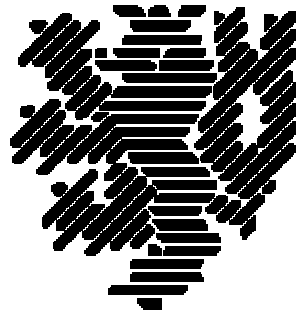


**The Impact of NMVOC Emissions from Traffic and
Solvent Use on Urban Air in Wuppertal –
An Experimental Study**



Thesis submitted to the Faculty of Mathematics and Natural Sciences
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Referee: Prof. Dr. K. H. Becker

Co-referee: Prof. Dr. P. Wiesen

Do kraju tego, gdzie winą jest duża
Popsować gniazdo na gruszy bocianie,
Bo wszystkim służą...

Cyprian Kamil Norwid

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Abstract

In Europe road traffic and solvent use are by far the most important emission sources of anthropogenic non-methane volatile organic compounds (NMVOC). However, the relative importance of these two source categories is still afflicted with a large uncertainty mainly due to the lack of measurements of larger hydrocarbons and oxygenated species. In order to clarify the contribution of solvent use to the total NMVOC emissions in Germany, the NMVOC composition of the city air of Wuppertal was investigated.

During three campaigns in September 2001, August/September 2002 and October 2003 NMVOC concentrations were measured at different locations in the city of Wuppertal. The measurements covered volatile hydrocarbons in the range of C₃-C₁₀ and oxygenated compounds such as alcohols, ketones and esters. Samples were collected using Carbotrap and Carbosieve SIII solid adsorption tubes and analysed off-line by thermal desorption and GC-FID analysis in the laboratory.

The data obtained from the measurements carried out in Wuppertal were analysed with respect to the composition of the NMVOC mixture, the ratio of individual compounds to benzene and the NMVOC/NO_x ratio. The average percental contributions of alkanes, alkenes and alkynes, aromatic hydrocarbons and oxygenated compounds for all measurement points in Wuppertal were 32, 16, 37 and 15%, respectively, which agrees with the results from other urban studies. Among the alkanes 2-methylpentane and i-pentane, among the alkenes and alkynes i-butene and 1-butene, among the aromatic hydrocarbons toluene followed by m- and p-xylene, and among the oxygenated compounds butyl acetate and acetone showed the largest abundance. For sites in dense traffic areas the NMVOC/NO_x ratio was found to be (0.56 ± 0.06) ppbC/ppbV. For the measurements performed at the various location in the city the NMVOC/NO_x ratios were quite variable with values ranging from 1.76 up to 7.93 ppbC/ppbV. These results agree well with the results from other studies in traffic and urban areas. The measured toluene/benzene ratio of (3.83 ± 0.22) ppbC/ppbC is significantly higher than the previously measured ratios at traffic sites. This finding can be explained by an over proportional decrease in the benzene emissions compared with other aromatic compounds since the year 2000, when the new European regulations on the benzene content in gasoline were implemented.

An assessment of the contribution from different emission sources to the observed NMVOC concentrations was attempted with the Chemical Mass Balance (CMB) modelling technique. Two emission source categories were investigated, namely road traffic and solvent use. The emission profiles required by the CMB model of both investigated sources were recalculated from the concentration profiles measured at sites representative either for traffic or for solvent use. Emission profiles for traffic were obtained from measurements performed in a

traffic tunnel, at a down-town street intersection and during drives through the city and on free-ways. Solvent emission profiles were investigated in the vicinity of different solvent factories and workshops in Wuppertal. For traffic, one average source profile from all measurements representing different driving conditions was derived, whereas for solvents four different emission profiles from special industrial source areas had to be used. The concentrations of more than 100 compounds were measured and used as input data for the CMB calculations. Apportionment analysis was performed for several receptor points located down-wind from the city centre, in residential areas, in dense traffic areas and in industrial areas.

The outcomes of the CMB analysis with the application of source profiles and receptor concentrations obtained from the city measurements showed that traffic emission rather than solvent use determines the ambient NMVOC composition. The contribution of traffic emission was dominant at all investigated points located down-wind from the city centre, with a relative contribution on average of about 90%. It has been shown that in dense traffic areas the traffic emission is still responsible for almost 100% of the NMVOC concentrations. A significant influence of solvent emissions could only be observed in close vicinity of solvent factories, where the impact of the investigated solvent sources amounted on average to about 45% of the measured NMVOC concentrations. The NMVOC concentrations calculated using the CMB model accounted on average for about 77% of the concentrations actually measured at the receptor points. The remaining part of the mass could not be explained with the investigated two emission sources.

The maximal contribution of solvent use to the NMVOC emission estimated on the basis of experimentally obtained results amounts to about 23% in the whole city area of Wuppertal. This value is an approximation, but it can be considered as an upper limit for the solvent use contribution to the total NMVOC emission. Accordingly, it can be concluded that the contribution of solvent use to the NMVOC concentrations in German cities falls in the range of a few to about 20%, provided that Wuppertal can be considered as a typical German urban area with certain proportions of domestic activities, traffic and various industries.

The results of the present study confirm the finding of two other experimental studies which were previously carried out in Berlin and Augsburg. The present work clearly shows that the experimentally observed proportions between traffic and solvent use emissions are in strong disagreement with the German Emission Inventory which states, that at present (reference year 2000) about 62% of the total NMVOC emissions originate from solvent use and only 18% from road traffic. Nevertheless more measurements and calculations are necessary in order to improve the emission profiles for solvent use and to include additional emission sources into the CMB apportion analysis. It is hoped that the outcome of the present work will also initiate further experimental studies aimed at improving the NMVOC emission inventories in Europe.

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Chapter 1

INTRODUCTION

1.1 State of knowledge

Since centuries the Earth's atmosphere is affected by emissions from human activities. Yearly, thousands of terra grams (Tg) from different anthropogenic sources are injected into the atmosphere as gaseous and particulate pollutants (Seinfeld and Pandis, 1998; Finlayson-Pitts and Pitts, 2000). Total emissions of gases such as carbon monoxide (CO), organic compounds calculated as organic carbon, sulphur dioxide (SO₂), nitrous oxide (N₂O), nitrogen oxides (NO_x) and others, range annually between 4000 and 5000 Tg, whereas man-made emissions differ significantly from compound to compound (Ehhalt, 1999; Prather *et al.*, 2001). Primary particles are emitted to the atmosphere with a strength of about 4000 Tg yearly (Georgii and Warneck, 1999; Penner *et al.*, 2001).

All substances emitted to the atmosphere undergo chemical transformations and removal processes which influence the atmospheric environment. Climate change (Houghton *et al.*, 2001), stratospheric ozone depletion (Crutzen, 1971; Molina and Rowland, 1974), changing of oxidation capacity (Thompson, 1992), long range transport of chemicals (Bidleman, 1988; Derwent and Jenkin, 1991), secondary air pollution (Logan, 1985; Crutzen, 1995; Odum *et al.*, 1996; Jenkin and Clemitshaw, 2000) and acidification of the environment (Brimblecombe, 1992) are the typical examples of long-range and long-term effects of air pollution.

1.1.1 NMVOC in the atmosphere

Among the species emitted to the atmosphere, the group of non-methane volatile organic compounds (NMVOCs) plays a very important role in affecting air quality, human health, plants and materials. Typical total NMVOC concentrations range in heavy polluted urban

areas from 500 to 1500 $\mu\text{g}/\text{m}^3$, in suburban areas from 100 to 250 $\mu\text{g}/\text{m}^3$ and from 30 to 200 $\mu\text{g}/\text{m}^3$ in forest, rural and remote areas (Ciccioli *et al.*, 1999).

The interest in NMVOC emissions has grown because they are the precursors for the photochemical production of ground-level ozone in the presence of NO_x . The first episodes of photochemical smog in Los Angeles during the late 1940s (Haagen-Smit, 1952) demonstrated the impact of reactive organic substances in the atmosphere. It is known, that volatile organic compounds together with nitrogen oxides (NO_x : $\text{NO} + \text{NO}_2$) under the influence of sunlight undergo a series of photochemical reactions leading to formation of secondary pollutants with ozone (O_3) as a main product, peroxyacetyl nitrate (PAN), hydrogen peroxide, organic peroxides, organic acids and many others oxidising species (LeBras (ed.), 1997; Wayne, 2000). The driving reagents for these processes are hydroxyl radicals (OH) during the day and nitrate radicals (NO_3) at night (Wayne *et al.*, 1991). OH and NO_3 can oxidise hydrocarbons in the troposphere producing species like peroxy radicals (RO_2) and hydroperoxy radicals (HO_2) that convert NO into NO_2 . Photolysis of NO_2 occurring at wavelengths <420 nm generates O_3 which can accumulate in the atmosphere.

Once emitted to the atmosphere VOCs can not only undergo chemical reactions with hydroxyl radicals (OH) and nitrate radicals (NO_3), as already mentioned, but also with ozone (O_3) and ground state oxygen atoms ($\text{O}(^3\text{P})$) (Atkinson, 1997; 2000; Calvert *et al.*, 2000; Calvert *et al.*, 2002; Atkinson and Arley, 2003). Some oxygenated volatile organic compounds such as aldehydes and ketones can also be photolysed at wavelengths <340 nm. VOCs can additionally react with Cl atoms, but these reactions are relevant only in marine areas (Jobson *et al.*, 1994). The detailed channels and reaction mechanisms depend on the structure of the individual organic compounds, whereby the reaction with OH is always important and is the dominant atmospheric loss process. Due to this, various classes of VOC and even different substances contribute with different weight to the photochemical air pollution. Detailed reviews of mechanisms and rate constants of atmospheric reactions of particular groups of compounds can be found in Atkinson (1997; 2000), Calvert *et al.* (2000), Wayne (2000), Calvert *et al.* (2002) and Atkinson and Arley (2003) and references therein.

Besides tropospheric ozone formation, VOCs contribute also to the formation of secondary organic aerosols (SOA). This process involves again oxidation of the volatile precursors by OH , O_3 and NO_3 to form semi-volatile products and eventually particles (Odum *et al.*, 1996; Seinfeld and Pandis, 1998; Dusek, 2000). The organic aerosols formed by gas-phase photochemical reactions of hydrocarbons have been identified in both urban and rural atmosphere and their contribution to the total organic aerosols can be as much as 70-80% during smog episodes (Turpin *et al.*, 1991; Turpin and Huntzicker, 1995; Castro *et al.*, 1999; Shell *et al.*, 2001; Lim and Turpin, 2002; Derwent *et al.*, 2003; Na *et al.*, 2004).

In addition to their activity in photochemical air pollution processes, some VOCs are also found to have a direct harmful influence on human health. Compounds like benzene, 1,3-butadiene, styrene, formaldehyde, acetaldehyde and polycyclic aromatic hydrocarbons (PAHs)

are toxic. Their effects, especially in indoor air, include eye, nose and throat irritation and central nervous system responses such as dizziness, headaches and loss of short-term memory. Long-term exposure may cause serious diseases, mutations and cancer (Wallace, 1993).

Due to the complexity of tropospheric formation of photo-oxidants and secondary organic aerosols the detailed knowledge about the degradation pathways of individual VOC compounds and about the atmospheric concentrations and emissions of particular precursors is of paramount importance in order to be able to develop effective abatement strategies.

In Europe the emissions of ozone precursors, including NMVOC, decreased between 1990-2000 by about 30% (EEA, 2003a) In spite of this, the ozone concentrations in the lower atmosphere still continue to exceed the target values set by European Union legislation (Directive 92/72/EEC; Directive 2002/3/EC) to protect human health and prevent damage to vegetation. Particularly, the very hot summer of 2003, when the measured ozone concentrations exceeded in some places the one-hour ozone concentration of $360 \mu\text{g}/\text{m}^3$, which is the threshold value for warning the population (EEA, 2003b), showed that the problems of ground level ozone formation, photochemical air pollution and NMVOC emissions, are still very actual in Europe. However, the high ozone values of over $600 \mu\text{g}/\text{m}^3$, observed in 1976 in Germany, have not been observed during recent years (Becker *et al.*, 1985). Recalculated historical ozone measurements from 1870s and 1880s in Paris seem to indicate that ozone levels have more than doubled in central Europe since the 19th century (Volz and Kley, 1988).

1.1.2 Emission sources of NMVOC

NMVOCs are emitted to the atmosphere from both natural and anthropogenic sources. The annual global NMVOC flux is estimated at about 1500 Tg (Gunther *et al.*, 1995; Middleton, 1995; Ehhalt, 1999). The biogenic contribution to the NMVOC emission is difficult to evaluate because of the great variability of plant types, complexity of the emission processes and the strong dependence on meteorological conditions, landcover and geographical regions (Steinbrecher and Smiatek, 2004). Nevertheless, the total global biogenic NMVOC emission has been estimated to be about 1300 Tg per year (Gunther *et al.*, 1995; Fall, 1999) and exceeds by far those of anthropogenic sources. Human activity is responsible for about 10% of the total NMVOC emission on a global scale and is estimated at about 150 Tg per year (Piccot *et al.*, 1992; Middleton, 1995). The NMVOC emissions on a global scale, in the USA, Europe and Germany and the proportions between anthropogenic and biogenic sources are summarised in table 1.1.

Table 1.1: Approximate emissions of NMVOCs in kt/year from anthropogenic and natural sources

scale	basis	natural		anthropogenic		total
		kt	%	kt	%	kt
global ^{a,b,c}	-	1300*10 ³	90	150*10 ³	10	1450*10 ³
USA ^d	1997	28190	60	18880	40	48000
Europe ^{e,f}	1996	13000	47	14644	53	27700
Germany ^{g,h}	1998	658	27	1735	73	2400

^a Gunther *et al.*, 1995; ^b Middelton, 1995; ^c Ehhalt, 1999; ^d EPA, 2000; ^e Simpson *et al.*, 1999; ^f EEA, 2003c; ^g Schnitzler *et al.*, 2002; ^h UBA, 2002

As observed in table 1.1, on the different scales, the proportions between natural and man-made emission vary significantly. In the USA the contribution of anthropogenic emissions amounts to about 40%, in Europe to more than 50% and in Germany to more than 70%.

An overview of the anthropogenic NMVOC emission sources in Europe is presented in table 1.2.

Table 1.2: Emissions of NMVOCs in kt/year as a total from 31 European countries (EEA31¹) over the time period from 1990 to 2001 for the major source categories (SNAP97 level 1²) according to European Environmental Agency (EEA, 2003c; EEA, 2004)

categories	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001
combustion in energy and transformation industries	90	91	91	85	91	91	95	92	91	95	109	96
non-industrial combustion plants	1272	1289	1215	1203	1147	1132	1181	1133	1091	1070	1008	1028
combustion in manufacturing industry	241	235	220	198	210	179	184	175	174	167	170	200
production processes	1599	1543	1499	1416	1353	1366	1406	1452	1479	1358	1302	1235
extracting and distributing of fossil fuels and geothermal energy	1496	1432	1427	1365	1399	1385	1345	1351	1280	1218	1209	1222
solvent and other product use	4846	4542	4350	4201	4131	4074	4014	4001	3995	3958	4020	3983
road transport	6891	6473	6344	6051	5753	5470	5201	4855	4573	4219	3600	3423
other mobile sources and machinery	793	764	745	708	726	703	701	711	724	714	696	677
waste treatment and disposal	181	190	180	181	178	170	171	170	168	169	166	167
agriculture	833	808	749	702	762	768	707	704	683	692	652	673
total	18241	17367	16819	16111	15750	15338	15005	14644	14259	13659	12933	12702

¹EEA31 - 31 European Environmental Agency member countries: Austria, Belgium, Denmark, Finland, France, Germany, Greece, Ireland, Italy, Luxembourg, Netherlands, Portugal, Spain, Sweden, United Kingdom, Czech Republic, Cyprus, Estonia, Hungary, Latvia, Lithuania, Malta, Poland, Slovenia, Slovak Republic, Bulgaria, Romania, Turkey, Iceland, Liechtenstein, Norway

²SNAP97 - Selected Nomenclature for Air Pollution; the hierarchical structure (3 levels - degrees of detail) of emission sources according to CORINAIR nomenclature (EEA, 2003c)

The number of processes from which the anthropogenic NMVOCs are emitted is very large, covering not only many branches of industry, but also transport, agriculture and domestic sources. In general the NMVOCs are emitted from combustion processes, production, treatment, storage and distribution of fossil fuels, application of volatile organic solvents and solvent containing products, industrial production processes and biological processes (Friedrich and Obermeier, 1999).

The total NMVOC emission and the proportions between particular source categories obviously differ from country to country. However, as observed in table 1.2, with respect to the European scale, road traffic and solvent use are by far the most important sources of anthropogenic NMVOC emissions. Particularly in Germany, the dominance of these two source categories can clearly be recognised in the emission inventories (figure 1.1). According to the German Environmental Agency emission inventory a significant reduction in NMVOC emission, from 3221 kt in 1990 to about 1600 kt in 2001, which is more than 50%, occurred. From the inventory it also follows that the relative importance of NMVOC emissions from solvent use has significantly increased in comparison to traffic sources over time (figure 1.1). Since 1992 more than 50% of anthropogenic NMVOC emissions in Germany have been attributed to sources related to solvents, with an increasing trend.

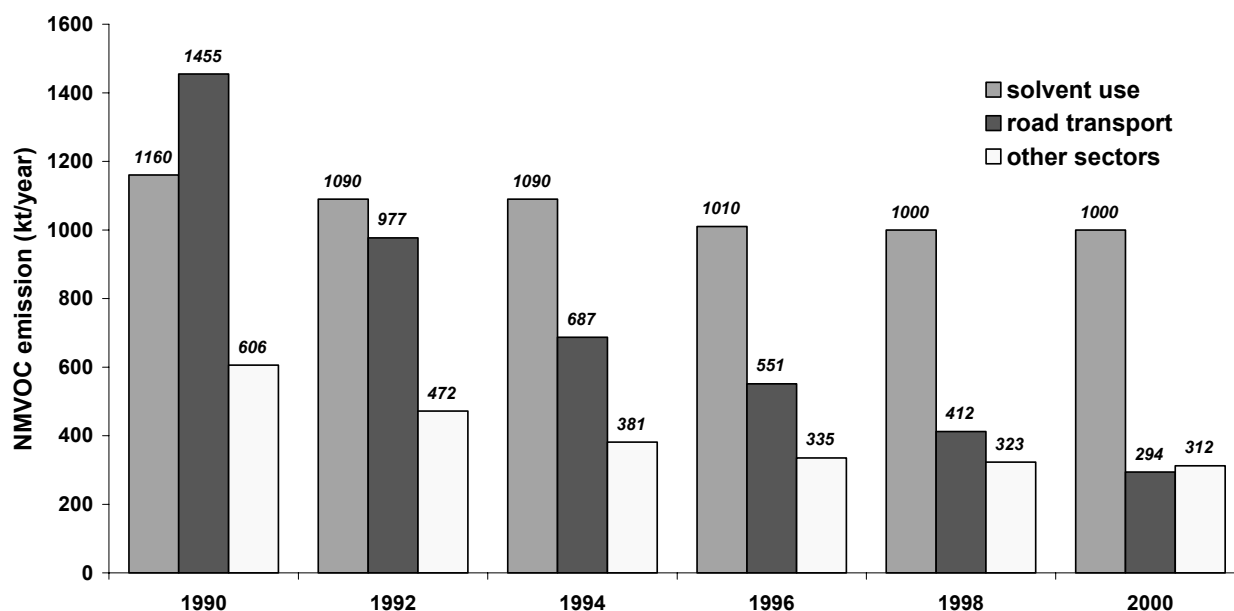


Figure 1.1: Annual emission of NMVOCs in kt in Germany during the time period from 1990 to 2000 for the major source categories according to the Federal Environmental Agency (UBA, 2002; UBA, 2003)

Motor vehicle emissions result not only from tailpipe exhaust but also from evaporation of fuel from various locations in the fuel tank-engine system, and the total emissions depend critically on the fuel type, operation mode, technical condition of the vehicle and the ambient temperature. Nevertheless, the road traffic emission is quite reasonably well established due to many dynamometer tests (Hassel *et al.*, 1994; Duffy *et al.*, 1999; Schmitz *et al.*, 2000; Heeb *et al.*, 2002; Zervas *et al.*, 2002; Mittermeier *et al.*, 2004), tunnel studies (Lonneman *et al.*, 1986; Pierson *et al.*, 1990; Zielinska *et al.*, 1996; Rogak *et al.*, 1998; Staehelin *et al.*, 1998; Kean *et al.*, 2001; Schmid *et al.*, 2001; Sturm *et al.*, 2001; Kurtenbach *et al.*, 2002; McGaughey *et al.*, 2004; Kristensson *et al.*, 2004; Stemmler *et al.*, 2005), roadside measurements (Doskey *et al.*, 1992; Conner *et al.*, 1995; Derwent *et al.*, 1995; Pierson *et al.*, 1996; Schmitz *et al.*, 1997; Thijsse *et al.*, 1999; Ho *et al.*, 2002) and model calculations (Kühlwein and Friedrich, 2000; Mensink *et al.*, 2000; Ntziachristos and Samaras, 2000; Friedrich *et al.*, 2002; Lewyckyj *et al.*, 2004). The about 50% estimated reduction in NMVOC emission from road transport in Europe over the last 15 years (EEA, 2004; Stemmler *et al.*, 2005) is mainly due to the regulation on exhaust gas composition, the introduction of catalysts on new cars and an increased use of diesel vehicles.

In the case of solvent use, the estimation of the emission strength is much more difficult than for road traffic. NMVOCs attributed to solvent use originate from many different sources, processes and activities and their emission is very dispersed and mostly uncontrolled. Moreover, they are also difficult to measure because, besides aliphatic and aromatic hydrocarbons, they contain many oxygenated species, which are more difficult to analyse (McInnes, 1996; Theloke *et al.*, 2001; Ullmann's Encyclopedia, 2001). Hence, relatively few measurements quantifying emissions due to solvent use are available and those which are available are normally limited to the aliphatic and aromatic hydrocarbons and the simple aldehydes and ketones (Thijsse *et al.*, 1999; Vega *et al.*, 2000; Choi and Ehrman, 2004).

Consequently, the solvent emissions reported in the inventories are estimated only on the basis of calculations using the production and consumption of solvents. Such estimations include surrogate indicators such as quantification of solvent use or solvent containing products, amount of manufactured goods, areas covered with solvent based coatings or even emissions calculated per capita in the case of domestic solvent use (Censullo *et al.*, 1996; Wickert *et al.*, 1999; Brandt *et al.*, 2000; Censullo *et al.*, 2000; Jenkin *et al.*, 2000; Klimont *et al.*, 2000; Placet *et al.*, 2000; Passant, 2002; EPA, 2004). In particular, calculation models differ from country to country. In Germany, the model of the Federal Environmental Agency was further developed by Theloke (Theloke *et al.*, 2000; 2001; Friedrich *et al.*, 2002; Theloke, 2004; Theloke and Friedrich, 2004). The calculations are based on statistical data on the inland production of solvent containing goods and their import and export. The emission factors are calculated by considering applications, control techniques and dispersion to other compartments (water and soil).

