel K., Arentze T., Janssens D., Wets G., (2009). The contribution of activity-based transport models to air quality modelling: a validation of the ALBATROSS - AURORA model chain. Science of the Total Environment, 407, 3814-3822.

Beusen B., Broekx S., Denys T., **Beckx C.**, Degraeuwe B., Gijsbers M., Scheepers K., Govaerts L., Torfs R., Int Panis L. (2009). Using on-board logging devices to study the long-term impact of an eco-driving course. Transportation Research Part D: Transport and Environment, 14, 514-520.

Beckx C., Int Panis L., Uljee I., Arentze T., Janssens D., Wets G. Disaggregation of nation-wide dynamic population exposure estimates in The Netherlands: applications of activity-based transport models. Atmospheric Environment, available from: http://dx.doi.org/10.1016/j.atmosenv.2009.07.035

Beckx C., Arentze T., Int Panis L., Janssens D. Vankerkom J., Wets G. An integrated activity-based modelling framework to assess vehicle emissions: approach and application. Environment and Planning B: Planning and Design. In press.

International publications without peer review (proceedings)

Int Panis L., Cosemans G., Torfs R., Liekens I., De Nocker L., Broekx S., **Beckx C.** (2005). Effect of a local traffic plan on exposure to local air pollution. In: Proceedings of the 14th Int Symp on Transport and Air Pollution, Graz, Austria, Vol. 85, n°2, pp. 13-21, ISBN: 3-902465-16-6.

Beckx C., Broekx S., Janssens D. (2005). Activity-based policies to reduce human exposure to traffic air pollution. In: Proceedings of the Colloquium Vervoersplanologisch Speurwerk, Antwerp, Belgium. pp 1955-1972.

Beckx C., Int Panis L., Wets G., Torfs R., Mensink C., Broekx S. and Janssens D. (2006). Impact of trip purpose on driving behaviour: case study on commuter behaviour in Belgium. In: Proceedings of the 15th International Symposium Transport and Air Pollution, Reims, France. Vol 107, n°2, pp. 332-337. ISBN: 2-85782-639-7.

Beckx, C., Arentze, T., Janssens, D. (2007). Travel behaviour and emission assessment in the Netherlands: a different approach. In: Proceedings of the Colloquium Vervoersplanologisch Speurwerk, Antwerp, Belgium.

Beckx C., Int Panis L., De Vlieger I., Wets G. (2007). Influence of gear changing behaviour on vehicular exhaust emissions. In: Highway and Urban Environment, Eds G.M. Morrison, S. Rauch (Springer, The Netherlands), pp. 45-51. ISBN: 978-1-40206009-0.

Beckx C., Int Panis L., Vanhulsel M., Wets G., Torfs R. (2007). Gender-linked disparity in vehicle exhaust emissions? Results from an activity-based survey. In: Highway and Urban Environment, Eds G.M. Morrison, S. Rauch (Springer, The Netherlands), pp. 63-70. ISBN: 978-1-40206009-0.

Beckx C., Int Panis L., Torfs R., Janssens D., Broekx S. (2007). The application of the simulation software VeTESS to evaluate the environmental impact of traffic measures. In: Proceedings of the 10th International Conference on Computers in Urban Planning and Urban Management, July 2007, Iguaçu, Brazil.

Beckx C., Int Panis L., Arentze T., Timmermans, H., Janssens D., Wets G. (2007). Applying an activity-based modelling framework to the evaluation of vehicle exhaust emissions. In: Proceedings of the 10th International Conference on Computers in Urban Planning and Urban Management, July 2007, Iguaçu, Brazil.

Int Panis L., **Beckx C.** and De Vlieger I. (2008). Where and when do electric vehicles have the largest environmental benefit? In: Proceedings of the EET-2008 European Ele-Drive Conference. 3rd European Ele-Drive Transportation Conference On the Way to Sustainable Development and Market Opening, March 2008, Geneva, Switzerland.

Beckx C., Arentze T., Int Panis L., Janssens D., Wets G. (2008). Assessing activity-related vehicle emissions through an integrated activity-based modelling framework. In: Proceedings of the iEMSs Fourth Biennial Meeting: International Congress on Environmental Modelling and Software (iEMSs 2008). International Environmental Modelling and Software Society, Barcelona, Catalonia, July 2008.

Beckx C., Int Panis L., Janssens D. and Wets G. (2009). Examining Gender-Linked Vehicle Emissions with GPS-Enabled Data Collection Tool. In: Proceedings of the Transportation Research Board 88th Annual Meeting, TRB 88th Annual Meeting Compendium of Papers DVD. Report n° 09-2460.

Beckx C., Arentze T., Timmermans H., Int Panis L., Janssens D. and Wets G. (2009). Application of an Activity-Based Model to Evaluate Dynamic Population Exposure to Air Pollution. In: Proceedings of the Transportation Research Board 88th Annual Meeting, TRB 88th Annual Meeting Compendium of Papers DVD. Report n° 09-2501.

PARTICIPATION AT INTERNATIONAL CONFERENCES

- Colloquium Vervoersplanologisch Speurwerk, Antwerp, Belgium, 24-25 November 2005

    Platform: Activity based policies to reduce human exposure to traffic air pollution.

- Colloquium International Association for Impact Assessement. Power, Poverty and Sustainability conference, Stavanger, Norway, 23-26 May 2006

  Platform: Do women drive sustainable mobility in the developed world? Results from an activity-based survey.

- 8th Highway and Urban Environment Symposium, Nicosia, Cyprus, 11-14 June 2006

  Platform: Gender-linked disparity in vehicle exhaust emissions? Results from an activity-based survey.

- 8th Highway and Urban Environment Symposium, Nicosia, Cyprus, 11-14 June 2006

  Platform: Influence of gear changing behaviour on fuel-use and vehicular exhaust emissions.

- 10th International Conference on Computers in Urban Planning and Urban Management, Iguaçu, Brazil, July 2007.

  Platform: The application of the simulation software VeTESS to evaluate the environmental impact of traffic measures.

- 10th International Conference on Computers in Urban Planning and Urban Management, Iguaçu, Brazil, July 2007.

  Platform: Applying an activity-based modelling framework to the evaluation of vehicle exhaust emissions.

- Colloquium Vervoersplanologisch Speurwerk, Antwerp, Belgium, 22-23 November 2007

  Platform: Travel behaviour and emission assessment in the Netherlands: a different approach.

- International Environmental Modelling and Software Society, Barcelona, Spain, July 2008

  Platform: Assessing activity-Related vehicle emissions through an integrated activity-based modelling framework.

- Joint Annual Conference of the International Society for Environmental Epidemiology and International Society for Exposure Analysis, Pasadena, USA, 12-16 October, 2008

  Platform: Establishing a dynamic exposure assessment with an activity-based modeling approach.

- Joint Annual Conference of the International Society for Environmental Epidemiology and International Society for Exposure Analysis, Pasadena, USA, 12-16 October, 2008

  Poster: Establishing a dynamic exposure assessment with an activity-based modeling approach.