According to the latest calculations (Theloke, 2004), the German NMVOC emissions from solvent use in 2000 amounted to about 700 kt. Important sources of solvent use emission include paint applications, degreasing processes, domestic solvent use, printing processes, application of glues and additives and preservation of wood. The percentage contribution for particular solvent sectors are presented by figure 1.2.

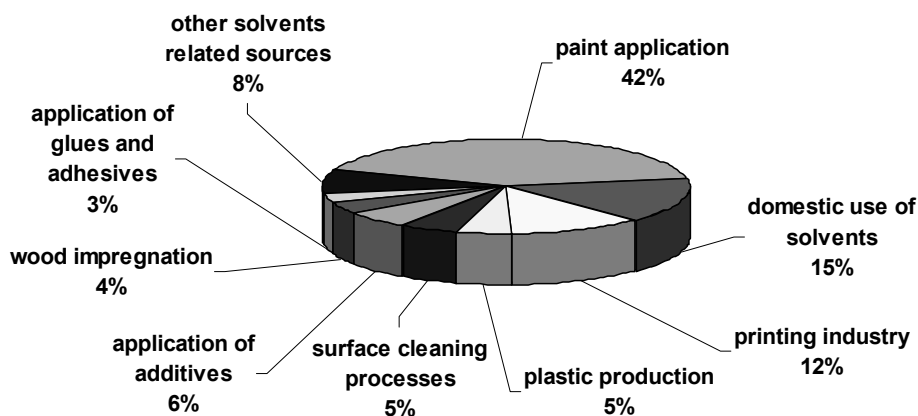


Figure 1.2: NMVOC emissions from solvent use in Germany in 2000 divided to main application groups (Theloke, 2004)

Data of ambient concentration measurements from different German cities always show that road traffic is still the dominant source of shorter (C_2 - C_{10}) hydrocarbons (Thijssse *et al.*, 1999; Mannschreck, 2000; Gomes, 2002; Kurtenbach *et al.*, 2002; Slemr *et al.*, 2002; Winkler *et al.*, 2002). These experimental observations disagree with the German emission inventory in which solvent use is the major source of NMVOC with a contribution of more than 60% to the total NMVOC emissions (UBA, 2003; Theloke *et al.*, 2001). This discrepancy between data from the emission inventories and the measurements has also been established by the results from the EVA (Evaluation of Highly Resolved Emission Inventories) experiment performed in the city of Augsburg (Mannschreck, 2000; Slemr *et al.*, 2002; Mannschreck *et al.*, 2005). The emission from solvent use calculated for Augsburg from the consumption of solvent containing products with a contribution of about 64% to the total NMVOC emission (Kühlwein *et al.*, 2002) could not be seen in the measurements. Particularly, large differences between measured and calculated values were found for some individual NMVOC species which are characteristic for solvent use. The solvent use contribution to the total NMVOC emission calculated from the experimental EVA data amounted at the most to about 10% (Mannschreck, 2000).

These disagreements may suggest that the officially accepted emission data from solvent use are currently overestimated or many components have not been covered by the ambient measurements. It should be stated that emission inventories in some other European countries show lower contribution from the solvent use sector. In the UK, for example, the estimated solvent use emissions amount only to about 32% of the total national NMVOC emissions and the contribution of road traffic to 22% (Dore *et al.*, 2001). The differences between the contributions of solvent use in Germany and the UK are presented in figure 1.3.

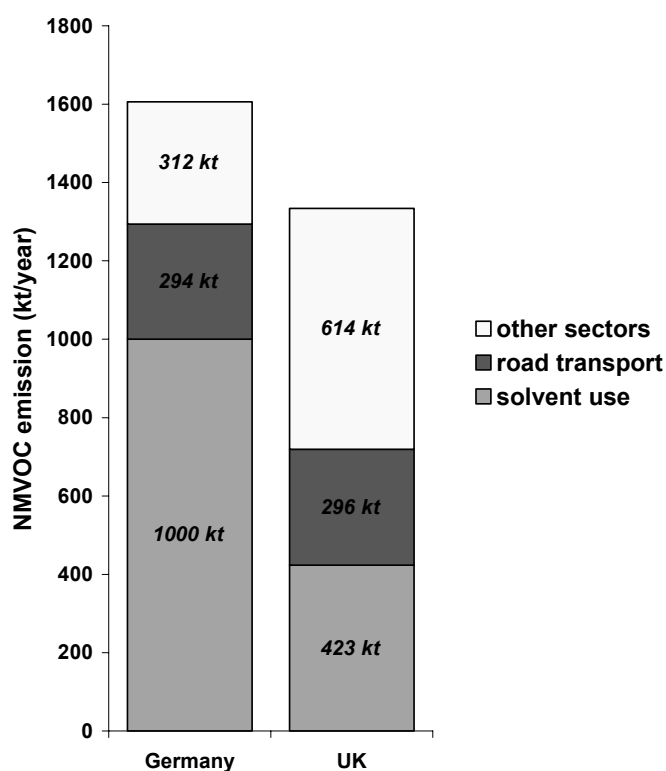


Figure 1.3: Annual emission of NMVOCs in kt in Germany and the United Kingdom in 2000 (UBA, 2002; Dore *et al.*, 2003)

The relative importance of two main NMVOC source categories, road traffic and solvent use, is still afflicted with a large uncertainty mainly due to the lack of measurements of larger hydrocarbons and oxygenated species.

1.2 Aim of the work

In order to clarify the contribution of solvent use to the total NMVOC emissions, an investigation on the composition of the city air of Wuppertal has been undertaken. In this work atmospheric concentrations of a large number of NMVOC compounds emitted by different anthropogenic sources including aliphatic and aromatic hydrocarbons and oxygenated species like alcohols, esters and ketones have been analysed.

The aim was to detect and quantify the contribution from solvent use in comparison to the emission from traffic in the city air of Wuppertal. A successive task was to create typical, real world NMVOC source profiles of road traffic and solvent use and through the implementation of a chemical mass balance source apportionment technique (CMB) to calculate the contributions from this two source types to the measured total ambient NMVOC concentration.

For the road traffic NMVOC emission profiles, measurements were planned in areas representative for major traffic conditions. In the case of solvent use emissions, measurements near various solvents factories and workshops in Wuppertal were considered.

Chapter 2

EXPERIMENTAL PART

2.1 Investigated compounds

In this work the troposphere abundance of a large number of non-methane volatile organic compounds (NMVOCs) emitted by different anthropogenic sources, in particular from traffic exhaust and solvent use, have been investigated.

Whereas NMVOC emissions from combustion processes contain predominantly hydrocarbons (alkanes, alkenes and aromatics), organic solvents and their vapours show also large contributions of oxygenated compounds such as alcohols, ketones, esters, glycol derivatives, ethers and halogenated hydrocarbons, as observed in figure 2.1 (Friedrich and Obermeier, 1999; Ullmann's Encyclopedia, 2001). According to this, additionally to the number of hydrocarbons (table 2.1) oxygenated species were included into the group of investigated compounds.

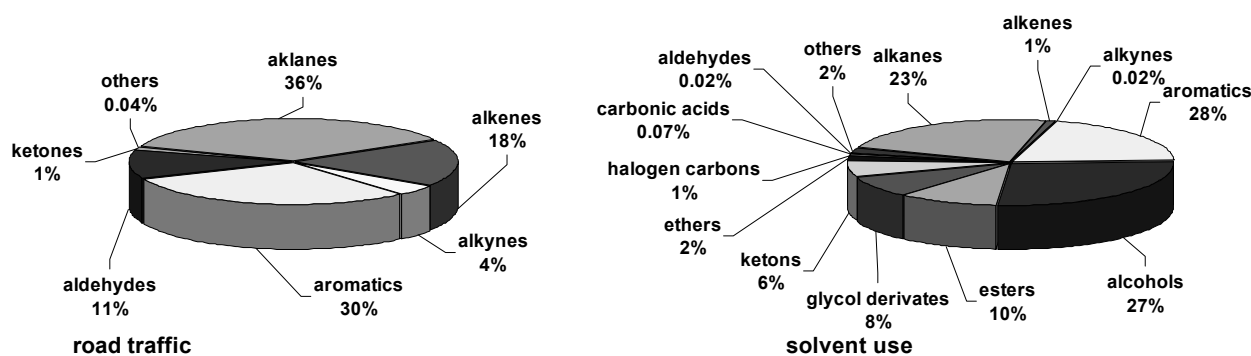


Figure 2.1: NMVOC split (wt%) for road traffic and solvent use in Germany (Friedrich, 2003)

The source category of solvent use is characterised not only by a large variety of solvent-containing products but also by a broad field of applications in industrial production as well as in commercial and private use (Ullmann's Encyclopedia, 2001). Among a large number of oxygenated species contained in solvents and solvent related products, the most common oxygenated compounds were assigned for the investigation. The choice is based on the known composition of products used in water-based architectural coatings, consumer products, paint applications, printing industry, dry cleaning (McInnes, 1996; Friedrich and Obermeier, 1999; Ullmann's Encyclopedia, 2001; Passant, 2002; EMEP/Corinair, 2003) and automotive performance coatings (DuPont, 2001). The most abundant compounds were evaluated with respect to their analytical monitoring.

The list of oxygenated compounds was completed by methyl *tert*-butyl ether, which is a typical species added to gasoline as an octane enhancer and in order to reduce emissions when gasoline is burned in the engine (European Fuel Oxygenated Association, 2003). Finally, 18 oxygenated species were selected for investigation (table 2.2).

Table 2.1.a: Characteristic properties of investigated hydrocarbons

hydrocarbons	formula	molecular weight (g/mol)	boiling point (°C)	melting point (°C)	k_{OH} ($\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$)
<i>Alkanes (24):</i>					
<i>ethane</i>	C_2H_6	30.07	-88.60	-183.30	$0.25 \cdot 10^{-12}$ (a)
<i>propane</i>	C_3H_8	44.10	-42.10	-187.70	$1.09 \cdot 10^{-12}$ (a)
<i>n-butane</i>	C_4H_{10}	58.12	-0.50	-138.40	$2.36 \cdot 10^{-12}$ (a)
<i>2-methylpropane (i-butane)</i>	C_4H_{10}	58.12	-11.70	-	$2.12 \cdot 10^{-12}$ (a)
<i>n-pentane</i>	C_5H_{12}	72.15	36.10	-129.70	$3.80 \cdot 10^{-12}$ (a)
<i>2-methylbutane (i-pentane)</i>	C_5H_{12}	72.15	30.00	-159.90	$3.60 \cdot 10^{-12}$ (a)
<i>2,2-dimethylbutane</i>	C_6H_{14}	86.18	49.70	-100.00	$2.23 \cdot 10^{-12}$ (a)
<i>2,3-dimethylbutane</i>	C_6H_{14}	86.18	58.00	-128.50	$5.78 \cdot 10^{-12}$ (a)
<i>cyclopentane</i>	C_5H_{10}	70.13	49.00	-94.00	$4.97 \cdot 10^{-12}$ (a)
<i>2-methylpentane</i>	C_6H_{14}	86.18	62.00	-154.00	$5.20 \cdot 10^{-12}$ (a)
<i>3-methylpentane</i>	C_6H_{14}	86.18	64.00	-118.00	$5.20 \cdot 10^{-12}$ (a)
<i>hexane</i>	C_6H_{14}	86.18	69.00	-95.00	$5.20 \cdot 10^{-12}$ (a)
<i>methylcyclopentane</i>	C_6H_{12}	84.16	71.80	-142.40	$6.80 \cdot 10^{-12}$ (c)
<i>cyclohexane</i>	C_6H_{12}	84.16	80.70	6.60	$6.67 \cdot 10^{-12}$ (a)
<i>2,3-dimethylpentane</i>	C_7H_{14}	100.20	90.00	-	$6.10 \cdot 10^{-12}$ (c)
<i>2-methylhexane</i>	C_7H_{14}	100.20	90.00	-188.00	$5.10 \cdot 10^{-12}$ (c)
<i>2,2,4-trimethylpentane</i>	C_8H_{18}	114.23	99.20	-107.00	$3.34 \cdot 10^{-12}$ (a)
<i>n-heptane</i>	C_7H_{16}	100.20	98.40	-90.60	$6.76 \cdot 10^{-12}$ (a)
<i>2,3,4-trimethylpentane</i>	C_8H_{18}	114.23	113.00	-109.00	$6.60 \cdot 10^{-12}$ (a)
<i>2-methylheptane</i>	C_8H_{18}	114.23	118.00	-109.00	$8.28 \cdot 10^{-12}$ (b)
<i>3-methylheptane</i>	C_8H_{18}	114.23	119.00	-121.00	$8.56 \cdot 10^{-12}$ (b)
<i>4-methylheptane</i>	C_8H_{18}	114.23	118.00	-121.00	$8.56 \cdot 10^{-12}$ (b)
<i>n-octane</i>	C_8H_{18}	114.23	126.00	-56.80	$8.11 \cdot 10^{-12}$ (a)
<i>n-decane</i>	$\text{C}_{10}\text{H}_{22}$	142.28	174.10	-29.70	$11.00 \cdot 10^{-12}$ (a)

^a Atkinson and Arley, 2003; ^b Kwok and Atkinson, 1995; ^c DeMore *et al.*, 1997; ^d Boodaghinas *et al.*, 1987; ^e Grosjean and Williams, 1992

Table 2.1.b: Characteristic properties of investigated hydrocarbons

hydrocarbons	formula	molecular weight (g/mol)	boiling point (°C)	melting point (°C)	k_{OH} ($cm^3 \text{ molecule}^{-1} s^{-1}$)
<i>Alkenes, Alkynes (30):</i>					
<i>ethene</i>	C ₂ H ₄	28.05	-103.70	-169.14	8.52*10 ⁻¹² (a)
<i>ethyne</i>	C ₂ H ₂	26.04	-28.10	-80.75	0.83*10 ⁻¹² (c)
<i>propene</i>	C ₃ H ₆	42.08	-47.40	-185.24	26.30*10 ⁻¹² (a)
<i>propadiene</i>	C ₃ H ₄	40.07	-34.50	-	9.82*10 ⁻¹² (a)
<i>propyne</i>	C ₃ H ₄	40.07	-23.00	-103.00	2.92*10 ⁻¹² (d)
<i>1-butene</i>	C ₄ H ₈	56.11	-6.10	-185.30	31.40*10 ⁻¹² (a)
<i>2-methylpropene (i-butene)</i>	C ₄ H ₈	56.11	-6.90	-140.30	51.40*10 ⁻¹² (a)
<i>1,3-butadiene</i>	C ₄ H ₆	54.09	-4.40	-108.90	66.60*10 ⁻¹² (a)
<i>trans-2-butene</i>	C ₄ H ₈	56.11	0.88	-	64.00*10 ⁻¹² (a)
<i>1-butyne</i>	C ₄ H ₆	54.09	8.00	-125.70	7.27*10 ⁻¹² (d)
<i>cis-2-butene</i>	C ₄ H ₈	56.11	3.70	-	56.40*10 ⁻¹² (a)
<i>3-methyl-1-butene</i>	C ₅ H ₁₀	70.13	20.00	-168.00	31.80*10 ⁻¹² (a)
<i>1-pentene</i>	C ₅ H ₁₀	70.13	30.00	-165.00	31.40*10 ⁻¹² (a)
<i>2-methyl-1,3-butadiene (isoprene)</i>	C ₅ H ₈	68.12	34.00	-120.00	100.00*10 ⁻¹² (a)
<i>trans-2-pentene</i>	C ₅ H ₁₀	70.13	37.00	-140.00	67.00*10 ⁻¹² (a)
<i>cis-2-pentene</i>	C ₅ H ₁₀	70.13	37.00	-151.00	65.00*10 ⁻¹² (a)
<i>2-methyl-2-butene</i>	C ₅ H ₁₀	70.13	39.00	-134.00	86.90*10 ⁻¹² (a)
<i>cyclopentene</i>	C ₅ H ₈	68.12	44.00	-135.00	67.00*10 ⁻¹² (a)
<i>1-hexene</i>	C ₆ H ₁₀	82.15	63.00	-139.80	37.00*10 ⁻¹² (a)
<i>2-ethyl-1-butene</i>	C ₆ H ₁₂	84.16	65.00	-132.00	56.00*10 ⁻¹² (e)
<i>2,3-dimethyl-1,3- butadiene</i>	C ₆ H ₁₀	82.15	69.00	-76.00	122.00*10 ⁻¹² (a)
<i>1-methyl-1- cyclopentene</i>	C ₆ H ₁₀	82.15	72.00	-	-
<i>2,3-dimethyl-2-butene</i>	C ₆ H ₁₀	82.15	73.00	-74.00	110.00*10 ⁻¹² (a)
<i>1,3-cyclohexadiene</i>	C ₆ H ₈	80.13	80.00	-98.00	164.00*10 ⁻¹² (a)
<i>cyclohexene</i>	C ₆ H ₁₀	82.15	83.00	-104.00	67.70*10 ⁻¹² (a)
<i>1-heptene</i>	C ₇ H ₁₄	98.19	93.30	-119.00	40.00*10 ⁻¹² (a)
<i>1,4-cyclohexadiene</i>	C ₆ H ₈	80.13	82.00	-49.20	99.50*10 ⁻¹² (a)
<i>1-methyl-cyclohexene</i>	C ₇ H ₁₂	96.17	110.00	-120.00	94.00*10 ⁻¹² (a)
<i>1-octene</i>	C ₈ H ₁₆	112.21	121.00	-101.70	38.00*10 ⁻¹² (e)
<i>α-pinene</i>	C ₁₀ H ₁₆	136.24	155.00	-64.00	52.30*10 ⁻¹² (a)
<i>Aromatics (14):</i>					
<i>benzene</i>	C ₆ H ₆	78.11	80.10	5.50	1.22*10 ⁻¹² (a)
<i>toluene</i>	C ₇ H ₈	92.14	110.60	3.14	5.63*10 ⁻¹² (a)
<i>ethylbenzene</i>	C ₈ H ₁₀	106.17	136.20	-94.90	7.00*10 ⁻¹² (a)
<i>p-xylene</i>	C ₈ H ₁₀	106.17	138.80	13.30	14.30*10 ⁻¹² (a)
<i>m-xylene</i>	C ₈ H ₁₀	106.17	139.10	-47.87	23.10*10 ⁻¹² (a)
<i>o-xylene</i>	C ₈ H ₁₀	106.17	144.00	-25.20	13.60*10 ⁻¹² (a)
<i>styrene</i>	C ₈ H ₈	104.15	145.20	-101.60	58.00*10 ⁻¹² (a)
<i>n-propylbenzene</i>	C ₉ H ₁₂	120.19	159.00	-100.0	5.80*10 ⁻¹² (a)
<i>4-ethyltoluene</i>	C ₉ H ₁₂	120.19	162.00	-62.00	11.80*10 ⁻¹² (a)
<i>1,3,5-trimethylbenzene</i>	C ₉ H ₁₂	120.19	165.00	-44.70	56.70*10 ⁻¹² (a)
<i>1,2,4-trimethylbenzene</i>	C ₉ H ₁₂	120.19	169.00	-43.80	32.50*10 ⁻¹² (a)
<i>tert-butylbenzene</i>	C ₁₀ H ₁₄	134.22	169.00	-58.00	4.50*10 ⁻¹² (a)
<i>1,2,3-trimethylbenzene</i>	C ₉ H ₁₂	120.19	175.00	-25.00	32.70*10 ⁻¹² (a)
<i>1,2,3,4- tetramethylbenzene</i>	C ₁₀ H ₁₄	134.22	205.00	-6.00	-

^a Atkinson and Arley, 2003; ^b Kwok and Atkinson, 1995; ^c DeMore *et al.*, 1997; ^d Boodaghinas *et al.*, 1987; ^e Grosjean and Williams, 1992

Table 2.2: Characteristic properties of investigated oxygenated compounds

oxygenated compounds	formula	molecular weight (g/mol)	boiling point (°C)	melting point (°C)	k_{OH} (cm ³ molecule ⁻¹ s ⁻¹)
<i>Alcohols:</i>					
<i>methanol</i>	CH ₄ O	32.04	64.60	-98.00	9.40*10 ⁻¹³ (a)
<i>ethanol</i>	C ₂ H ₆ O	46.07	78.30	-114.10	3.20*10 ⁻¹² (a)
<i>2-propanol</i>	C ₃ H ₈ O	60.10	82.40	-88.50	5.17*10 ⁻¹² (b)
<i>1-propanol</i>	C ₃ H ₈ O	60.10	97.20	-126.00	5.83*10 ⁻¹² (b)
<i>2-butanol</i>	C ₄ H ₁₀ O	74.12	99.50	-115.00	9.20*10 ⁻¹² (c)
<i>1-butanol</i>	C ₄ H ₁₀ O	74.12	117.70	-89.50	8.47*10 ⁻¹² (b)
<i>Ketones:</i>					
<i>acetone</i>	C ₃ H ₆ O	58.08	56.20	-94.30	1.70*10 ⁻¹³ (a)
<i>2-butanone</i>	C ₄ H ₈ O	72.11	79.60	-86.30	1.22*10 ⁻¹² (h)
<i>4-methyl-2-pentanone (hexanone)</i>	C ₆ H ₁₂ O	100.16	117.40	-80.00	13.00*10 ⁻¹² (a)
<i>2-hexanone</i>	C ₆ H ₁₂ O	100.16	127.00	-57.00	9.10*10 ⁻¹² (a)
<i>cyclohexanone</i>	C ₆ H ₁₀ O	98.14	155.60	-47.00	6.40*10 ⁻¹² (a)
<i>Esters:</i>					
<i>methyl acetate</i>	C ₃ H ₆ O ₂	74.08	56.90	-98.00	8.50*10 ⁻¹³ (d)
<i>ethyl acetate</i>	C ₄ H ₈ O ₂	88.11	77.10	-83.60	1.70*10 ⁻¹³ (e)
<i>isopropyl acetate</i>	C ₅ H ₁₀ O ₂	102.13	90.00	-73.40	3.77*10 ⁻¹² (f)
<i>propyl acetate</i>	C ₅ H ₁₀ O ₂	102.13	102.00	-96.00	3.56*10 ⁻¹² (e)
<i>isobutyl acetate</i>	C ₆ H ₁₂ O ₂	116.16	118.00	-99.00	6.33*10 ⁻¹² (f)
<i>butyl acetate</i>	C ₆ H ₁₂ O ₂	116.16	126.10	-106.20	2.20*10 ⁻¹² (g)
<i>methyl tert-butyl ether</i>	C ₅ H ₁₂ O	88.15	55.20	-109.00	2.94*10 ⁻¹² (a)

^a Atkinson and Arley, 2003; ^b Yujing and Mellouki, 2001; ^c Chew and Atkinson, 1996; ^d Le Calve *et al.*, 1997a; ^e Picquet *et al.*, 1998; ^f Le Calve *et al.*, 1997b; ^g Veillerot *et al.*, 1996; ^h Le Calve *et al.*, 1998

2.2 Measurement procedure

The almost universal approach to the identification and quantification of the individual NMVOCs is gas chromatography (GC) with either flame ionisation detection (FID) or mass spectroscopy (MS). These techniques are regarded as the most cost effective methods for the measurements of VOCs because of the large number of compounds that can be determined in a single run (Ciccioli, 1993; Finlayson-Pitts and Pitts, 2000). GC-MS is used to establish the identity of a particular compound through the combination of retention times and mass spectra and can also be used for quantification. However, for a given type of air mass, GC-FID is commonly used for more extensive quantitative measurements after the individual peaks have been identified.

However, to reach the sensitivity necessary for detecting pollutants at ambient concentrations enriching procedure for sample collection must be combined with highly efficient chromatographic column and selective detection (Ciccioli, 1993). Cryogenic focusing on empty tubes, adsorption on traps filled with solid sorbents or a combination of both techniques are procedures commonly adopted for the enriching of atmospheric samples. Thermal desorption carried out under the flow rate of inert gas to prevent chemical

transformation is the preferred techniques to transfer analytes from the enriching system to the GC.

To establish the appropriate analytical procedure for the purpose of these studies preparative laboratory experiments based on an extensive literature search were performed. Finally, the measurements of hydrocarbons and oxygenated species were performed with the method based on the US EPA Compendium Method TO-17 entitled “*Determination of Volatile Organic Compounds in Ambient Air Using Active Sampling Onto Sorbent Tubes*” (Woolfenden and McClenny, 1999).

The procedure was as follows:

- ambient air collection by active sampling on glass tubes packed with adsorption materials,
- thermal desorption of the sampled tubes,
- sample preconcentration with a cryo-trap,
- gas chromatography-flame ionisation detection analysis.

Recent results from the studies using an improved method of peak deconvolution from double-column gas chromatography (Lewis *et al.*, 2000; Schoenmakers *et al.* 2000; Xu *et al.* 2003) suggest that the conventional GC techniques can only cover around one-third of the total mass of volatile carbon. According to these and due to the fact that none of existing columns is capable to separate all the compounds abundant in air, the analysis of hydrocarbons and oxygenated species were performed separately, by means of different capillary columns. The partition of analytical procedure followed from application of different adsorption tubes, through separated sampling, desorption, preconcentration to application of different GC systems.

In the following a more detailed description of the experimental procedure is given.

2.2.1 Adsorption tubes

Adsorption materials

Different types of solid adsorbents for thermal desorption have been tested and used for collecting various VOCs since the mid-1970s (Ciccioli, 1993; Woolfenden, 1997; Woolfenden and McClenny, 1999; Harper, 2000). Based on the published data and own studies two adsorption materials were selected for the purpose of the present work, Carbotrap graphitised carbon and Carbosieve SIII carbon molecular sieve. Because a single adsorbent cannot efficiently collect a wide range of VOCs (Pollack *et al.*, 1993), multi-adsorbent sampling with a combination of those materials were used. Alternatively, a train of single-sorbent tubes coupled together in a series may also be used. According to the literature data, tubes consisting of Carbotrap and Carbosieve SIII are suitable for compounds ranging in volatility from C₂ to C₁₂ including oxygenated compounds (Camel and Caude, 1995; Matisova and Skrabakova, 1995; Woolfenden, 1997; Hallama *et al.*, 1998; Cao and Hewitt, 1999;

Woolfenden and McClenny, 1999; Manura, 1999; Harper, 2000). The main characteristics of the employed sorbents are presented in table 2.3.

Table 2.3: Characteristics of adsorption materials used for VOCs sampling (Woolfenden and McClenny, 1999)

adsorbent	max. temp (°C)	specific area (m ² /g)	hydrophobicity
Carbotrap	>400	100	yes
Carbosieve SIII	400	800	no

Carbotrap graphitised carbon black (*Supelco*) is a non-specific, non-porous adsorbent with a high surface homogeneity and hydrophobic properties. Carbotrap has a surface area of 100 m²/g and can be used for monitoring many C₅-C₁₂ compounds in ambient air. Water does not effect the breakthrough volume for compounds trapped on these adsorbent. Also ozone, in mixing ratios range below 100 ppb, does not produce artefacts from the sorbent itself (Helmig and Vierling, 1995; Camel and Caude, 1995; Supelco 1997; Woolfenden, 1997; Harper, 2000).

Carbosieve SIII carbon molecular sieve (*Supelco*) has a large surface area of 800 m²/g and high porosity. Carbosieve is well suited for the trapping of small molecules such as C₂ compounds. The pure carbon framework allows the thermal desorption of these small molecules without loss. Carbosieve retains also water what can affect the sampling efficiency in high relative humidity, however, the save sampling volume should typically be reduce by a factor of 10 at 90-95% relative humidity (Supelco, 1992; Helmig and Vierling, 1995; Camel and Caude, 1995; Woolfenden and McClenny, 1999; Harper, 2000).

Tubes construction

Glass tubes with 6 mm o.d., wall thickness of 1 mm and 114 mm length, supplied by *Supelco* were used. They were filled with solid adsorbents up to the bed length of 40 mm. Glass wool plugs were used to separate and hold the adsorbent in place. For hydrocarbons multi-bed tubes packed with 125 mg Carbotrap graphitised carbon and 150 mg Carbosieve SIII carbon molecular sieve (figure 2.2) were selected. Tubes were packed in the order of increasing sorbent strength, first Carbotrap followed by Carbosieve SIII. The higher molecular weight compounds were retained on the front, on the least retentive sorbent; the more volatile compounds were retained further into the packing on the stronger adsorbent. By this rule, higher molecular weight compounds did not encounter the stronger adsorbents, thereby improving the efficiency of the thermal desorption process (Cao and Hewitt, 1999; Woolfenden and McClenny, 1999; Harper, 2000).

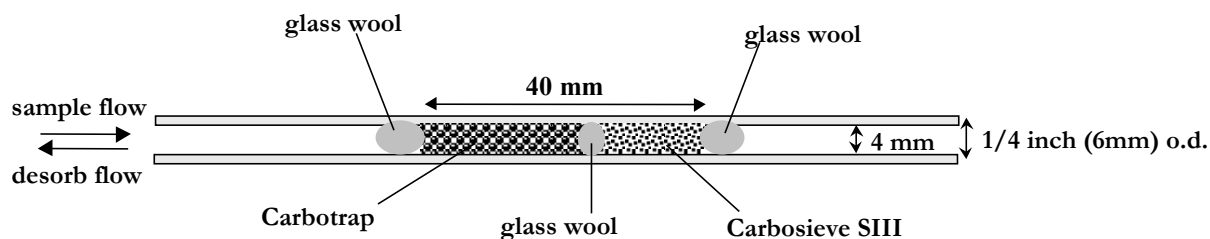


Figure 2.2: Construction of adsorbent tubes used for sampling of hydrocarbons

For oxygenated compounds a combination of two adsorbent tubes was used: tube packed with 190 mg Carbotrap and tube with 350 mg Carbosieve SIII (figure 2.3). During the sample collection tubes are located in the same way as in the multi-bed tube: first a Carbotrap tube as a less retentive sorbent, than a Carbosieve SIII tube as a stronger adsorbent.

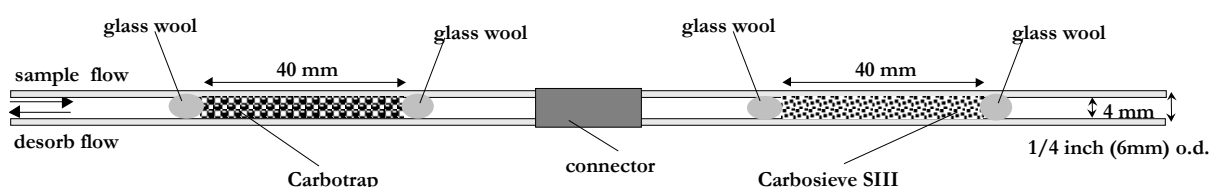


Figure 2.3: Construction of adsorbent tubes used for sampling of oxygenated compounds

Newly packed tubes were conditioned for 3 h at 390°C by flashing with 60 ml/min of helium as carrier gas. Conditioning was carried out in a thermal desorber (*Thermal Desorption Unit Model 890 from Supelco*).

Tube parameters

The common problem connecting with the application of sorbent tubes with thermal desorption and GC analysis is that artefacts from the adsorption material may falsify the results of the analytes. This can be minimised or eliminated by selecting the sorbent or series of sorbents of appropriate strength for the particular target and by appropriate preparation, sampling, storage and desorption procedure.

To avoid artefact formation tubes were handled carefully according to guidelines given in EPA Compendium Method TO-17 (Woolfenden and McClenny, 1999). Quality assurance and performance criteria for the adsorption sampling in ambient air by means of selected tubes were tested by specification of the following parameters:

- tube backgrounds,
- breakthrough volume,
- save sampling volume,
- analytical precision of duplicate pairs,
- sample recovery,
- storage stability.

To establish the artefact level of adsorption tubes, conditioned and unsampled tubes (laboratory blanks) were analysed with the same desorption and GC programme as calibration and field samples. All employed tubes were tested in the same way. Received GC signals were accepted as particular tube backgrounds and were than subtracted from the measurement results. Background peaks with an area of 10% or more of the area of average component peaks in the sample were marked as artefacts.

Breakthrough volume (BV) is defined as volume sampled when the amount of analyte passing through the adsorption tube reaches a certain percentage of total amount, collected and missed. Typically BV for a given sorbent/analyte combination is considered to the sample volume at which 5% of analyte passed the sampling tube. For the purpose of this study the breakthrough volume was tested during the laboratory experiments. Different amounts of analytes were sampled from dry gas mixture (custom made gas mixtures: RM2, Annex B, table B.2) at room temperature through the adsorption tube directly to the GC system. By variation of the volume and the concentration of sampled gas mixture both breakthrough affecting parameters, namely total sampling volume and total sampled mass of particular compounds were checked. Table 2.4 presents the breakthrough percentage for different sampled mass for different analysed compounds.

Table 2.4.a: Breakthrough percentage in dependence of sampling mass

compounds	sampled mass (ng)	break-through (%)	sampled mass (ng)	break-through (%)	sampled mass (ng)	break-through (%)	sampled mass (ng)	break-through (%)
<i>ethene</i>	0.47	7.4	2.34	50.9	140.16	98.4	280.31	99.5
<i>ethyne</i>	0.43	23.2	2.16	62.8	129.80	99.9	259.61	99.5
<i>ethane</i>	0.49	21.3	2.47	83.2	148.32	99.3	296.65	99.5
<i>propene</i>	0.54	0.0	2.70	0.0	162.03	2.3	324.05	4.8
<i>propane</i>	0.74	0.0	3.71	0.0	222.54	0.5	445.09	1.0
<i>i-butane</i>	1.03	0.0	5.14	0.0	308.53	0.0	617.06	0.1
<i>i-butene</i>	0.89	0.0	4.43	0.0	265.94	0.1	531.88	0.2
<i>n-butane</i>	0.95	0.0	4.76	0.0	285.80	0.0	571.59	0.1
<i>trans-2-butene</i>	0.70	0.0	3.49	0.0	209.43	0.1	418.86	0.1
<i>cis-2-butene</i>	0.73	0.0	3.63	0.0	218.04	0.0	436.08	0.1
<i>i-pentane</i>	0.73	0.0	3.67	0.0	220.14	0.1	440.28	0.1
<i>1-pentene</i>	0.10	0.0	0.50	0.0	30.21	0.4	60.42	0.7
<i>n-pentane</i>	1.17	0.0	5.84	0.0	350.12	0.1	700.24	0.3
<i>isoprene</i>	0.16	0.0	0.82	0.0	49.41	0.2	98.82	0.4
<i>trans-2-pentene</i>	0.21	0.0	1.03	0.0	61.82	0.1	123.65	0.2
<i>cis-2-pentene</i>	0.10	0.0	0.48	0.0	28.50	0.0	57.00	0.2
<i>2,2-dimethylbutane</i>	1.64	0.0	8.18	0.0	490.67	0.4	981.34	0.3
<i>cyclopentene</i>	0.21	0.0	1.07	0.0	64.29	0.1	128.57	0.1
<i>methyl-tert-butyl ether, 2,3-dimethylbutane, cyclopentane</i>	3.24	0.0	16.21	0.0	972.61	0.1	1945.22	0.2

Table 2.4.b: Breakthrough percentage in dependence of sampling mass

compounds	sampled mass (ng)	break-through (%)	sampled mass (ng)	break-through (%)	sampled mass (ng)	break-through (%)	sampled mass (ng)	break-through (%)
<i>2-methylpentane</i>	1.37	0.0	6.86	0.0	411.32	0.3	822.65	0.2
<i>3-methylpentane</i>	1.32	0.0	6.60	0.0	396.07	0.4	792.14	0.3
<i>1-hexene</i>	0.45	0.0	2.27	0.0	136.09	0.4	272.17	0.2
<i>n-hexane, 2-ethyl-1-butene</i>	2.39	0.0	11.96	0.0	717.88	0.2	1435.76	0.2
<i>2,3-dimethyl-1,3-cyclohexadiene</i>	0.70	0.0	3.51	0.0	210.89	0.5	421.78	0.3
<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	2.14	0.0	10.72	0.0	643.04	0.2	1286.07	0.2
<i>2,3-dimethyl-2-butene</i>	0.73	0.0	3.63	0.0	217.51	0.4	435.03	0.3
<i>benzene</i>	1.33	0.0	6.65	0.0	399.06	0.4	798.12	0.2
<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	4.11	0.0	20.57	0.0	1234.16	0.2	2468.31	0.2
<i>2-methylhexane</i>	2.26	0.0	11.32	0.0	678.99	0.3	1357.98	0.2
<i>cyclohexene</i>	1.22	0.0	6.10	0.0	365.99	0.5	731.98	0.3
<i>1-heptene</i>	1.38	0.0	6.90	0.0	413.73	0.1	827.46	0.2
<i>2,2,4-trimethylpentane</i>	2.78	0.0	13.89	0.0	833.19	0.2	1666.39	0.2
<i>n-heptane</i>	1.52	0.0	7.58	0.0	455.02	0.1	910.05	0.2
<i>1,4-cyclohexadiene</i>	0.97	0.0	4.84	0.0	290.62	0.6	581.24	0.2
<i>2,3,4-trimethylpentane</i>	2.66	0.0	13.32	0.0	799.30	0.2	1598.61	0.2
<i>toluene, 2-methylpentane</i>	3.41	0.0	17.05	0.0	1022.71	0.1	2045.41	0.2
<i>3-methylpentane</i>	2.77	0.0	13.85	0.0	831.25	0.1	1662.50	0.1
<i>4-methylpentane, 1-methyl-1-cyclohexene</i>	4.67	0.0	23.36	0.2	1401.41	0.2	2802.81	0.2
<i>1-octene</i>	2.66	0.0	13.28	0.0	796.89	0.1	1593.78	0.1
<i>n-octane</i>	2.31	0.0	11.54	0.0	692.43	0.1	1384.85	0.1
<i>ethylbenzene</i>	1.33	0.0	6.66	0.0	399.60	0.2	799.21	0.2
<i>m, p-xylene</i>	2.64	0.0	13.22	0.0	793.05	0.1	1586.09	0.1
<i>styrene</i>	2.45	0.0	12.26	0.0	735.85	0.2	1471.70	0.2
<i>o-xylene</i>	1.50	0.0	7.51	0.0	450.43	0.2	900.87	0.2
<i>a-pinene</i>	5.70	0.0	28.50	0.2	1710.16	0.2	3420.32	0.3
<i>n-propylbenzene</i>	1.59	0.0	7.94	0.0	476.24	0.2	952.48	0.2
<i>4-ethyltoluene</i>	1.19	0.0	5.97	0.0	358.22	0.2	716.44	0.2
<i>1,3,5-trimethylbenzene</i>	1.88	0.0	9.39	0.0	563.54	0.2	1127.08	0.2
<i>n-decane</i>	1.09	0.0	5.46	0.0	327.80	0.1	655.60	0.1
<i>1,2,4-trimethylbenzene, tert-butylbenzene</i>	2.95	0.0	14.73	0.0	883.81	0.2	1767.62	0.2
<i>1,2,3-trimethylbenzene</i>	1.20	0.0	5.98	0.0	358.87	0.2	717.74	0.2
<i>1,2,3,4-tetramethylbenzene</i>	0.93	0.0	4.64	0.0	278.12	0.2	556.23	0.2

As observed in table 2.4, for all analysed compounds apart from ethane, ethene and ethyne no breakthrough above 5% were found in the sampled mass interval from ca. 0.5 ng up to ca. 3400 ng. The sampling efficiency of C₂ hydrocarbons were very low already by small concentrations. For sampling of about 0.5 ng of each the breakthrough reached 21, 7 and 23% for ethane, ethene and ethyne, respectively. Such ineffectiveness of the sampling process disables the correct quantitative analysis. According to this, the C₂ hydrocarbons were excluded from further analysis.

The total sampling volume varied during the experiment from 100 to 12000 ml. To test the influence of the sampling volume on the sampling/desorption efficiency the area of peaks obtained after sampling and thermal desorption/GC-FID analysis were plotted against the sampled mass for different volume/concentration combinations. Figures 2.4, 2.5 and 2.6 present the graphical representation of these plots for some exemplary compounds.

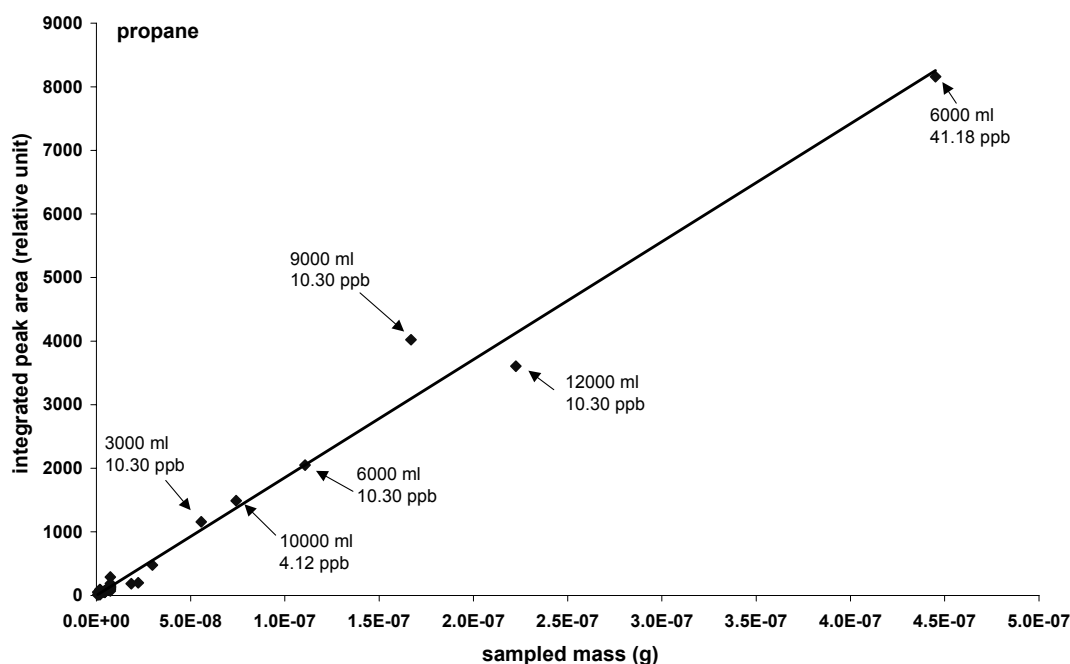


Figure 2.4: Correlation plot of area of propane peaks obtained after sampling and thermal desorption/GC-FID analysis against sampled mass; descriptions of the points present sampling volume and mixing ratio of sampled gas

For the presented compounds (figures 2.4, 2.5 and 2.6) the linear correlation between peaks area and sampled mass could be observed for all tested sampling volumes and total sampled masses. This indicates no losses and thereby no breakthrough of analytes for all tested sampling parameters. The same trend is observed for all others investigated compounds.

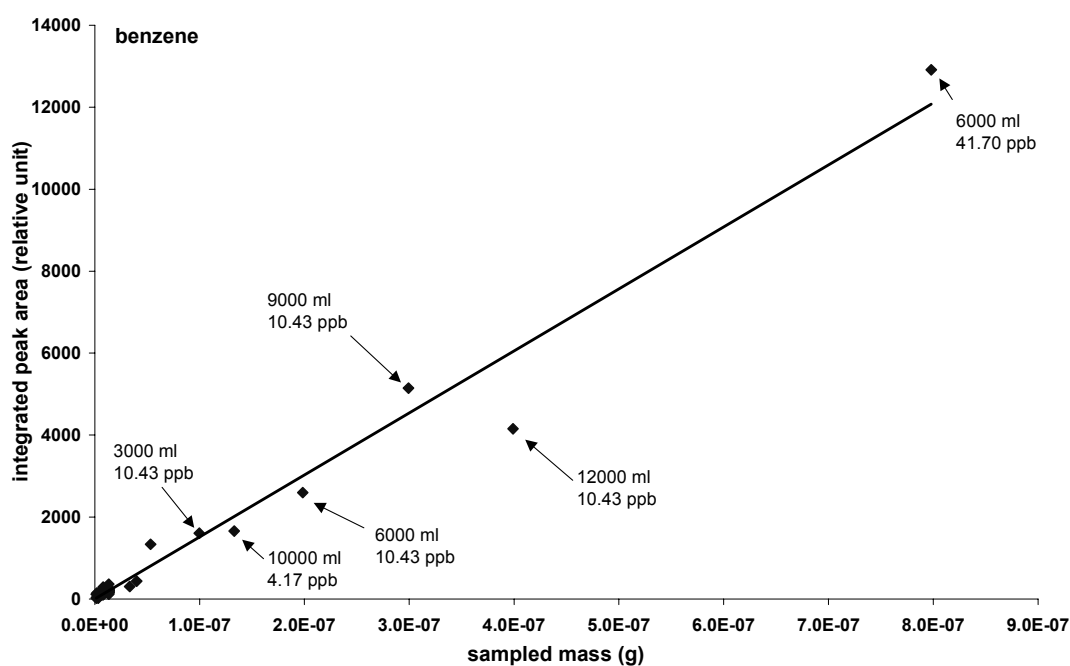


Figure 2.5: Correlation plot of area of benzene peaks obtained after sampling and thermal desorption/GC-FID analysis against sampled mass; descriptions of the points present sampling volume and mixing ratio of sampled gas

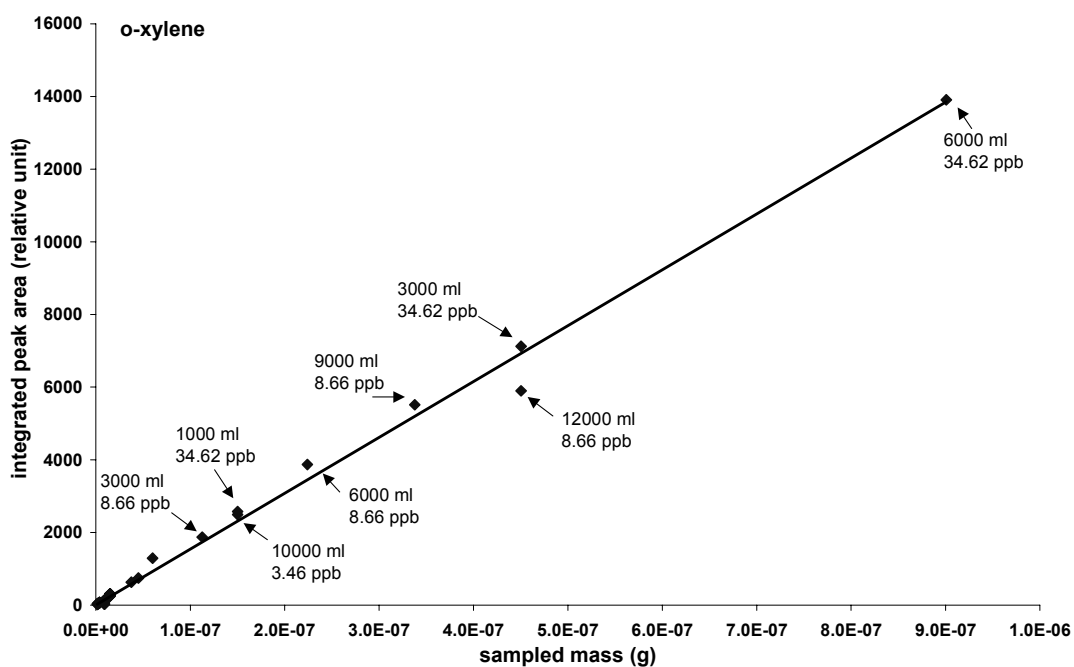


Figure 2.6: Correlation plot of area of o-xylene peaks obtained after sampling and thermal desorption/GC-FID analysis against sampled mass; descriptions of the points present sampling volume and mixing ratio of sampled gas

Safe sampling volume (SSV) was calculated as two-thirds of the breakthrough volume (Woolfenden and McClenny, 1999). According to the performed tests of breakthrough the highest sampled mass was assumed as a breakthrough mass and used for the calculation of the save sampling mass. This mass of particular tested compounds was recalculated to the corresponding volume for different atmospheric concentrations. Table 2.5 presents safe sampling volume for various atmospheric conditions.

Table 2.5.a: Save sampling volume (in ml) at different atmospheric concentrations

compounds	up to 500 ppb (car exhaust emission)	up to 250 ppb (strongly polluted area)	up to 10 ppb (normal urban area)	up to 1 ppb (normal rural area)	up to 2.5 ppb (forest area)
<i>propene</i>	348	697	17414	174142	69657
<i>propane</i>	342	684	17092	170919	68368
<i>i-butane</i>	498	995	24884	248844	99538
<i>i-butene</i>	296	592	14788	147879	59152
<i>n-butane</i>	342	683	17076	170761	68305
<i>trans-2-butene</i>	233	466	11646	116456	46582
<i>cis-2-butene</i>	261	521	13027	130273	52109
<i>i-pentane</i>	203	406	10143	101434	40573
<i>1-pentene</i>	27	54	1353	13531	5413
<i>n-pentane</i>	323	645	16132	161325	64530
<i>isoprene</i>	46	91	2277	22766	9106
<i>trans-2-pentene</i>	59	117	2933	29332	11733
<i>cis-2-pentene</i>	26	53	1313	13133	5253
<i>2,2-dimethylbutane</i>	452	904	22609	226088	90435
<i>cyclopentene</i>	48	96	2411	24108	9643
<i>methyl-tert-butyl ether, 2,3- dimethylbutane, cyclopentane</i>	713	1426	35643	356427	142571
<i>2-methylpentane</i>	379	758	18953	189527	75811
<i>3-methylpentane</i>	297	594	14853	148532	59413
<i>1-hexene</i>	102	204	5103	51034	20413
<i>n-hexane, 2-ethyl-1- butene</i>	551	1103	27568	275676	110270
<i>2,3-dimethyl-1,3- cyclohexadiene</i>	162	324	8098	80985	32394
<i>methylcyclopentane, 1-methyl-1- cyclopentene</i>	506	1012	25298	252976	101191
<i>2,3-dimethyl-2- butene</i>	169	338	8454	84542	33817
<i>benzene</i>	306	613	15324	153244	61298
<i>cyclohexane, 2,3- dimethylpentane, 1,3-cyclohexadiene</i>	1021	2043	51064	510640	204256
<i>2-methylhexane</i>	548	1095	27385	273854	109542
<i>cyclohexene</i>	236	472	11804	118035	47214
<i>1-heptene</i>	326	651	16277	162766	65106
<i>2,2,4- trimethylpentane</i>	548	1097	27424	274240	109696
<i>n-heptane</i>	257	515	12874	128738	51495
<i>1,4-cyclohexadiene</i>	187	375	9373	93727	37491
<i>2,3,4- trimethylpentane</i>	645	1290	32238	322381	128952
<i>toluene, 2- methylpentane</i>	660	1319	32983	329831	131933

Table 2.5.b: Save sampling volume (in ml) at different atmospheric concentrations

compounds	up to 500 ppb (car exhaust emission)	up to 250 ppb (strongly polluted area)	up to 10 ppb (normal urban area)	up to 1 ppb (normal rural area)	up to 2.5 ppb (forest area)
<i>3-methylpentane</i>	470	941	23518	235181	94073
<i>4-methylpentane, 1-methyl-1-cyclohexene</i>	793	1586	39649	396493	158597
<i>1-octene</i>	490	979	24480	244801	97920
<i>n-octane</i>	399	798	19943	199432	79773
<i>ethylbenzene</i>	226	452	11306	113058	45223
<i>m, p-xylene</i>	483	966	24141	241406	96562
<i>styrene</i>	448	896	22400	223996	89598
<i>o-xylene</i>	280	559	13977	139772	55909
<i>a-pinene</i>	1041	2082	52058	520579	208232
<i>n-propylbenzene</i>	226	452	11297	112972	45189
<i>4-ethyltoluene</i>	193	385	9632	96316	38526
<i>1,3,5-trimethylbenzene</i>	303	606	15152	151521	60608
<i>n-decane</i>	176	353	8814	88136	35254
<i>1,2,4-trimethylbenzene, tert-butylbenzene</i>	402	803	20076	200755	80302
<i>1,2,3-trimethylbenzene</i>	193	386	9649	96491	38596
<i>1,2,3,4-tetramethylbenzene</i>	150	299	7478	74778	29911

As observed in table 2.5, the save sampling volume recalculated from save sampling mass differs strongly for different atmospheric conditions. For measurements of car exhaust emission the sampling volume would be cut down to about 500 ml, whereas in rural areas the volume of 100 l would be adequate. Due to the fact that the NMVOC mixing ratios in the city air of Wuppertal correspond to the normal urban area conditions (Schmitz *et al.*, 1997; Gomes, 2002) the save sampling volume for the present measurements were assumed for the mixing ratios up to about 10 ppb. Additionally, because the maximal laboratory tested sampling volume was 12 l, two-thirds of this volume, namely 8 l, was accepted as the maximal sampling volume used during the present study.

Sample recovery gives a information what part of mass of a particular compound trapped on the adsorption tube could be thermally restored and measured by GC-FID analysis.

The recovery experiments were carried out with custom made standard gas mixture (RM2, table B.2 in Annex B). Adsorption tubes were sampled with different amount of analytes, under different conditions and than thermally desorbed to the gas chromatograph. Desorption and analysis was performed either directly after sampling or after some time of storage. The quantitative recoveries were calculated by comparison with a standard gas mixtures sampled directly to the GC system. Results are presented in table 2.6.

Table 2.6: Recovery rates (%) for adsorption tubes sampling and thermal desorption/GC-FID analysis for different compounds in dependence of storage time

compounds	direct	1 day	2 days	1 week	2 weeks	2 months
	%	%	%	%	%	%
<i>ethene</i>	18	23	36	50	63	52
<i>ethyne</i>	7	16	6	11	8	12
<i>ethane</i>	4	7	10	19	27	21
<i>propene</i>	108	72	106	104	121	107
<i>propane</i>	63	69	73	72	83	83
<i>i-butane</i>	73	53	56	68	61	51
<i>i-butene</i>	94	63	99	89	120	104
<i>n-butane</i>	89	55	75	92	86	66
<i>trans-2-butene</i>	78	57	51	71	66	35
<i>cis-2-butene</i>	81	51	49	58	65	37
<i>i-pentane</i>	46	45	54	94	82	97
<i>1-pentene</i>	24	38	33	32	48	59
<i>n-pentane</i>	15	52	37	35	55	50
<i>isoprene</i>	17	60	29	47	54	45
<i>trans-2-pentene</i>	23	50	40	31	47	43
<i>cis-2-pentene</i>	29	54	35	27	37	71
<i>2,2-dimethylbutane</i>	21	59	34	43	61	68
<i>cyclopentene</i>	50	33	63	94	58	87
<i>methyl-tert-butyl ether, 2,3-dimethylbutane, cyclopentane</i>	15	60	43	52	66	69
<i>2-methylpentane</i>	25	77	55	72	85	91
<i>3-methylpentane</i>	26	77	57	69	84	87
<i>1-hexene</i>	31	88	66	92	112	99
<i>n-hexane, 2-ethyl-1-butene</i>	28	83	60	72	83	87
<i>2,3-dimethyl-1,3-cyclohexadiene</i>	28	81	62	76	81	84
<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	18	69	48	55	69	74
<i>2,3-dimethyl-2-butene</i>	16	72	46	66	74	77
<i>benzene</i>	25	87	77	93	112	140
<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	30	70	50	57	68	69
<i>2-methylhexane</i>	42	89	74	80	87	89
<i>cyclohexene</i>	14	66	37	46	65	68
<i>1-heptene</i>	60	97	80	89	91	91
<i>2,2,4-trimethylpentane</i>	61	96	81	89	89	90
<i>n-heptane</i>	65	99	81	89	89	87
<i>1,4-cyclohexadiene</i>	17	72	34	53	49	30
<i>2,3,4-trimethylpentane</i>	65	96	83	88	90	90
<i>toluene, 2-methylpentane</i>	75	101	89	94	95	95
<i>3-methylpentane</i>	68	99	86	94	92	93
<i>4-methylpentane, 1-methyl-1-cyclohexene</i>	63	96	80	86	89	89
<i>1-octene</i>	86	103	89	96	94	95
<i>n-octane</i>	90	101	92	94	95	95
<i>ethylbenzene</i>	79	103	89	96	96	99
<i>m, p-xylene</i>	91	105	92	97	96	98
<i>styrene</i>	99	121	100	105	102	107
<i>o-xylene</i>	88	106	86	94	93	92
<i>a-pinene</i>	75	101	82	88	87	91
<i>n-propylbenzene</i>	93	107	92	94	92	98
<i>4-ethyltoluene</i>	103	119	93	94	91	102
<i>1,3,5-trimethylbenzene</i>	99	115	87	83	82	89
<i>n-decane</i>	124	121	110	112	112	120
<i>1,2,4-trimethylbenzene, tert-butylbenzene</i>	97	108	99	104	102	105
<i>1,2,3-trimethylbenzene</i>	100	105	118	118	118	125
<i>1,2,3,4-tetramethylbenzene</i>	107	114	105	99	101	114

As observed in table 2.6, the recovery rates for the presented compounds differ significantly from each other. The lowest recovery were found for C₂ hydrocarbons, what is connected with the very low breakthrough volume of those compounds, as reported above. Also compounds like i-butane, trans-2-butene, cis-2-butene, isoprene, trans-2-pentene and 1,4-cyclohexadiene gave lower recovery. For higher hydrocarbons, larger than C₇, better recovery was found with a rate about 100%.

An important factor which can limit the application of adsorption tubes for ambient air measurements is the capability to store sampled tubes for a certain time without changes in the sample composition and concentration. Therefore, the influence of storage time on the recovery of test compounds (RM2 mixtures) after thermal desorption was investigated for different time periods, from direct desorption up to two months of storage. Among sampling and analysis tightly capped tubes were stored by a container in a clean environment of a refrigerator.

Surprisingly, the lowest recovery were found for desorption performed direct (up to few hours) after sampling for almost all analysed compounds, whereas the recovery after one day up to two months were significantly higher (table 2.6). This trend is also presented by figures 2.7 and 2.8, where the recovery rates for some compounds are plotted.

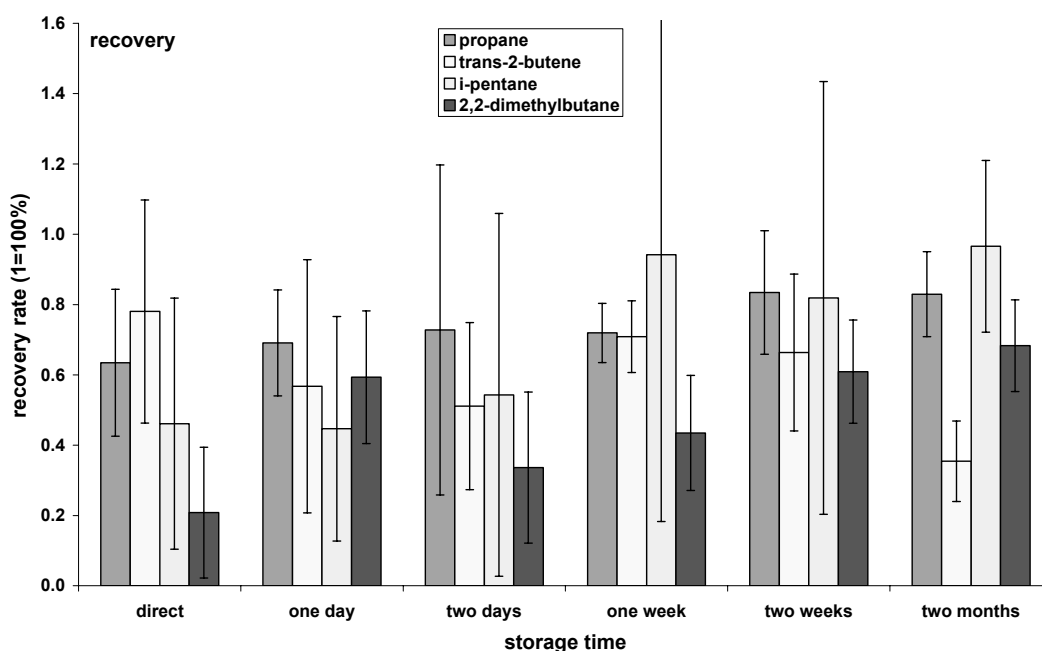


Figure 2.7: Recovery rates for propane, trans-2-butene, i-pentane and 2,2-dimethylbutane in dependence of storage time

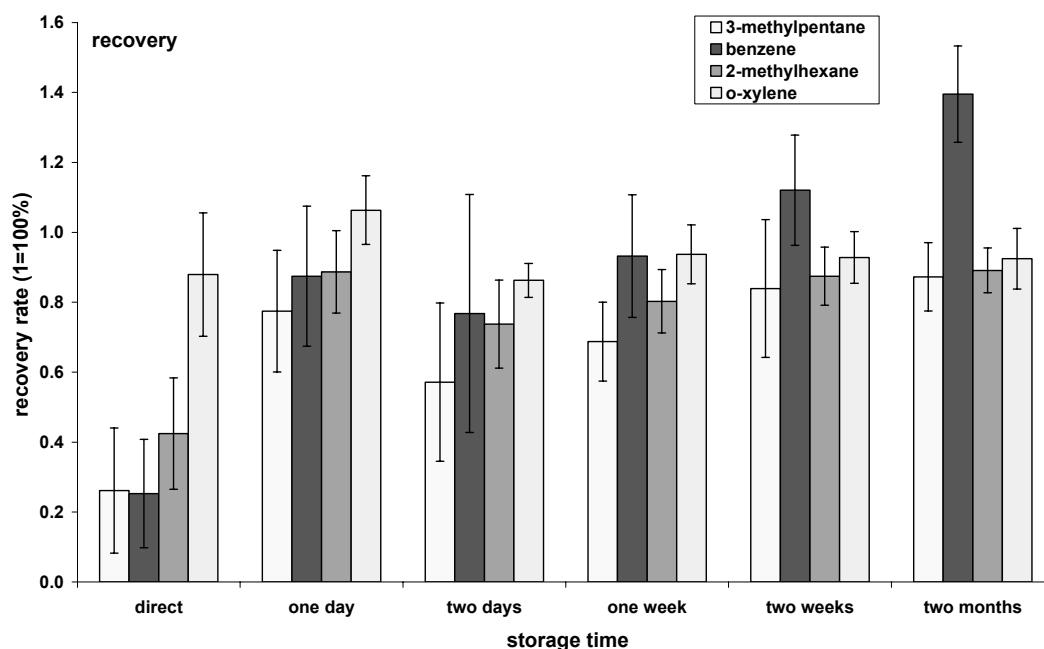


Figure 2.8: Recovery rates for 3-methylpentane, benzene, 2-methylhexane and o-xylene in dependence of storage time

Lower recoveries obtained after direct sample desorption, in comparison with the results of desorption after some days of storage could be explained by the influence of humidity on the process. The experiments were performed with dry gas mixture, nevertheless, during the storage some moisture could migrate to the tubes and thereby improve the desorption process. Similar results were reported in some previous work (Sunesson *et al.*, 1995; Peng and Batterman, 2000) where an increasing of sample recovery with rising the relative humidity was reported.

No sample losses with storage time were observed except trans-2-pentene and cis-2-pentene. For all other tested compounds a good storage stability for time periods from one day up to two months were found.

In praxis, tubes sampled in the ambient air were analysed after two days up to one month after sampling. For all investigated compounds the results obtained from thermal desorption and GC-FID analysis were corrected with the appropriate recovery rates.

Analytical precision of duplicate pairs (p_{dp}) is one of the performance criteria. It is the absolute value of relative difference between two identical samples. The samples are trapped with the same flow rate over the same time period and analysed after the same time (Woolfenden and McClenny, 1999). It is expressed by the following equation:

$$p_{dp} = \frac{X_1 - X_2}{X_a} * 100\% \quad [2.1]$$

with p_{dp} : analytical precision of duplicate pairs,
 X_1 : measured values from the first sampled tubes,
 X_2 : values from the second sampled tubes,
 X_a : average of X_1 and X_2 .

These parameters describe the precision achieved for the sampling and analysis procedure including sampling, thermal desorption and GC-FID analysis. The precision was tested for many sets of two different absorption tubes, thereby describing the whole analytical system consisting of about 50 sampling tubes. To meet the performance criteria analytical precision of duplicate pairs should stay within 20% (Woolfenden and McClenny, 1999). Table 2.7 presents the average analytical precision of duplicate pairs measured during laboratory experiments for different compounds.

Table 2.7.a: Analytical precision of duplicated pairs and audit accuracy for sampling tube for different compounds

compounds	analytical precision of duplicated pairs	
	%	±
<i>ethene</i>	25.90	14.75
<i>ethyne</i>	18.44	3.52
<i>ethane</i>	19.72	15.90
<i>propene</i>	30.75	15.13
<i>propane</i>	18.99	13.89
<i>i-butane</i>	19.96	11.39
<i>i-butene</i>	15.14	18.95
<i>n-butane</i>	21.72	16.78
<i>trans-2-butene</i>	20.16	5.32
<i>cis-2-butene</i>	16.49	8.38
<i>i-pentane</i>	33.35	7.88
<i>1-pentene</i>	21.23	15.80
<i>n-pentane</i>	31.43	13.14
<i>isoprene</i>	27.71	16.61
<i>trans-2-pentene</i>	32.68	12.96
<i>cis-2-pentene</i>	36.11	10.10
<i>2,2-dimethylbutane</i>	26.39	14.59
<i>cyclopentene</i>	21.20	11.99
<i>methyl-tert-butyl ether, 2,3-dimethylbutane, cyclopentane</i>	22.36	13.18
<i>2-methylpentane</i>	16.96	12.35
<i>3-methylpentane</i>	21.92	14.51
<i>1-hexene</i>	17.02	10.92
<i>n-hexane, 2-ethyl-1-butene</i>	17.54	8.94
<i>2,3-dimethyl-1,3-cyclohexadiene</i>	16.88	10.26
<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	19.63	11.37
<i>2,3-dimethyl-2-butene</i>	21.04	10.83
<i>benzene</i>	22.22	12.65
<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	17.97	12.31
<i>2-methylhexane</i>	11.11	4.69
<i>cyclohexene</i>	24.57	15.10
<i>1-heptene</i>	10.99	4.68

Table 2.7.b: Analytical precision of duplicated pairs and audit accuracy for sampling tube for different compounds

compounds	analytical precision of duplicated pairs	
	%	±
<i>2,2,4-trimethylpentane</i>	9.36	5.05
<i>n-heptane</i>	9.71	8.42
<i>1,4-cyclohexadiene</i>	19.20	16.84
<i>toluene, 2-methylpentane</i>	8.41	5.67
<i>3-methylpentane</i>	7.63	7.04
<i>4-methylpentane, 1-methyl-1-cyclohexene</i>	8.65	4.34
<i>1-octene</i>	8.03	5.11
<i>n-octane</i>	8.23	6.23
<i>ethylbenzene</i>	8.13	2.62
<i>m, p-xylene</i>	7.66	2.90
<i>styrene</i>	9.03	4.81
<i>o-xylene</i>	7.66	4.00
<i>a-pinene</i>	7.86	4.48
<i>n-propylbenzene</i>	7.71	3.54
<i>4-ethyltoluene</i>	8.07	3.46
<i>1,3,5-trimethylbenzene</i>	8.37	3.59
<i>n-decane</i>	9.21	3.67
<i>1,2,4-trimethylbenzene, tert-butylbenzene</i>	6.32	3.97
<i>1,2,3-trimethylbenzene</i>	7.91	3.42
<i>1,2,3,4-tetramethylbenzene</i>	7.88	5.78

On average, the precision of duplicate pairs of the tested hydrocarbons was 17% (alkanes - 17%, alkenes - 21% and aromatics - 9%). In general the precision of the analysed compounds meet the criterion of 20%. Only some compounds like propene, i-pentane, n-pentane, trans-2-pentene and cis-2-pentene had lower precision, with the average absolute value of relative difference between two identical samples higher than 30%.

2.2.2 Sampling collection

Sampling collection was performed for four air samples in parallel. Two samples were assigned for the analysis of hydrocarbons and two for oxygenated compounds. Double sampling option were used according to quality assurance of the method (Woolfenden and McClenny, 1999). The collection was carried out by a fixed flow of 100 ml/min with independent rate control for each channel. The sampling time varied according to the expected NMVOC concentrations in the sample gas, however, the total sampled volume ranged from 1000 to 7000 ml. The sampling train included, from the front to the back: sampling tubes, connection line, flow controllers and pump (figure 2.9). The placement of the sorbent tube as the first element reduced the possibility of contamination from further elements. A membrane pump operating up to 5000 ml/min was applied. To regulate the sampling rate mass flow controllers from *Bronkhorst HI-TEC*, calibrated for synthetic air, were

employed. Between sampling tubes and flow controllers 3 m (6 mm o.d.) PVC lines were used as a connection.

After sampling the adsorption tubes were tightly capped and transported to the laboratory. Until the time of analysis sampled tubes were stored in a clean container placed in a refrigerator. Storage times differed from a day up to months.

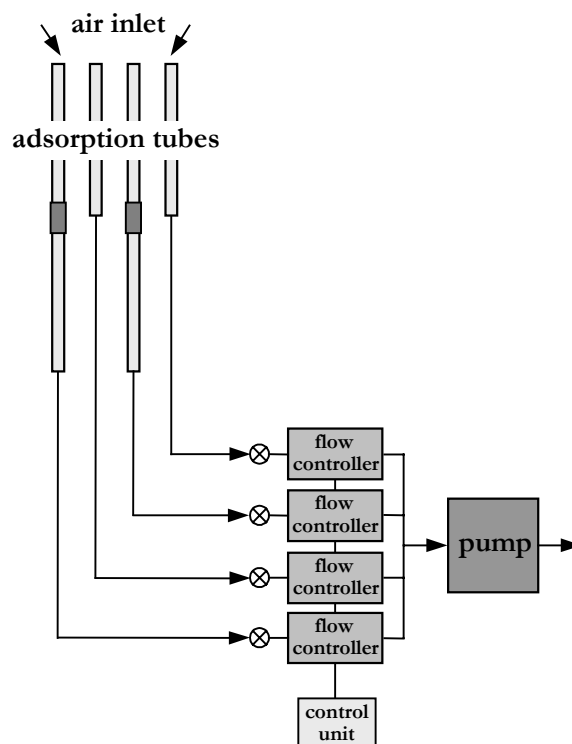


Figure 2.9: Schematic diagram of the sampling train

2.2.3 Steps in sample analysis

After the sampling and storage the tubes were analysed through a sequence of analytical steps (figure 2.10). As mentioned before, the analysis of hydrocarbons and oxygenated species were performed separately. There were some variations in the way of treatment of hydrocarbons and oxygenates compound, however, the main steps were the same:

- dry purge of sampled adsorption tubes,
- thermal desorption of sampled tubes,
- analyte refocusing on secondary trap,
- GC-FID analysis.

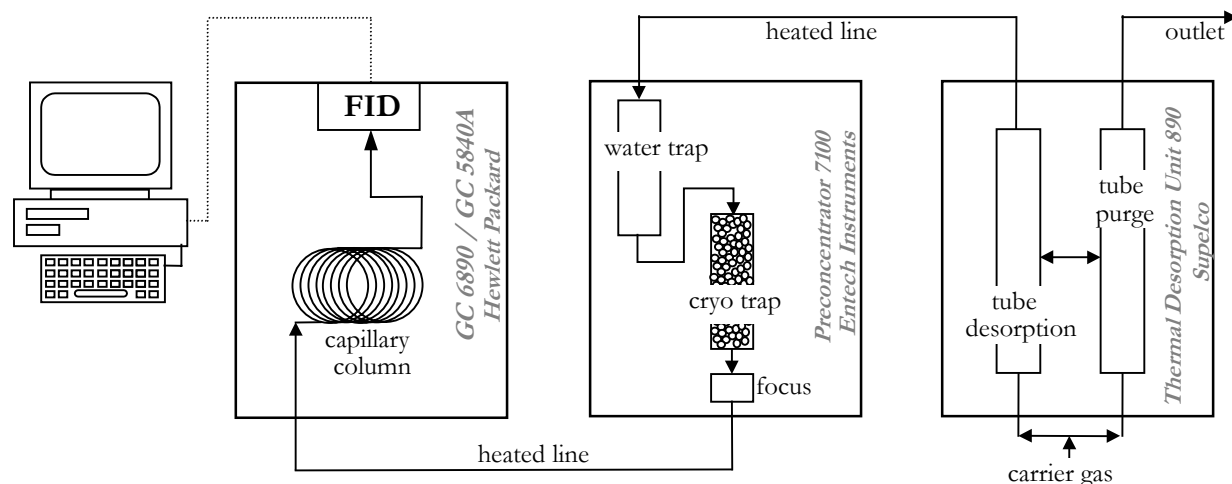


Figure 2.10: Schematic view of the sample analysis steps

Thermal tube desorption

As a first step in the sample analysis dry purge of sampled adsorption tubes was performed. This step is necessary to remove water vapour and oxygen from the tube, in order to avoid disturbance of the analytical process and artefact formation (Woolfenden, 1997; Harper, 2000).

Both, multi-bed tubes assigned for the analysis of hydrocarbons and separate Carbotrap and Carbosieve SIII tubes for oxygenated species were purged under the same conditions. The treatment was carried out in the *Thermal Desorption Unit Model 890 from Supelco* over 10 min, in helium flow of 60 ml/min, in the temperature range of 40 – 50°C. Figure 2.11 shows the configuration of the thermal desorber during purging the tube.

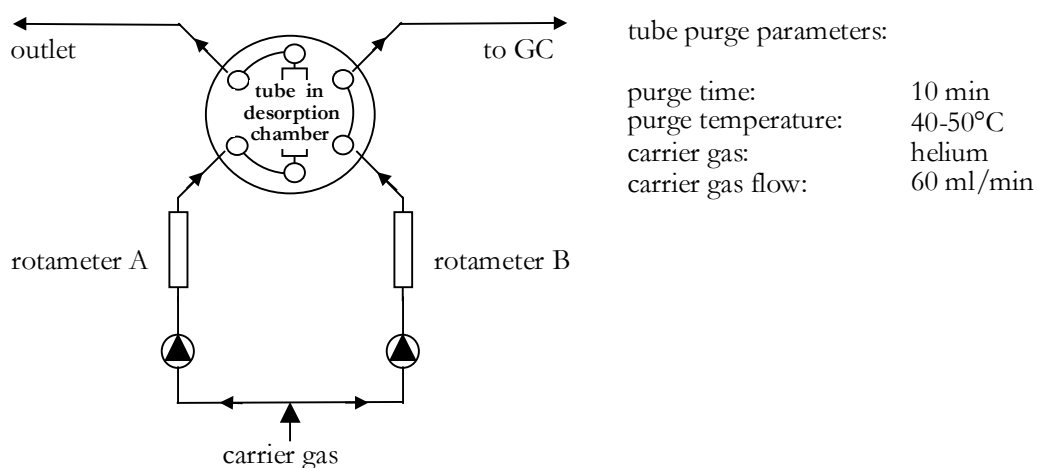


Figure 2.11: Desorber configuration during the tube purge

The thermal desorption process was performed in thermal desorber directly after purging of the tube. Analytes were desorbed from the tube in backflush mode, with the gas flow in reverse direction of the air flow during sampling.

There were some differences in the analysis of hydrocarbons and oxygenated species. Multi-bed tubes with hydrocarbons were desorbed at 350°C. For Carbotrap and Carbosieve SIII tubes with oxygenated compounds a desorption temperature of 300°C was used. The appropriate desorption temperature was adjusted on the basis of preparatory experiments and literature data (Hallama *et al.*, 1998; Pierini *et al.*, 1999). Lower temperature of desorption for oxygenated species was used due to the possibility of analyte degradation at higher temperatures (Mastrogiacomo *et al.*, 1998).

The desorption in all cases was performed in a helium flow of 40 ml/min, over 5 min. Figure 2.12 presents the configuration of the thermal desorption process of the multi-bed tubes with hydrocarbons and Carbotrap and Carbosieve SIII tubes with oxygenated compounds.

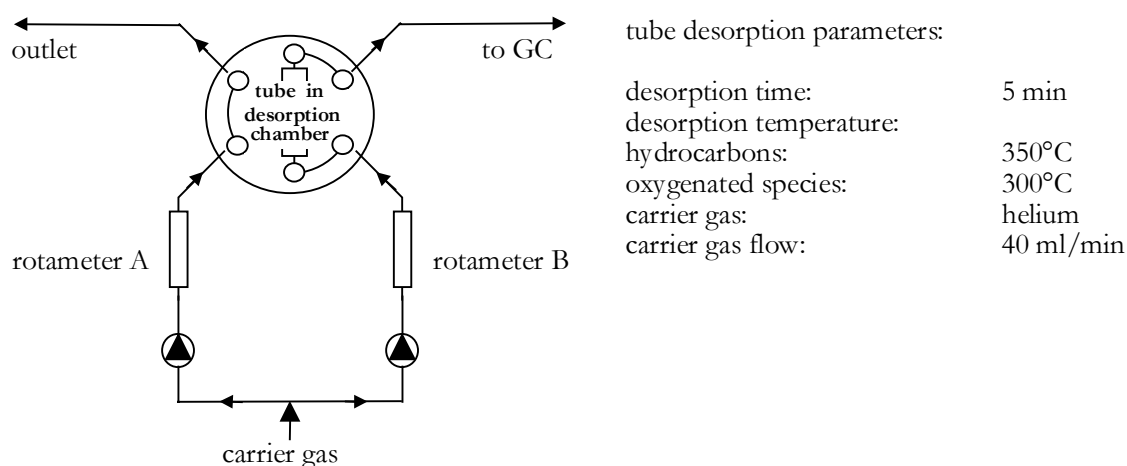


Figure 2.12: Desorber configuration during the thermal desorption of sampled tubes

Sample preconcentration

After thermal desorption of the adsorption tubes the analyte was concentrated in a second step. As an enrichment technique cryo-focusing was applied. This step was performed by a *Preconcentrator 7100* from *Entech Instruments*, an automatic sampler, cryo-focuser and injector. The instrument can be used with one, two or three traps: water trap, cryo-trap and focusing trap. Figure 2.13 presents the schematic view of the system. As a cooling device liquid nitrogen was used.

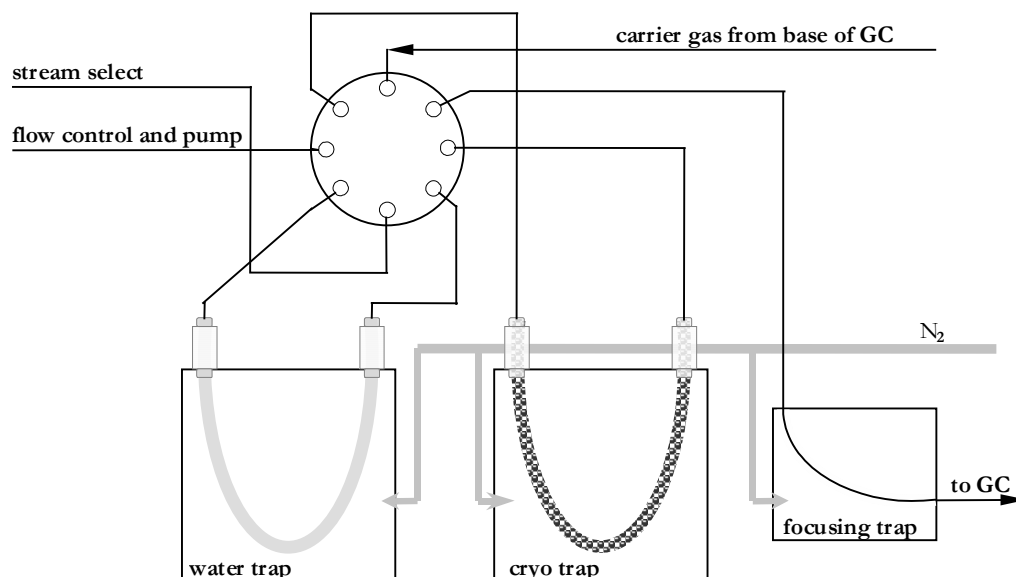


Figure 2.13: Schematic view of the *Preconcentrator 7100*

As a water trap a 1/8 inch empty silkosteel tube was used. This step was employed in order to remove water from the sample before cryogenic collection. Water has to be removed from the sample because its presence can cause some problems by further analysis, like plugging the cryo-trap and affecting the GC separation and FID sensitivity (Lai *et al.*, 1993; Camel and Caude, 1995). Water trapping could be used optionally. If used, the temperature of the water trap by sampling, desorption and the injection was kept at -20°C . A water loop was used only for the analysis of hydrocarbons. In this case the water trapping at temperatures above -30°C does not cause any condensation of $\text{C}_2\text{-C}_{10}$ hydrocarbons and does not affect the sampling efficiency (Lai *et al.*, 1993; Schmitz *et al.*, 1997). For the oxygenated compounds analysis, the water trap was not employed due to the possibility of analyte loss through condensation or absorption in water.

The cryo-trap was constructed of a 1/8 inch U-shape silkosteel tube packed with 60-80 mesh untreated glass balls. For hydrocarbons as well as for oxygenated species the trapping was performed at -180°C during the whole sampling time. As the accomplished experiments showed, all analysed species were effectively collected at this temperature.

After cryo-concentration and prior to the desorption, the cryo-trap was purged with helium in order to possibly remove remaining oxygen. Afterwards rapid desorption at 180°C , over 5 min, was performed and the target analytes were injected into the gas chromatograph or transferred to the focusing trap.

The third trap (figure 2.13) could be operated optionally as focusing trap, in addition to the cryo-concentration. This trap was placed between the cryo-loop and the GC column and was built of a 1/16 inch silkosteel tube. The additional focusing was employed to reduce the sample in size and to generate narrow hydrocarbons peaks (Lai *et al.*, 1993; Moschonas and Glavas, 1997). The focusing trap was only used for analysis of oxygenated species. The sample was desorbed from the cryo-trap and transferred to the focusing trap cooled down to -80°C. Afterwards the focussing trap was heated up to the 80°C and the sample, reduced in volume was injected into the GC column. In the case of hydrocarbons analysis, the additional focusing was not necessary and the desorbed sample was direct injected into the GC column. The effect of narrow bands was obtained through the focusing on the GC column due to the very low (-50°C) initial column temperature.

After final sample injection all traps of the *Preconcentrator 7100* were baked out in order to remove possible contaminations and to prepare for the next sample preconcentration. The bake out was performed by heating the water, cryo and focussing trap up to 130, 190 and 80°C, respectively, and using the helium to flush them.

Table 2.8 gives an overview of the performance parameters for the preconcentration process.

Table 2.8: Parameters of the preconcentration process

parameters	<i>hydrocarbons</i>	<i>oxygenated</i>
sampling volume	420 ml	420 ml
sampling flow	60 ml/min	60 ml/min
carrier gas	helium	helium
cooling device	liquid nitrogen	liquid nitrogen
water trap temperature	- 20°C	off
cryo-trap temperature	- 180°C	- 180°C
focusing	off	on (-80°C)
desorption temperature	180°C	180°C
desorption/GC injection time	5 min	5 min
valves and transfer line	100°C	100°C

Gas chromatography-flame ionisation detection analysis

Separation and detection of the analysed compounds were performed using high resolution capillary gas chromatography with flame ionisation detection (GC-FID). Two different gas chromatographs were used. The hydrocarbons were analysed with a *Hewlett Packard GC 6890* equipped with a 90 m HP-1 (100% dimethylpolysiloxane, non-polar) capillary column, the oxygenated species were analysed with a *Hewlett Packard GC 5840A* with a 60 m DB-WAX (CARBOWAX, polar) capillary column.

As mentioned before, two separated GC systems were employed because two different capillary columns are required. It was not possible to successfully separate all analytes of interests with one capillary column. The parameters of the employed GC systems are presented in table 2.9.

Table 2.9: Parameters of the GC-FID process

parameters	<i>HP GC 6890</i>	<i>HP GC 5840A</i>
capillary column	HP-1 (non-polar)	DB-WAX (polar)
• film material	dimethylpolysiloxane	carbowax
• column length	90 m (3 x 30 m)	60 m
• column diameter	0.32 mm	0.25 mm
• film thickness	3.00 µm	0.25 µm
carrier gas	helium	helium
inlet temperature	100°C	100°C
column pressure (setpoint)	2 bar	2 bar
oven parameters during GC run:		
• start temperature	- 50°C over 10 min	30°C over 30 min
• ramp	5°C/min up to 200°C	5°C/min up to 200°C
• end temperature	200°C over 20 min	200°C over 6 min
• total GC run	80 min	70 min
• column back flashing	on after 64 min	-
detector (FID) parameters:		
• detector temperature	300°C	300°C
• hydrogen flow	40 ml/min	24 ml/min
• synthetic air flow	350 ml/min	340 ml/min
• helium flow (make-up gas)	30 ml/min	30 ml/min

No split option was used, the whole sample from the enrichment system was injected either to the *HP GC 6890* with a non-polar column for analysis for hydrocarbons or to a *HP GC 5840A* with polar column for oxygenated species. The injection direction was regulated through the head valve of *HP GC 6890*. The valve construction gave the possibility of connecting the second GC system (*HP GC 5840A*) to the injection line coming from the *Preconcentrator 7100*. By changing the valve position the injection stream could be switched between the two GC systems. A schematic view of the GCs connection with the enrichment system are presented by figures 2.14 and 2.15.

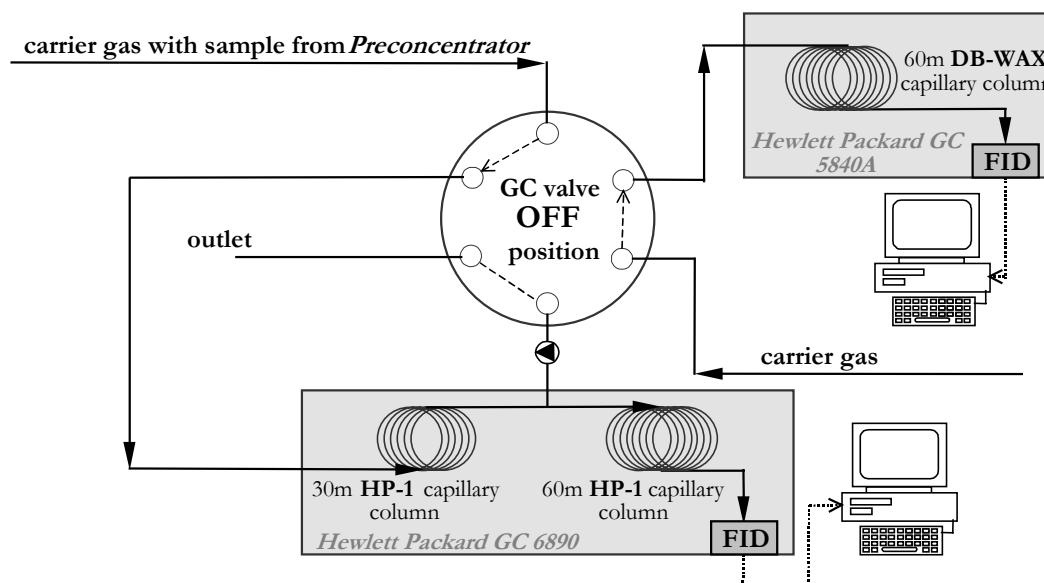


Figure 2.15: Schematic view of GC systems for the analysis of hydrocarbons

Figure 2.14 presents the valve position (OFF) and the stream directions during the analysis of hydrocarbons. In this case the whole sample from the enrichment system was injected into the 90 m HP-1 capillary column of *HP GC 6890*. The second GC at this time was kept in the standby modus at room temperature with helium flushing the capillary column.

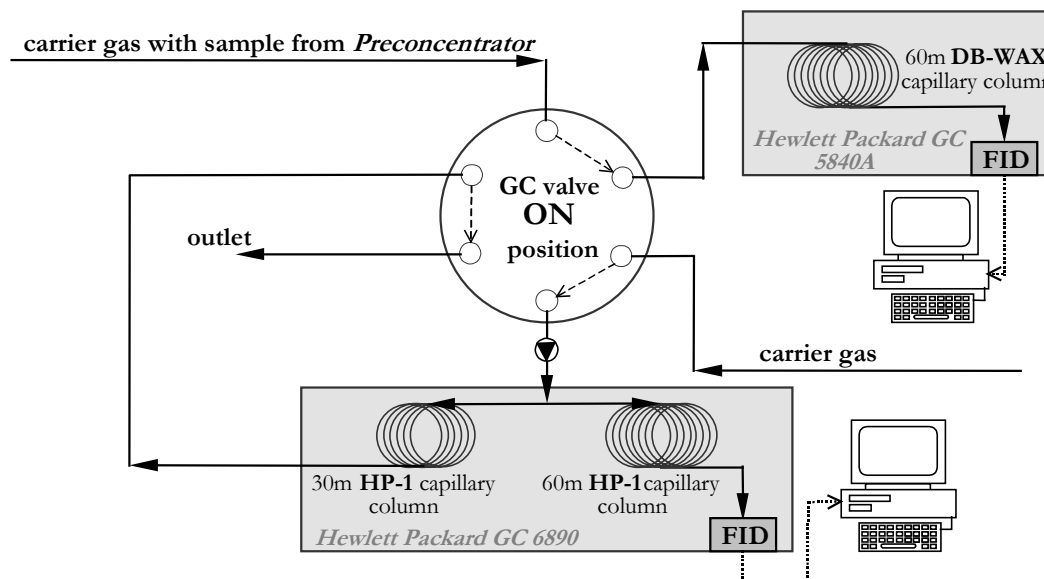


Figure 2.15: Schematic view of GC systems for the analysis of oxygenated species

Figure 2.15 presents the valve position (ON) and the stream directions during the analysis of oxygenated compounds. By this position the sample from enrichment system was injected into the 60 m DB-WAX capillary column of *HP GC 5840A*. In this case the second GC was kept in the standby modus at 60°C with helium flushing the capillary column in a backflush modus.

The temperature programmes for both columns were optimised in order to obtain the best resolution. The finally selected parameters are presented in table 2.9. Also parameters of the FID's were optimised for the best sensitivity.

2.2.4 Calibration procedure

During the whole measurement period the hydrocarbons were calibrated with a standard gas mixture containing 30 C₂-C₉ compounds prepared and certified by the National Physical Laboratory (NPL), England. The mixing ratios of all NPL compounds ranged from 5 to 47 ppbV. The content of the NPL gas mixture is presented in table B.1 in Annex B.

The calibration was performed by standard gas sampling to the preconcentrator/GC system from the gas cylinder. The standard mixture was dynamically diluted with synthetic air by dilution factors from 0.01 to 0.5, equivalent to the mixing ratios measured in ambient air. The GC systems were regularly calibrated during the measurements. The standard samples were analysed by the same procedure as the ambient samples. The response factors of the individual hydrocarbons were calculated on a gram basis, given as integrated peak area (relative unit) per sampled mass (g).

Figure 2.16 shows a typical calibration curve for toluene with different concentration.

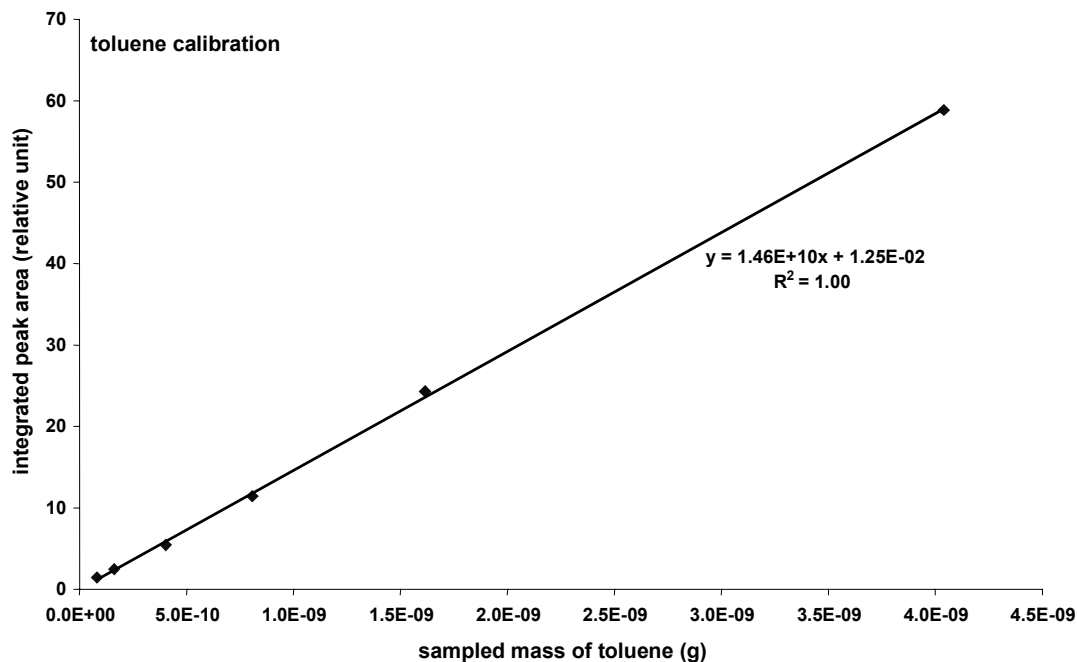


Figure 2.16: Calibration curve for toluene

Table 2.10 summarises the regression parameters obtained for the calibration of NPL compounds.

Table 2.10: List of parameters of the linear regression for the calibration of different hydrocarbons (NPL compounds) using HP GC 6890

	compounds	b (area/g)	± (area/g)	R ²
1	<i>ethene</i>	1.31E+10	5.77E+08	0.99
2	<i>ethyne</i>	1.44E+10	2.12E+08	1.00
3	<i>ethane</i>	1.53E+10	3.05E+08	1.00
4	<i>propene</i>	1.20E+10	2.02E+08	1.00
5	<i>propane</i>	1.31E+10	3.65E+08	1.00
6	<i>propyne</i>	7.49E+09	4.24E+08	0.99
7	<i>i-butane</i>	1.29E+10	4.39E+08	1.00
8	<i>1-butene</i>	1.28E+10	1.39E+08	1.00
9	<i>i-butene</i>	1.28E+10	1.39E+08	1.00
10	<i>1,3-butadiene</i>	1.10E+10	6.58E+08	0.99
11	<i>n-butane</i>	1.53E+10	1.23E+09	0.97
12	<i>trans-2-butene</i>	1.16E+10	3.57E+08	1.00
13	<i>cis-2-butene</i>	1.26E+10	3.09E+08	1.00
14	<i>i-pentane</i>	1.32E+10	4.12E+08	1.00
15	<i>n-pentane</i>	1.22E+10	3.74E+08	1.00
16	<i>isoprene</i>	1.11E+10	3.87E+08	1.00
17	<i>trans-2-pentene</i>	1.23E+10	1.79E+08	1.00
18	<i>cis-2-pentene</i>	1.17E+10	2.90E+08	1.00
19	<i>2-methylpentane</i>	1.35E+10	1.30E+08	1.00
20	<i>3-methylpentane</i>	1.42E+10	1.09E+08	1.00
21	<i>n-hexane</i>	1.33E+10	1.64E+08	1.00
22	<i>benzene</i>	1.45E+10	1.14E+08	1.00
23	<i>cyclohexane</i>	1.45E+10	9.91E+07	1.00
24	<i>n-heptane</i>	1.36E+10	7.70E+07	1.00
25	<i>toluene</i>	1.46E+10	1.42E+08	1.00
26	<i>ethylbenzene</i>	1.40E+10	1.57E+08	1.00
27	<i>m-xylene</i>	1.43E+10	1.68E+08	1.00
28	<i>o-xylene</i>	1.34E+10	1.34E+08	1.00
29	<i>1,3,5-trimethylbenzene</i>	1.26E+10	1.23E+08	1.00
30	<i>1,2,4-trimethylbenzene</i>	1.08E+10	7.66E+08	0.98

The response factors of all calibrated compounds agreed quite well, as it can be seen in table 2.10. The relative standard deviation of the average value was 12%. According to this, the common response factor for all compounds have been calculated as a slope from the linear regression of the calibration plot of all NPL compounds (figure 2.17). The slope value of $(1.36E+10 \pm 1.54E+08)$ area/g (table 2.11) was further used as a response factor for all investigated hydrocarbons determined with *HP GC 6890*, also for unknown hydrocarbons.

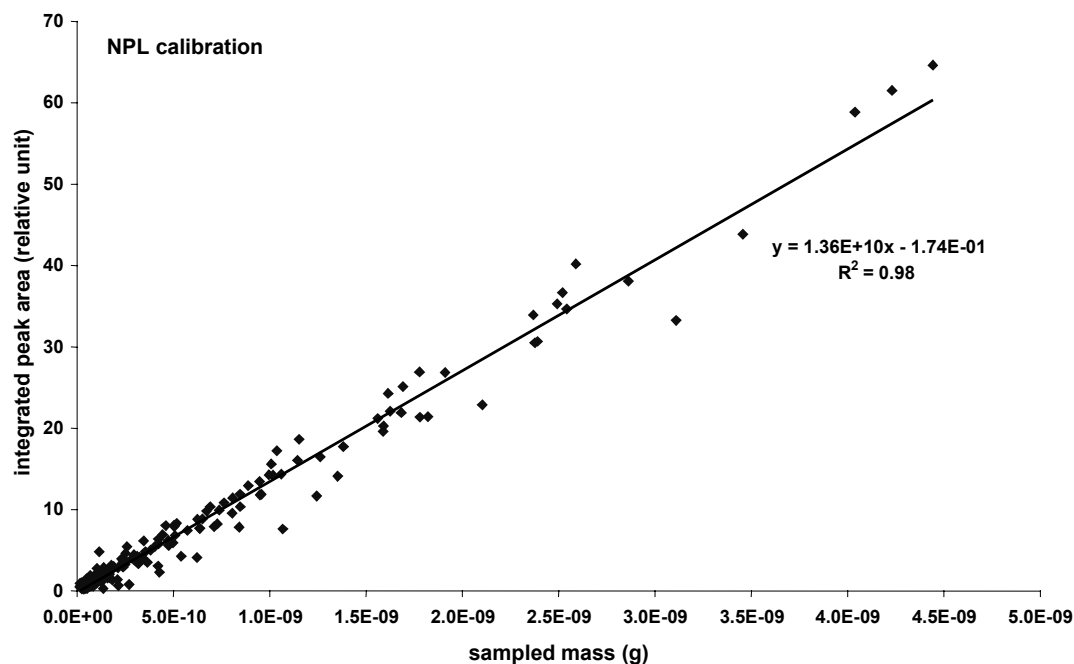


Figure 2.17: Calibration curve for all NPL compounds

In the case of oxygenated species, investigated with *HP GC 5840A*, no certified standards were available. For calibration pure liquid substances delivered by *Aldrich*, *Lancaster* or *Merck* were used. Calibration procedure involved:

- substrate preparation in a 405 l reaction chamber under atmospheric conditions, 298 K and 760 Torr,
- determination of substrate concentration by FTIR absorption spectroscopy (*Nicolet Magna 550*),
- active sampling onto adsorption tubes,
- thermal desorption and GC-FID analysis.

These procedures allowed the calibration of the whole measurement system, from the sampling tubes to the gas chromatograph. The calibration samples were analysed with the same procedure as the ambient samples. As a reference compound for all oxygenated species analysed with *HP GC 5840A* 1-propanol was used. The calibration curve of this compound with the response factor ($1.09E+14 \pm 5.06E+12$) area/g is presented by figure 2.18.

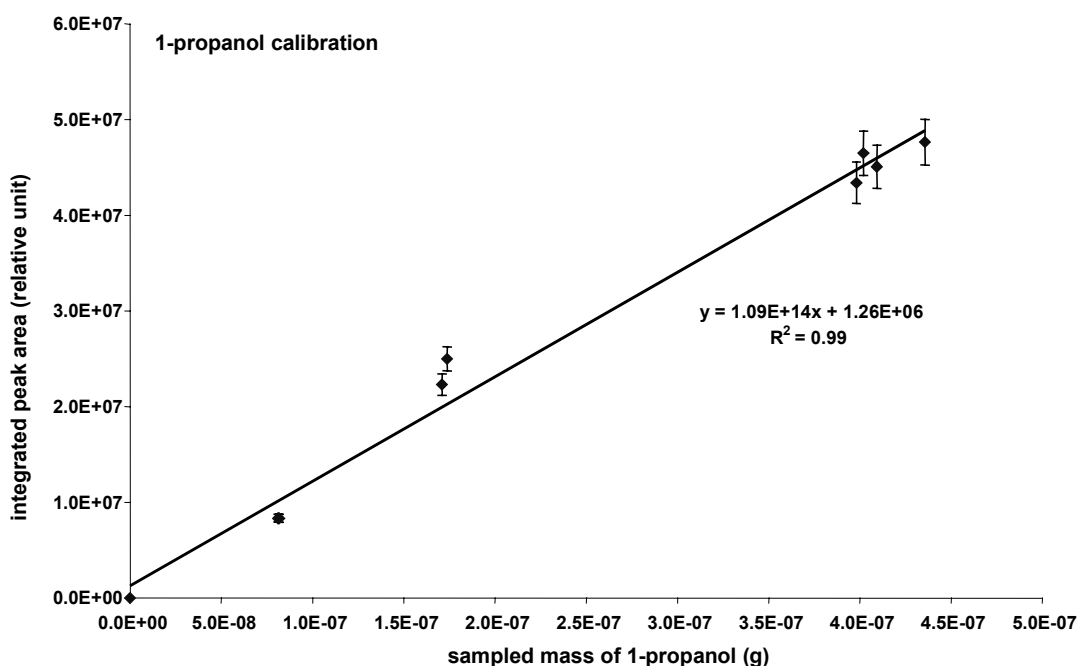


Figure 2.18: Calibration curve for 1-propanol

Table 2.11: Response factors of hydrocarbons (*HP GC 6890*) and oxygenated species (*HP GC 5840A*)

compounds	RF (area/g)	± (area/g)
hydrocarbons <i>HP GC 6890</i>	1.36E+10	1.54E+08
oxygenated species <i>HP GC 5840A</i>	1.09E+14	5.06E+12

2.2.5 Detection limits and precision

Detection limit

The detection limit of an analytical procedure understood as the lowest amount of analyte in a sample which can be detected and the quantitation limit understood as the lowest amount of analyte in a sample which can be quantitatively determined with suitable precision and accuracy were determined according to DIN 32645. The detection limit of the component can be determined by a blank method or by a calibration method. In the present study the calibration method was used. The following formula was applied:

$$x_{dl} = \frac{y_c - a}{b} \quad [2.2]$$

with x_{dl} : detection limit in g,
 a : intercept of the calibration function (in g),
 b : slope of the calibration function (in area/g),
 y_c : critical value of the signal (in area).

The critical value y_c was calculated as a sum of the intercept a of the calibration function and three times the standard deviation ($3\sigma_a$) of this intercept. To obtain the detection limits the calibration was performed in the concentration range not higher than $10x x_{dl}$. As quantitation limit x_{qt} three times of the calculated detection limits were taken. As a calibration standard for hydrocarbons the NPL gas mixture (table B.1, Annex B) was used. The sample was introduced directly into the preconcentrator/GC system, omitting the analytical steps of adsorption tube sampling and thermal desorption.

Tables 2.12 shows a list of detection limits determined for different hydrocarbons.

Table 2.12: Detection limits and quantitation limits of different hydrocarbons (NPL compounds, *HP GC 6890*)

	compounds	detection limit		quantitation limit	
		(g)	($\mu\text{g}/\text{Nm}^3$) ¹ in 6000 ml sample	(g)	($\mu\text{g}/\text{Nm}^3$) ¹ in 6000 ml sample
1	<i>ethene</i>	3.75E-11	0.006	7.50E-11	0.013
2	<i>ethyne</i>	4.76E-11	0.008	9.53E-11	0.016
3	<i>ethane</i>	9.06E-11	0.015	1.81E-10	0.030
4	<i>propene</i>	4.71E-11	0.008	9.43E-11	0.016
5	<i>propane</i>	6.30E-11	0.010	1.26E-10	0.021
6	<i>propyne</i>	7.11E-11	0.012	1.42E-10	0.024
7	<i>i-butane</i>	5.47E-11	0.009	1.09E-10	0.018
8	<i>1-butene</i>	3.20E-11	0.005	6.41E-11	0.011
9	<i>i-butene</i>	3.22E-11	0.005	6.45E-11	0.011
10	<i>1,3-butadiene</i>	4.64E-10	0.077	9.28E-10	0.155
11	<i>n-butane</i>	1.33E-10	0.022	2.66E-10	0.044
12	<i>trans-2-butene</i>	4.86E-11	0.008	9.71E-11	0.016
13	<i>cis-2-butene</i>	5.46E-11	0.009	1.09E-10	0.018
14	<i>i-pentane</i>	6.70E-11	0.011	1.34E-10	0.022
15	<i>n-pentane</i>	4.20E-11	0.007	8.39E-11	0.014
16	<i>isoprene</i>	8.02E-11	0.013	1.60E-10	0.027
17	<i>trans-2-pentene</i>	5.88E-11	0.010	1.18E-10	0.020
18	<i>cis-2-pentene</i>	7.40E-11	0.012	1.48E-10	0.025
19	<i>2-methylpentane</i>	1.27E-11	0.002	2.53E-11	0.004
20	<i>3-methylpentane</i>	3.12E-11	0.005	6.25E-11	0.010
21	<i>n-hexane</i>	2.54E-11	0.004	5.08E-11	0.008
22	<i>benzene</i>	3.67E-11	0.006	7.34E-11	0.012
23	<i>cyclohexane</i>	1.80E-11	0.003	3.60E-11	0.006
24	<i>n-heptane</i>	1.62E-12	0.000	3.25E-12	0.001
25	<i>toluene</i>	4.67E-11	0.008	9.33E-11	0.016
26	<i>ethylbenzene</i>	5.16E-11	0.009	1.03E-10	0.017
27	<i>m-xylene</i>	3.11E-11	0.005	6.22E-11	0.010
28	<i>o-xylene</i>	4.18E-11	0.007	8.36E-11	0.014
29	<i>1,3,5-trimethylbenzene</i>	1.79E-11	0.003	3.58E-11	0.006
30	<i>1,2,4-trimethylbenzene</i>	1.15E-10	0.019	2.31E-10	0.038

¹ concentration calculated for normal conditions (273,15 K and 1 atm)

For the non-NPL hydrocarbons and for unknown compounds determined with *HP GC 6890* the detection limit of 2.54E-11 g (0.004 $\mu\text{g}/\text{m}^3$ in 6000 ml sample) and the quantitation limit of 5.08E-11 g (0.008 $\mu\text{g}/\text{m}^3$ in 6000 ml sample), calculated from the calibration curve of all NPL compounds (figure 2.17), were taken.

For oxygenated compounds the detection limit was calculated on the basis of the baseline noise of the chromatograms measured by *HP GC 5840A*. The smallest area which could be unambiguously detected as a compound peak was accepted as detection limit. Consequently, the detection limit of $9.17\text{E-}12$ g ($0.002 \mu\text{g}/\text{m}^3$ in 6000 ml sample) and the quantitation limit of $2.75\text{E-}11$ g ($0.005 \mu\text{g}/\text{m}^3$ in 6000 ml sample) were taken.

Precision

The precision of the method defined as a measure of agreement (the standard deviation) among the results from repeated measurements of the same concentration under identical condition were determined by using the standard gas mixtures (NPL, table B.1, Annex B and custom made gas mixture with 17 oxygenated compounds OXY, table B.3, Annex B). This parameter describes the precision of preconcentrator/GC system without considering of the tube sampling and thermal desorption. Table 2.13 presents the results of these measurements using the NPL and OXY gas mixtures.

Table 2.13: The average precision for the measurements of different hydrocarbons (NPL compounds) and oxygenated species (OXY compounds)

	hydrocarbons	precision (%)	oxygenated	precision (%)
1	<i>ethene</i>	6.68	<i>acetone</i>	8.19
2	<i>ethyne</i>	2.66	<i>methyl acetate</i>	8.71
3	<i>ethane</i>	6.00	<i>ethyl acetate</i>	10.64
4	<i>propene</i>	5.85	<i>methanol</i>	12.07
5	<i>propane</i>	4.28	<i>2-butanone</i>	11.69
6	<i>propyne</i>	4.72	<i>isopropyl acetate</i>	14.16
7	<i>i-butane</i>	7.40	<i>2-propanol</i>	12.52
8	<i>1-butene</i>	3.61	<i>ethanol</i>	13.20
9	<i>i-butene</i>	3.61	<i>propyl acetate</i>	8.80
10	<i>1,3-butadiene</i>	3.94	<i>isobutyl acetate</i>	12.00
11	<i>n-butane</i>	4.98	<i>hexanone</i>	10.37
12	<i>trans-2-butene</i>	5.14	<i>2-butanol</i>	7.59
13	<i>cis-2-butene</i>	4.40	<i>1-propanol</i>	8.95
14	<i>i-pentane</i>	4.38	<i>butyl acetate</i>	12.37
15	<i>n-pentane</i>	3.22	<i>2-hexanone</i>	11.21
16	<i>isoprene</i>	5.35	<i>1-butanol</i>	6.24
17	<i>trans-2-pentene</i>	3.40	<i>cyclohexanone</i>	9.40
18	<i>cis-2-pentene</i>	5.62		
19	<i>2-methylpentane</i>	3.08		
20	<i>3-methylpentane</i>	2.93		
21	<i>n-hexane</i>	2.30		
22	<i>benzene</i>	3.12		
23	<i>cyclohexane</i>	3.47		
24	<i>n-heptane</i>	4.23		
25	<i>toluene</i>	3.53		
26	<i>ethylbenzene</i>	6.94		
27	<i>m-xylene</i>	4.96		
28	<i>o-xylene</i>	9.04		
29	<i>1,3,5-trimethylbenzene</i>	4.18		
30	<i>1,2,4-trimethylbenzene</i>	6.75		

On average, the precision of the hydrocarbon measurements was 5% (alkanes – 6%, alkenes – 4% and aromatics – 5%) whereas for oxygenated species the obtained precision was 11% (alcohols – 11%, esters – 10%, ketones – 11%). The low reproducibility of isopropyl acetate was caused by some difficulties with the peak integration of this compound.

The precision of the preconcentrator/GC system was compared with the precision of the duplicated pairs of sampling tubes, which describes a measure of agreement among the results from repeated measurements using all sampling tubes followed by thermal desorption, preconcentration and GC/FID analysis (chapter 2.2.1 Adsorption tubes, Tube parameters). The comparison shows that the use of absorption tubes as sampling device lowers the average measurement precision of investigated compounds from 8 to 17%.

2.2.6 Identification and integration

The identification of hydrocarbons and oxygenated species were basically performed by the GC retention time of single compounds, by comparing the ambient air chromatograms with the chromatograms of standard gas mixtures. Peaks of hydrocarbons were identified by the National Physics Laboratory (NPL) standard gas mixture with 30 compounds (table B.1 in Annex B). Additionally a custom made synthetic air mixture with 62 compounds (RM2, table B.2 in Annex B) was used to identify the investigated species. In the case of unknown peaks, synthetic air mixtures of single compound were prepared in a 405 l reaction chamber under atmospheric conditions (298 K and 760 Torr) and analysed by direct injection to the Preconcentrator/GC system. Since the capillary column used for hydrocarbons separation was non-polar (HP-1, chapter 2.2.3: Steps in sample analysis) the specific retention times of most of the compounds were correlated with their boiling points and chemical structure.

The 62-compounds gas mixture (RM2) was frequently analysed during the measurement series to check the stability of retention time of analysed compounds and to proof the identification and integration quality. The typical chromatogram of RM2 is presented by figure 2.19.

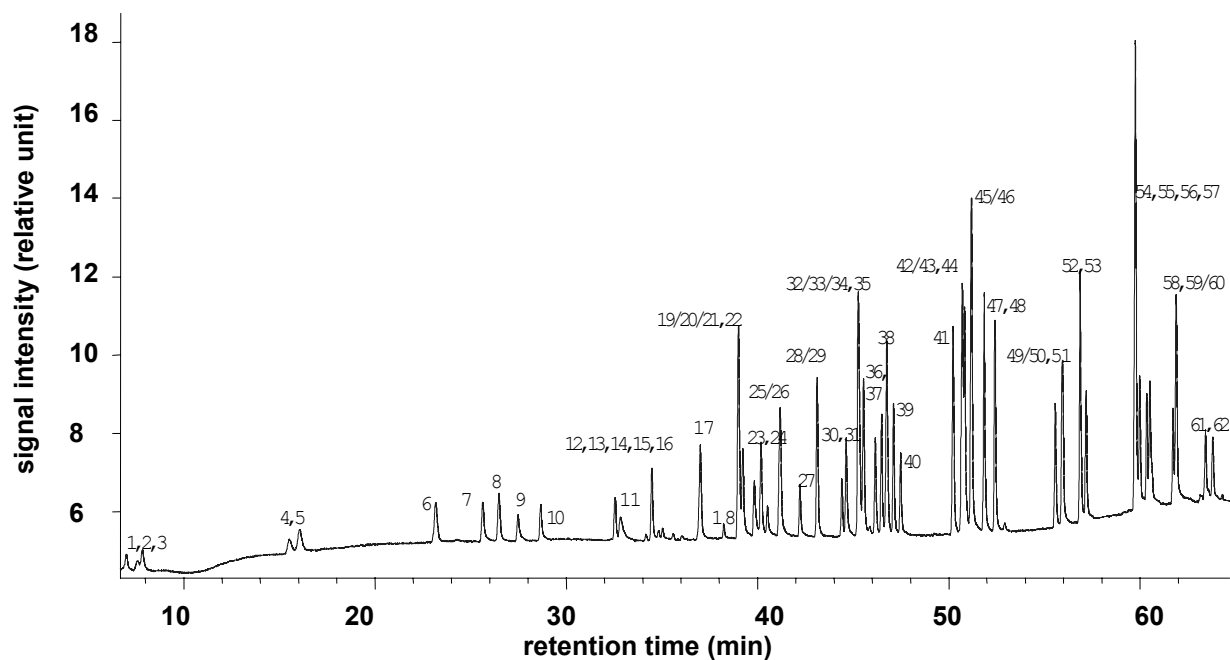


Figure 2.19: A typical chromatogram of RM2 gas mixture containing 62 C₂-C₁₀ hydrocarbons

compounds: ¹ethene, ²ethyne, ³ethane, ⁴propene, ⁵propane, ⁶i-butane, ⁷i-butene, ⁸n-butane, ⁹trans-2-butene, ¹⁰cis-2-butene, ¹¹i-pentane, ¹²1-pentene, ¹³n-pentane, ¹⁴isoprene, ¹⁵trans-2-pentene, ¹⁶cis-2-pentene, ¹⁷2,2-dimethylbutane, ¹⁸cyclopentene, ¹⁹methyl-tert-butyl ether, ²⁰2,3-dimethylbutane, ²¹cyclopentane, ²²2-methylpentane, ²³3-methylpentane, ²⁴1-hexene, ²⁵n-hexane, ²⁶2-ethyl-1-butene, ²⁷2,3-dimethyl-1,3-cyclohexadiene, ²⁸methylcyclopentane, ²⁹1-methyl-1-cyclopentene, ³⁰2,3-dimethyl-2-butene, ³¹benzene, ³²cyclohexane, ³³2,3-dimethylpentane, ³⁴1,3-cyclohexadiene, ³⁵methylhexane, ³⁶cyclohexene, ³⁷1-heptene, ³⁸2,2,4-trimethylpentane, ³⁹n-heptane, ⁴⁰1,4-cyclohexadiene, ⁴¹2,3,4-trimethylpentane, ⁴²toluene, ⁴³2-methylpentane, ⁴⁴3-methylpentane, ⁴⁵4-methylpentane, ⁴⁶1-methyl-1-cyclohexene, ⁴⁷1-octene, ⁴⁸n-octane, ⁴⁹ethylbenzene, ⁵⁰m-xylene, ⁵¹p-xylene, ⁵²styrene, ⁵³o-xylene, ⁵⁴α-pinene, ⁵⁵n-propylbenzene, ⁵⁶4-ethyltoluene, ⁵⁷1,3,5-trimethylbenzene, ⁵⁸n-decane, ⁵⁹1,2,4-trimethylbenzene, ⁶⁰tert-butylbenzene, ⁶¹1,2,3-trimethylbenzene, ⁶²1,2,3,4-tetramethylbenzene

It was observed that the retention time was stable within small deviations, the relative standard deviation (1σ) for all NPL compounds stayed during the whole measurement period (2001-2004) between 0.1–3.5%. However, some baseline changes were observed. According to this, the automatic integration performed by the *HP GC 6890* software, the *HP Chem Station*, was often not satisfying. Therefore, every chromatogram was additionally hand-integrated. In the case of some coeluted compounds the peak separation was performed by means of the *Origin* programme. The software fits the Gauss curves in coeluted peaks and separates them without significant losses or gains of the integrated peak area. Figure 2.20 shows a typical example of *Origin* separation.

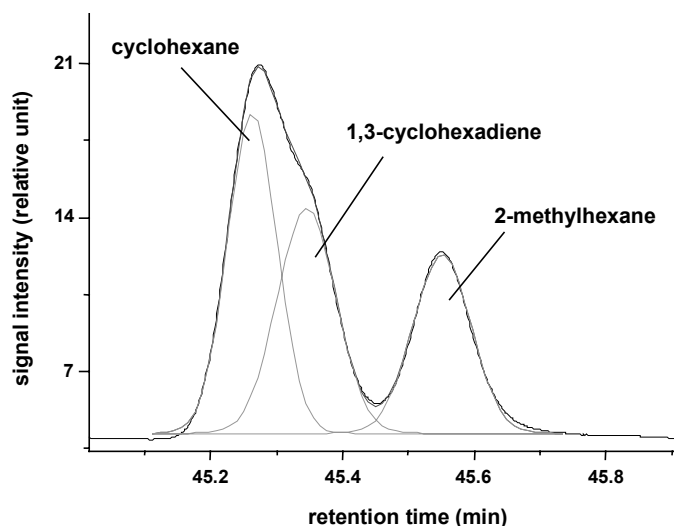


Figure 2.20: Separation of the coeluted peaks using the *Origin* programme

The peak identification for oxygenated compounds was made by comparing the retention times of the analysed compounds with those of pure liquid standards. Synthetic air mixtures were prepared in a 405 l reaction chamber under atmospheric conditions (298 K and 760 Torr) and analysed by direct injection into the preconcentrator/GC system. Additionally, for 17 selected compound the synthetic air gas mixture was prepared in a 20 l steel gas cylinder (OXY mixture, table B.3 in Annex B). This mixture was afterwards used to check the stability of the retention time of the analysed compounds and to proof the identification and integration quality. The typical chromatogram of OXY is shown by figure 2.21.

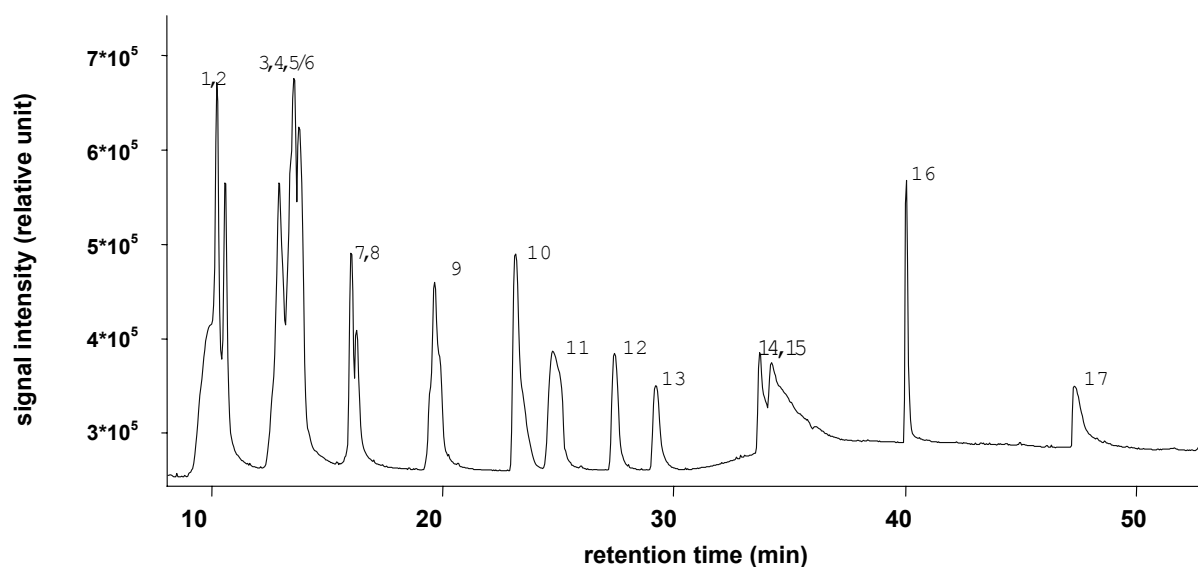


Figure 2.21: A typical chromatogram of OXY gas mixture containing 17 oxygenated compounds

compounds: ¹acetone, ²methyl acetate, ³ethyl acetate, ⁴methanol, ⁵2-butanone, ⁶isopropyl acetate, ⁷2-propanol, ⁸ethanol, ⁹propyl acetate, ¹⁰isobutyl acetate, ¹¹hexanone, ¹²2-butanol, ¹³1-propanol, ¹⁴butyl acetate, ¹⁵2-hexanone, ¹⁶1-butanol, ¹⁷cyclohexanone

Since the capillary column used for separation of oxygenated compounds was polar (DB-WAX, chapter 2.2.3: Steps in sample analysis), the specific retention times of oxygenated components were correlated with their boiling points. The integration was performed with the *Borwin* software. Similarly as for hydrocarbons, the automatic integration could not be used because of baseline changes. Every chromatogram had to be integrated by hand. Finally, from about 200 peaks detected in the GC-FID signals from ambient air analysis, 68 hydrocarbons and 18 oxygenates species could be identified, integrated and quantified.

2.2.7 Concentration determination

The concentrations ($\mu\text{g}/\text{m}^3$) of the individual hydrocarbons and oxygenated species were in practice determined by comparing the response factor (peak area/g, chapter 2.2.4: Calibration procedure) of the component, calculated from the calibration with the peak area produced from the sample analysis.

In a first step the obtained integrated peak area of a particular compound was reduced by the area of the background tube signal (chapter 2.2.1: Adsorption tubes, Tube parameters) for corresponding species, according to the formula:

$$PAC_i = PA_i - PAB_i \quad [2.3]$$

with PAC_i : corrected area of i -component,
 PA_i : integrated peak area for that component,
 PAB_i : integrated peak area for i -component in a particular tube background signal.

Thereafter, the absolute mass of the sampled compound was calculated from the formula:

$$m_i = \frac{PAC_i}{RF_i * RR_i} \quad [2.4]$$

with m_i : total sampled mass of i -component in g,
 PAC_i : corrected peak area for that component,
 RF_i : response factor in peak area pro g,
 RR_i : tube recovery rate (chapter 2.2.1: Adsorption tubes, Tube parameters) of i -compound.

To obtain the ambient air concentration ($\mu\text{g}/\text{m}^3$) of a particular compound the received total sampled mass (g) was recalculated per sampling volume using the following formula:

$$c_i = \frac{m_i * 1E + 06 * 1E + 06}{V_i} \quad [2.5]$$

with c_i : ambient concentration of i -component,
 V_i : sampled air volume in Nml (ml in normal conditions: 273.15K and 1 atm),
 1E+06: recalculation factor from g to μg ,
 1E+06: recalculation factor from ml to m^3 .

The statistical error for the determined concentration of the compound was performed using the Gauss law of error propagation, which defines the standard error. The final formula for the concentration of the component i is the following:

$$c_i = \frac{PAC_i * 1E + 12}{RF_i * RR_i * V_i} \quad [2.6]$$

The standard error Δc_i was calculated as the square root over the sum of the products of the square of the partial derivative of function c_i with respect to the particular variable and its square of the standard error:

$$\Delta c_i = \sqrt{\left(\frac{\partial c_i}{\partial PAC_i}\right)^2 * \Delta PAC_i^2 + \left(\frac{\partial c_i}{\partial RF_i}\right)^2 * \Delta RF_i^2 + \left(\frac{\partial c_i}{\partial RR_i}\right)^2 * \Delta RR_i^2 + \left(\frac{\partial c_i}{\partial V_i}\right)^2 * \Delta V_i^2} \quad [2.7]$$

After some simplification, the relative error $\frac{\Delta c_i}{c_i}$ was calculated from the following formula:

$$\frac{\Delta c_i}{c_i} = \sqrt{\left(\frac{\Delta PAC_i}{PAC_i}\right)^2 + \left(\frac{\Delta RF_i}{RF_i}\right)^2 + \left(\frac{\Delta RR_i}{RR_i}\right)^2 + \left(\frac{\Delta V_i}{V_i}\right)^2} \quad [2.8]$$

with $\frac{\Delta PAC_i}{PAC_i}$ the relative error of the peak area of the manual integration, which was 1 - 5%,

$\frac{\Delta RF_i}{RF_i}$ the relative error of response factor coming from the calibration, the standard deviation value and in the case of oxygenated species additionally the error coming from FTIR measurements and liquid standard; for the hydrocarbons the error was in the range 10 - 20% and for oxygenated species it was 20%,

$\frac{\Delta RR_i}{RR_i}$ the relative error of the tube recovery rate, the standard deviation value in the range 10 - 20%,

$\frac{\Delta V_i}{V_i}$ the relative error of the sampling volume, which was 1 - 2%.

For the NMVOC concentrations below the detection limits the error was assumed as half of the detection limit value.

2.2.8 Comparison with other analytical system

The comparison of the measurement method with other analytical systems is very important for the quality assurance of the measurements and provides information about the appropriateness of the accepted analytical procedures.

The measurement system for hydrocarbons, consisting of adsorption tubes, an enrichment device (*Preconcentrator 7100*) and a gas chromatograph (*HP GC 6890*) with a non-polar column and a FID detector was compared with the quasi-online instrument *Airmovac 2010* gas chromatograph from *Airmotec*. This instrument was also equipped with a non-polar capillary column (DB-5), adsorption tubes as a sampling device, an enrichment system (cryo-trap) and a FID detector. The detection limit of *Airmovac 2010* for investigated hydrocarbons was in the pptV range (Gomes, 2002).

For comparison measurements were taken, which have been obtained during the ARTEMIS (Assessment and Reliability of Transport Emission Models and Inventory Systems, EU project) campaign carried out in the Mersey traffic tunnel in Liverpool, England, in February 2003. Parallel measurements of the tunnel air were executed by using one common sampling line.

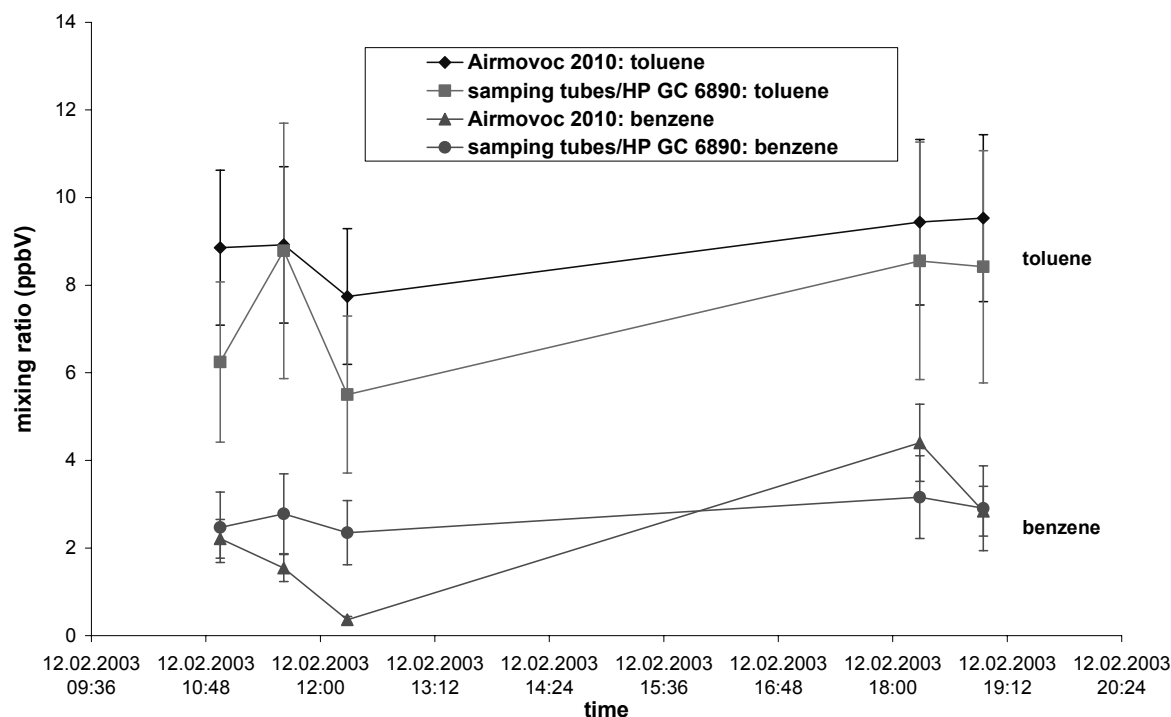


Figure 2.22: Mixing ratio - time correlation plots of toluene and benzene measured by two different analytical instruments, ARTEMIS 2003

The results of the measurements using tube sampling/GC-FID analysis and quasi-online GC-FID analysis show a quite good correlation for measured hydrocarbons, as it can be seen in figure 2.22 where time correlation plots for toluene and benzene are presented. The average correlation factor for 2-methylpentane, 3-methylpentane, n-hexane, benzene, toluene, ethylbenzene, m,p-xylene, and o-xylene amounted to 0.80 ± 0.10 for HP GC 6890/Airmovoc 2010.

In the case of oxygenated species the intercomparison with other systems was performed during the ZITTEX campaign (DBU project: "Atmospheric Diagnostic") carried out in Zittau, Germany, in May 2002 (Wiesen (ed.), 2002). The method used for the purpose of this study, based on adsorption tube sampling, enrichment process (*Preconcentrator 7100*) and gas chromatography analysis (*HP GC 6890*) with polar column and FID detector was compared with the derivatisation/GC-ECD/MS method. The carbonyl measurements were performed by the Technical University Darmstadt, based on the sampling of carbonyl compounds on cartridges activated with pentafluorobenzylhydriochloride (PFBAH), analyte elution with hexane and gas chromatography analysis with electron capture detection (ECD) and mass spectroscopy identification (Schlowski, 2000). As the reference compound 2-butanone in ambient air was used. Figure 2.23 presents time-correlation plots for both methods.

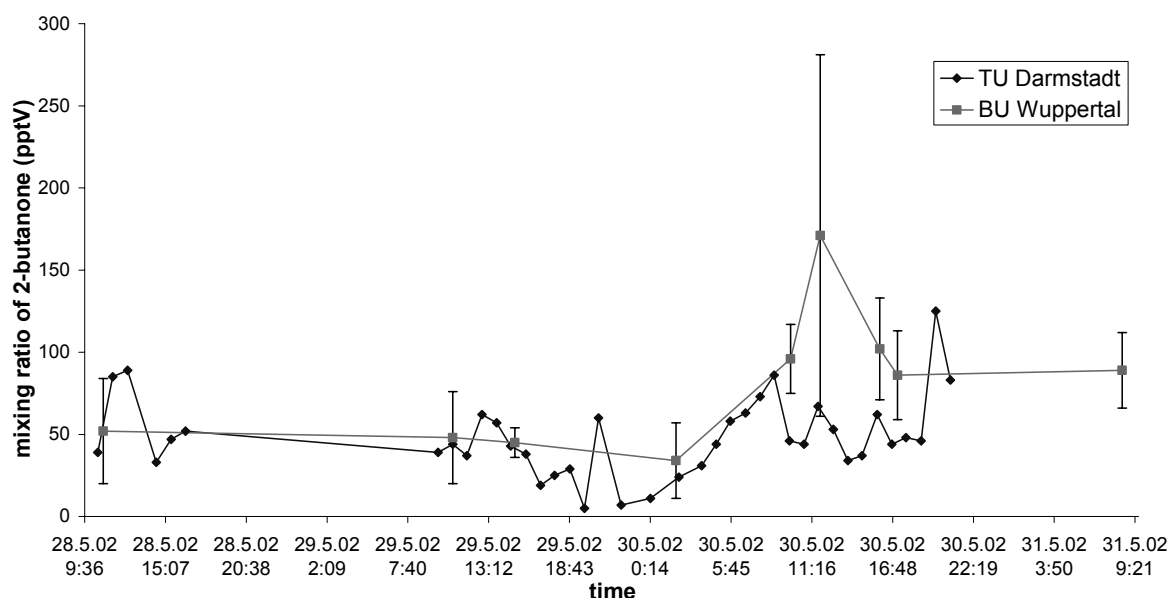


Figure 2.23: Mixing ratio - time correlation plots of 2-butanone measured by two different methods, ZITTEX 2002

The results of the 2-butanone measurements by tube sampling/GC-FID analysis and derivatisation/GC-ECD/MS analysis show a quite good correlation. Even with the different time resolution of both method, the same trend in diurnal variations can be observed.

Both field measurements indicate the suitability of the selected GC/FID method and the application of adsorption tubes as sampling device for the measurements of hydrocarbons and oxygenated compounds under low ambient concentrations.

2.3 Equipment for measuring CO, CO₂, NO_x, SF₆ and meteorological parameters

To obtain a better characterisation of the city air of Wuppertal, besides NMVOC some other atmospheric compounds were also measured in the frame of this work. During the campaigns the measurements were performed by means of automatic analysers for:

- carbon monoxide,
- carbon dioxide,
- nitrogen oxides (nitrogen monoxide and nitrogen dioxide),
- sulphur hexafluoride.

Additionally, meteorological parameters were determined. Measurements were carried out by a car equipped with the hydrocarbons sampling system and other automatic analysers.

2.3.1 Carbon monoxide

The carbon monoxide (CO) was analysed with the automatic gas analyser from *Aero-Laser GmbH*, model *AL 5002*. The measurement method is based on the fluorescence of CO excited by a CO-lamp (VUV light at 150 nm). The fluorescence in the wavelength range between 160 – 190 nm is detected by a photomultiplier connected to a fast counter. Calibration of the instrument was made with the standard gas of CO. The measurement of *AL 5002* ranged from 1 ppbV up to 100 ppmV.

2.3.2 Carbon dioxide

The measurements of carbon dioxide (CO₂) were performed with a compact automatic analyser *Carbondio 1000* from *Pewatron AG*. As a method for CO₂ detection the dual wavelength infrared method (NDIR) is used. The absorption spectra are measured in a wavelength range where CO₂ absorbs light (4.26 µm) and the reference spectra are measured outside of this range. Calibration of the instrument was made with the standard gas of CO₂. An example of the calibration curve is shown in figure 2.24. Measurement range of *Carbondio 1000* was up to 1000 ppmV.

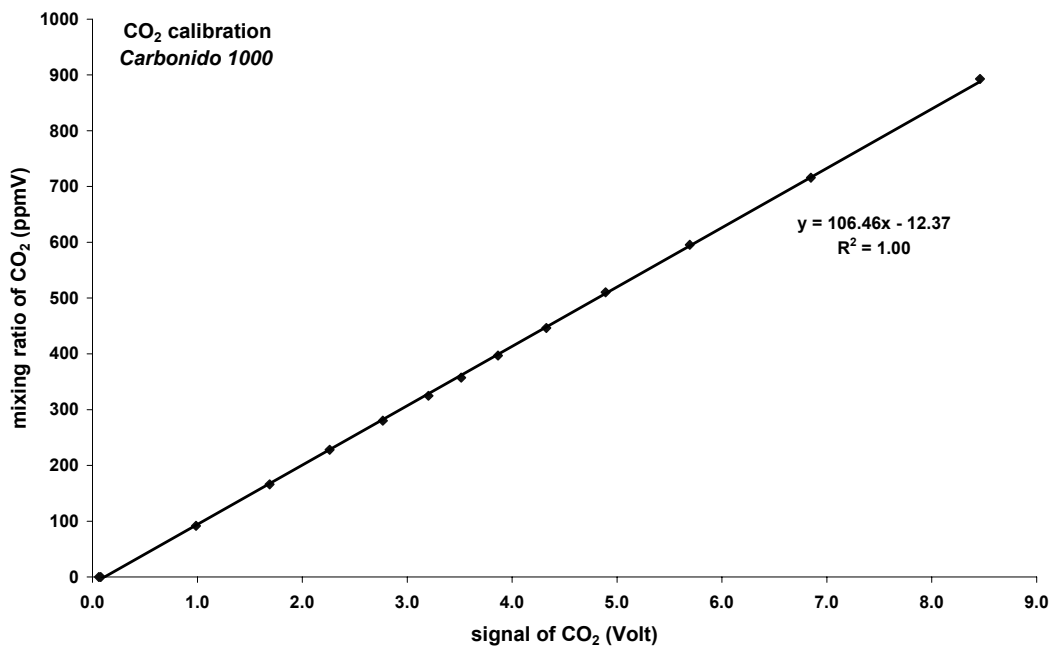


Figure 2.24: Calibration curve for CO₂ using the *Carbondio 1000* instrument

2.3.3 Nitrogen oxides

Nitrogen oxide (NO) and nitrogen dioxide (NO₂) were measured with a *LMA-3D* analyser from *Unisearch Associates INC.* The instrument detects the presence of NO₂ via chemiluminescence. The chemiluminescence in the region of 425 nm is produced by luminol in contact with NO₂ in the presence of O₂. The chemiluminescence is measured by a photomultiplier and converted into a signal that is proportional to the mixing ratio of NO₂ in the sampled air. The measurements of NO_x (NO + NO₂) are performed by using a chrome oxide converter, which oxidises NO to NO₂, before the luminol oxidation. Calibration of the instruments was made with standard mixtures of NO and NO₂. The measurement of the instrument ranged from 10 pptV up to 2 ppmV. An example of the calibration curve of NO₂ using *LMA-3D* is presented by figure 2.25.

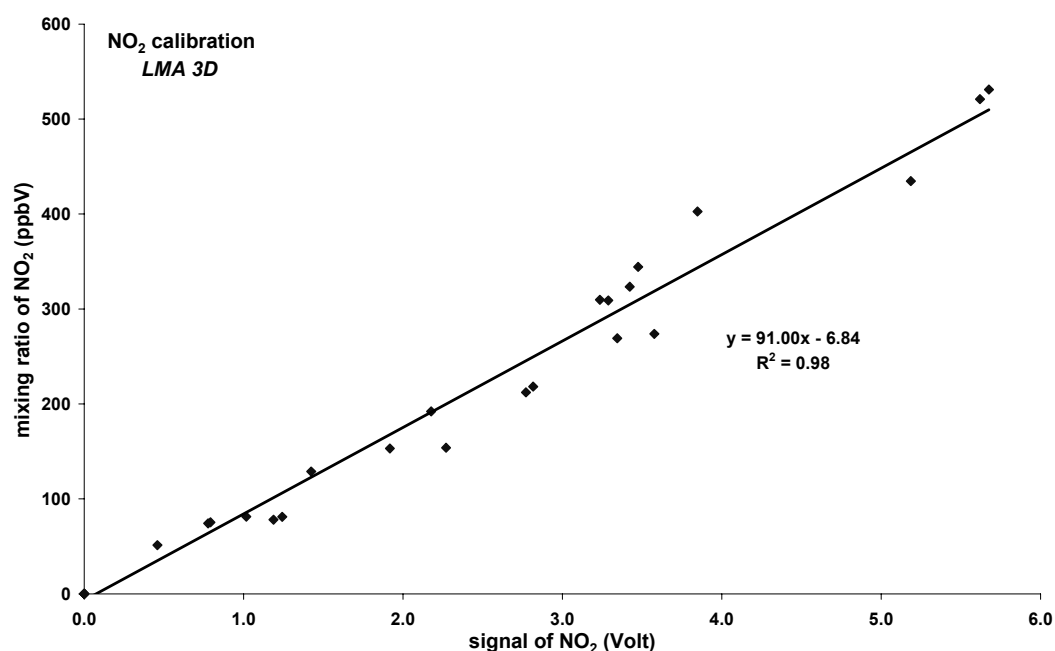


Figure 2.25: Calibration curve for NO₂ using the *LMA 3D* instrument

2.3.4 Sulphur hexafluoride

Sulphur hexafluoride (SF₆) was used as a tracer for a contaminated plume. SF₆ was emitted up-wind from the investigated emission point and measured down-wind. To analyse the SF₆ a *GC A-TCD/ECD* monitor from *Chromato Sud* was used. It contains a multi-valve port, a 1.3 m precolumn (Porapak Q 80-100 mesh) and a 2 m analytical column (Porapak Q 80-100 mesh) with a electron capture detector (ECD). The system was calibrated with standard SF₆ gas.

2.3.5 Meteorological parameters

For the measurement of meteorological parameters the compact *Meteo-station* from *Conrad Electronic GmbH* was used. The instrument measured the following parameters:

- temperature,
- air pressure,
- wind direction,
- wind speed,
- relative humidity.

2.4 Measurement sites in Wuppertal

During three campaigns performed in September 2001, August/September 2002 and October 2003 concentrations were measured in different city areas of Wuppertal and near known sources of NMVOCs. Measurements were carried out from a car (figure 2.26) equipped with a NMVOC sampling system (chapter 2.2.2: Sampling collection) and automatic analysers for the detection of carbon monoxide, carbon dioxide, nitrogen oxides and sulphur hexafluoride. In addition, a small meteorological station was installed in the car (chapter 2.3: Measurement equipment for CO, CO₂, NO_x, SF₆ and meteorological parameters). Table 2.14 summarised the measurements performed during all campaigns.



Figure 2.26: View of the car installed with the instruments used for the measurements carried out in Wuppertal

Table 2.14: Summary of the measurements performed during the measurement campaigns carried out in Wuppertal

	sampling sites	sampling time		measured compounds
September 2001	Kiesberg Tunnel, traffic	18.09.01	11:20-12:20	NMVOC
	Blücher Str., PPG	18.09.01	13:20-14:20	NMVOC
	Hatzfelder Str., Du Pont	18.09.01	15:20-16:20	NMVOC
	Girardet Str., ambient air	19.09.01	11:10-12:10	NMVOC
August/ September 2002	Uni, ambient air	22.08.02	15:06-16:06	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Kiesberg Tunnel, traffic	23.08.02	9:51-10:36	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Kiesberg Tunnel, traffic	23.08.02	10:53-11:38	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Kiesberg Tunnel, traffic	25.08.02	17:50-18:35	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Kiesberg Tunnel, traffic	25.08.02	18:44-19:29	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Bundesallee, intersection	26.08.02	15:35-16:35	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Bundesallee, intersection	26.08.02	16:40-17:40	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Im Johannistal, ambient air	27.08.02	15:55-17:05	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Im Johannistal, ambient air	27.08.02	17:12-18:24	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Wilkhaus Str., DuPont	29.08.02	13:06-14:10	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Hatzfelder Str., DuPont	29.08.02	14:55-15:55	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Simon Str., Bayer	03.09.02	10:35-11:40	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Bissing Str., PPG	03.09.02	12:52-13:52	NMVOC, CO, CO ₂ , NO ₂ , NO, meteo
	Lützwow Str., PPG	04.09.02	14:29-15:30	NMVOC, CO, NO ₂ , NO, meteo
	Viehhof Str., Conrads	04.09.02	16:17-17:17	NMVOC, CO, NO ₂ , NO, meteo
	Conrads-Uni, driving	04.09.02	17:31-17:45	NMVOC, CO, NO _x
	A46, driving	05.09.02	13:06-13:27	NMVOC, CO, CO ₂ , NO _x
	Bundesallee, driving	05.09.02	14:11-14:57	NMVOC, CO
	A46/A3, driving	05.09.02	17:12-18:11	NMVOC, CO, CO ₂ , NO _x
	A3/A46, driving	06.09.02	09:23-10:23	NMVOC, CO, CO ₂ , NO ₂ , NO
October 2003	Bissing Str., PPG	13.10.03	13:06-14:06	NMVOC+background, CO ₂ , NO ₂ , NO, SF ₆ , meteo
	Hatzfelder Str., DuPont	15.10.03	12:55-14:00	NMVOC+background, CO ₂ , NO ₂ , NO, SF ₆ , meteo
	Simon Str., Gorn	17.10.03	09:45-10:55	NMVOC+background, CO ₂ , NO ₂ , NO, meteo

2.4.1 Road traffic

In order to create the NMVOC emission profiles for road traffic, measurements were performed in areas representative for major traffic conditions. Air samples were taken:

- in a traffic tunnel (Kiesberg Tunnel),
- downtown at a street intersection,
- during the drives in the city centre of Wuppertal and on free-ways.

Kiesberg Tunnel

The Kiesberg Tunnel is located in the city of Wuppertal and connects the free-way A46 between Düsseldorf and Wuppertal with the centre of Wuppertal Elberfeld. The tunnel has a length of 1.1 km and consist of two independent tubes in east-west direction. During the measurements the samples were collected inside the tunnel, roughly 10 meters from the outlet of the tube direction Wuppertal Elberfeld, as it can be seen on figure 2.27(a).

Due to the close position of the free-way A46 it was assumed that the cars passing the tunnel were under “warm” driving conditions. It was also assumed that the air at the measurement point was well mixed over the whole tunnel length by the turbulence caused by the traffic flow.

The investigation of the tunnel air were performed during the first campaign, 18.09.01 and the second campaign, 23.08.02 (Friday) and 25.08.02 (Sunday).



Figure 2.27: View of the sampling sites in the Kiesberg Tunnel (a) and at the street intersection at Bundesallee (b)

Street intersection

For the investigation of the traffic emission by “stop and go” driving conditions a larger street intersection located in the centre of Wuppertal Elberfeld was chosen. Samples were collected at the Bundesallee (B7), directly at the intersection, in-between two street lines. The

position of the sampling port is presented by figure 2.27(b). The measurements were performed during the second campaign, on 26.08.02.

Driving

To characterise the traffic emission samples were also collected during drives in the city centre of Wuppertal and on free-ways. During the second campaign, measurements were performed on 04.09.02 (driving in the city centre), 05.09.02 (driving at the free-way A46, in the city centre at B7, at the free-way A46/A3), 06.09.02 (driving at the free-way A3/A46). The sampling port was located outside the car, at about 1m above the road.

2.4.2 Solvent use

To obtain the NMVOC emission profiles for solvent use measurements were performed in the neighbourhood of various solvents factories and workshops in Wuppertal. The following factories were considered:

- DuPont Performance Coatings GmbH,
- PPG Industries Lacke GmbH,
- Bayer AG,
- Dr. Alfred Conrads Lackfabrick Nachf. KG,
- Karosseriebau Gorn GmbH.

Due to the fact that the emission from solvent factories is not limited only to point sources and is more likely spread over a larger area the direct determination of the emission strength was not possible. Because of this, the emission profiles of particular factories were measured down-wind of the source and in the background. Additionally, for better identification of the contaminated plume coming from the investigated source, tracer experiments were performed. Sulphur hexafluoride, used as a tracer gas, was emitted up-wind from the source and measured down-wind. The locations of the particular plants in Wuppertal are shown on maps C.1 – C.5 in Annex C.

DuPont Performance Coatings GmbH

DuPont Performance Coatings is the biggest producer of car coating products world-wide and the fourth biggest varnish factory. The branch in Wuppertal is specialised in the production of automotive coating systems, products for vehicle repair, coatings for plastic surface, coatings for metal surface, electrodeposition coatings, digital inks, protective coatings and special adhesives (DuPont Performance Coatings, 2004). DuPont Performance Coatings GmbH is located in Wuppertal Barmen and is the most important emitter of NMVOCs in Wuppertal with an annual emission (year 2000) of about 206 Mg (Landesumweltamt Nordrhein Westfalen, 2004).

To determine the emission profiles of the factory the measurements were performed at the sampling sites located close to the DuPont area (figure 2.28a). Measurements were carried out

during three campaigns (table 2.14), during the third campaign also background measurements and tracer experiments with SF₆ were carried out.

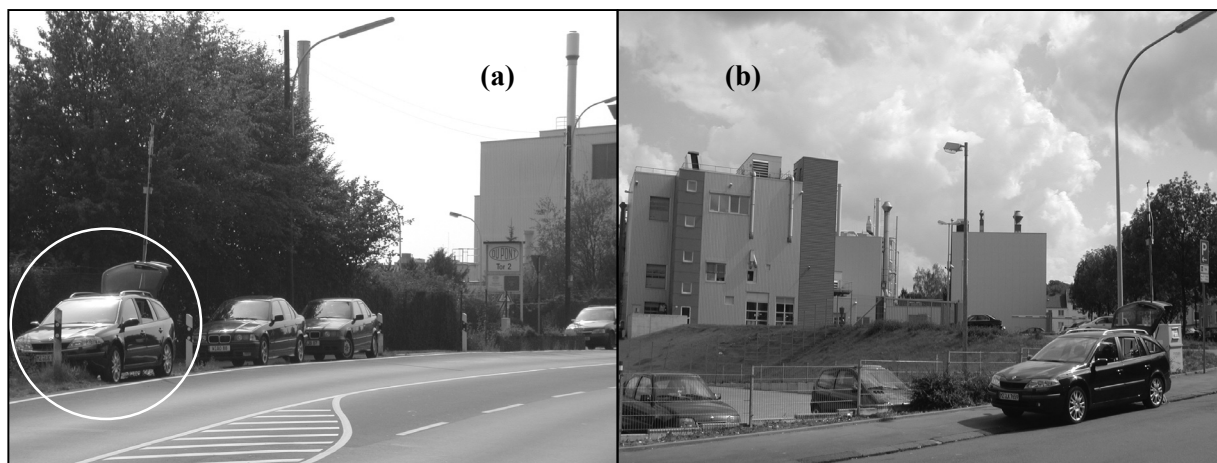


Figure 2.28: View of the sampling points for the DuPont Performance Coatings GmbH (a) and PPG Industries Lacke GmbH (b)

PPG Industries Lacke GmbH

PPG Industries Lacke GmbH is next of the biggest solvent producer in Wuppertal. The product range of the factory contains automobile and general industrial coatings, automobile repair coatings, coatings for the packaging industry, coil coating and coatings and sealings for the aircraft industry. PPG is located in Wuppertal Vohwinkel and belongs to the group of most important NMVOCs emitters in Wuppertal with an annual emission (year 2000) of about 6 Mg (Landesumweltamt Nordrhein Westfalen, 2004).

Measurements of the emission characteristics of PPG were performed during all campaigns (table 2.14). Sampling sites were located near the object (figure 2.28.b), down-wind from the factory. During the third campaign also background measurements and tracer experiments with SF₆ were carried out.

Bayer AG

The Bayer factory in Wuppertal is the oldest of the five plants of the Bayer AG in Germany. The Wuppertal Elberfeld branch produces pharmaceuticals but mainly chemical materials. The Bayer AG with its high emission of NMVOCs (about 51 Mg in year 2000) belongs also to the most important emitters in Wuppertal (Landesumweltamt Nordrhein Westfalen, 2004). To determine the NMVOC emission profiles of Bayer the measurements were performed during the second campaign (table 2.14). Sampling sites were located down-wind from the factory.

Dr. Alfred Conrads Lackfabrick Nachf. KG

Dr. Alfred Conrads Lackfabrick Nachf. KG is located in the Wuppertal Elberfeld and belongs to the 20 most important NMVOCs emitters in Wuppertal with an annual emission (year 2000) of about 2 Mg (Landesumweltamt Nordrhein Westfalen, 2004). Beside industrial and corrosion protection coatings, also a number of specialities for artists, architects and restorers belongs to the product assortment of the Conrads enterprise.

The investigation of the emission characteristic from the Conrads factory was performed during the second campaign (table 2.14). The sampling sites were located near the object, down-wind from the factory.

Gorn GmbH

The workshop Gorn located in Wuppertal Elberfeld was also investigated with respect to NMVOC emissions. The plant is mainly engaged in car repair coating. Measurements were performed during the second and third campaign (table 2.14). Sampling sites were located near the object, down-wind from the workshop.

2.4.3 Ambient air

To obtain the ambient NMVOC concentrations sampling were performed at different points located in Wuppertal. The sampling sites represented residential, industrial, mixed settings and areas down-wind from the city centre (table 2.15). The locations of the receptor points in Wuppertal, against the investigated solvent factories and workshops, are presented on map C.1 in Annex C.

Chapter 3

MEASUREMENT RESULTS

3.1 Ambient air mixing ratios

The measurements of NMVOCs, CO, CO₂, NO₂, NO and meteorological parameters were carried out in Wuppertal during three measurement campaigns performed in September 2001, August/September 2002 and October 2003 (chapter 2.4: Measurement sites in Wuppertal). Table 3.1 summarised the maximum, minimum, average and median mixing ratio of measured compounds.

Table 3.1.a: Overview of NMVOC and CO, CO₂, NO_x, NO, NO₂ mixing ratios (ppbV)¹ measured during the study carried out in Wuppertal

compounds	maximum	minimum	average	st. dev. ²	median
<i>propene</i>	1.060	0.056	0.345	0.250	0.234
<i>propane</i>	1.528	0.006	0.425	0.450	0.280
<i>propadiene</i>	0.091	0.001	0.008	0.017	0.002
<i>propyne</i>	0.055	0.001	0.011	0.015	0.007
<i>2-methylpropane</i>	0.739	0.018	0.236	0.190	0.172
<i>1-butene, i-butene</i>	2.570	0.279	0.861	0.530	0.712
<i>1,3-butadiene</i>	0.124	0.014	0.045	0.029	0.036
<i>n-butane</i>	1.161	0.026	0.408	0.346	0.283
<i>trans-2-butene</i>	0.227	0.022	0.068	0.053	0.049
<i>1-butyne</i>	0.047	0.001	0.008	0.008	0.007
<i>cis-2-butene</i>	0.191	0.016	0.057	0.048	0.037
<i>3-methyl-1-butene</i>	0.320	0.016	0.056	0.058	0.039
<i>2-methylbutane (i-pentane)</i>	5.485	0.224	1.197	1.228	0.818
<i>1-pentene</i>	1.827	0.029	0.203	0.334	0.131
<i>n-pentane, 2-methyl-1-butene</i>	9.763	0.095	1.128	1.791	0.637
<i>2-methyl-1,3-butadiene</i>	1.219	0.034	0.337	0.285	0.268
<i>trans-2-pentene</i>	2.130	0.013	0.197	0.398	0.081
<i>cis-2-pentene</i>	1.026	0.008	0.128	0.191	0.077
<i>2,2-dimethylbutane</i>	1.012	0.009	0.132	0.190	0.095
<i>cyclopentene</i>	0.293	0.005	0.044	0.056	0.024
<i>methyl tert-butyl ether</i>	1.190	0.010	0.273	0.259	0.181
<i>2,3-dimethylbutane, cyclopentane</i>	4.648	0.063	0.546	0.855	0.350
<i>2-methylpentane</i>	6.702	0.092	0.784	1.212	0.477
<i>3-methylpentane</i>	3.804	0.030	0.440	0.686	0.274
<i>1-hexene</i>	0.586	0.020	0.079	0.101	0.060

Table 3.1.b Overview of NMVOC and CO, CO₂, NO_x, NO, NO₂ mixing ratios (ppbV)¹ measured during the study carried out in Wuppertal

compounds	maximum	minimum	average	st. dev. ²	median
<i>n</i> -hexane, 2-ethyl-1-butene	3.747	0.081	0.527	0.690	0.384
2,3-dimethyl-1,3-butadiene	0.257	0.001	0.024	0.049	0.009
methylcyclopentane, 1-methyl-1-cyclopentene	5.239	0.055	0.580	0.954	0.355
2,3-dimethyl-2-butene	0.526	0.007	0.052	0.094	0.029
benzene	5.601	0.160	0.988	1.076	0.749
cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene	4.981	0.084	0.682	0.903	0.422
2-methylhexane	0.984	0.015	0.119	0.181	0.063
cyclohexene	0.105	0.003	0.018	0.019	0.013
1-heptene	0.865	0.019	0.115	0.153	0.078
2,2,4-trimethylpentane	2.891	0.040	0.322	0.520	0.196
<i>n</i> -heptane	1.843	0.048	0.274	0.338	0.163
1,4-cyclohexadiene	0.043	0.001	0.013	0.011	0.010
2,3,4-trimethylpentane	1.099	0.008	0.119	0.202	0.059
toluene	21.002	0.384	3.090	4.002	1.980
2-methylheptane	1.133	0.027	0.157	0.209	0.090
3-methylheptane	0.375	0.007	0.048	0.072	0.026
4-methylheptane, 1-methyl-1-cyclohexene	1.373	0.016	0.148	0.254	0.078
1-octene	0.369	0.018	0.090	0.085	0.061
<i>n</i> -octane	1.060	0.028	0.180	0.224	0.092
ethylbenzene	2.171	0.049	0.541	0.497	0.364
meta- and para-xylene	3.047	0.067	0.947	0.770	0.697
styrene	0.342	0.000	0.064	0.081	0.037
ortho-xylene	1.046	0.011	0.283	0.261	0.222
alpha-pinene	0.682	0.002	0.086	0.154	0.023
<i>n</i> -propylbenzene	0.233	0.001	0.049	0.056	0.033
4-ethyltoluene	0.177	0.000	0.038	0.047	0.021
1,3,5-trimethylbenzene	0.215	0.000	0.040	0.058	0.016
<i>n</i> -decane	0.120	0.001	0.018	0.023	0.012
1,2,4-trimethylbenzene, tetrabutylbenzene	0.799	0.001	0.132	0.192	0.071
1,2,3-trimethylbenzene	0.108	0.001	0.014	0.022	0.006
1,2,3,4-tetramethylbenzene	0.009	0.000	0.001	0.002	0.001
acetone	17.392	0.072	1.799	3.290	0.611
methyl acetate	1.225	0.005	0.160	0.274	0.086
ethyl acetate	0.385	0.001	0.051	0.084	0.005
methanol	1.003	0.004	0.167	0.264	0.050
2-butanone	0.418	0.001	0.048	0.078	0.021
isopropyl acetate	0.496	0.001	0.030	0.090	0.011
2-propanol	0.843	0.011	0.148	0.186	0.085
ethanol	12.467	0.003	0.777	2.363	0.106
propyl acetate	0.488	0.004	0.060	0.104	0.016
isobutyl acetate	0.280	0.001	0.021	0.053	0.008
4-methyl-2-pentanone	0.176	0.001	0.014	0.034	0.002
2-butanol	6.791	0.003	0.622	1.575	0.032
1-propanol	1.550	0.001	0.064	0.286	0.006
butyl acetate	87.022	0.003	3.138	16.136	0.013
2-hexanone	0.103	0.001	0.014	0.026	0.004
1-butanol	2.313	0.003	0.125	0.428	0.018
cyclohexanone	0.140	0.001	0.015	0.025	0.011
Σ NMVOC	159.609	6.581	27.896	32.718	18.596
CO	3473.111	144.683	1007.911	964.547	600.113
CO ₂	502145.976	352335.713	411728.147	50464.438	394741.252
NO _x	405.745	8.089	125.226	138.949	39.689
NO ₂	77.369	4.657	29.067	25.168	18.974
NO	338.840	2.843	85.007	127.863	15.456

¹ volume mixing ratio; ² st.dev. – standard deviationanalytical equipment used: for NMVOC: Hewlett Packard GC 6890 and 5840A; for CO: Carbondio 1000; for CO₂: AL 5002; for NO_x: LMA 3D

The measurement results of NMVOC in other units (ppbC and $\mu\text{g}/\text{m}^3$) are presented in tables D.1 and D.2 in Annex D.

Table 3.1 shows that among alkanes 2-methylpentane and i-pentane, among alkenes and alkynes i-butene/1-butene, among aromatic hydrocarbons toluene followed by m-, p-xylene and among oxygenated compounds butyl acetate and acetone have the largest mixing ratios. C_2 hydrocarbons were excluded from the results due to the impossible quantitative analysis (chapter 2.2.1: Adsorption tubes, Tubes parameters, Breakthrough volume).

The measurements were carried out at different sites, which were expected to be influenced by different NMVOC emission sources. Due to this, different characteristics of the measured NMVOC-mix could be observed at the different sites. As an example, the comparison of mixing ratios of few most abundant compounds in different areas is presented by the figure 3.1.

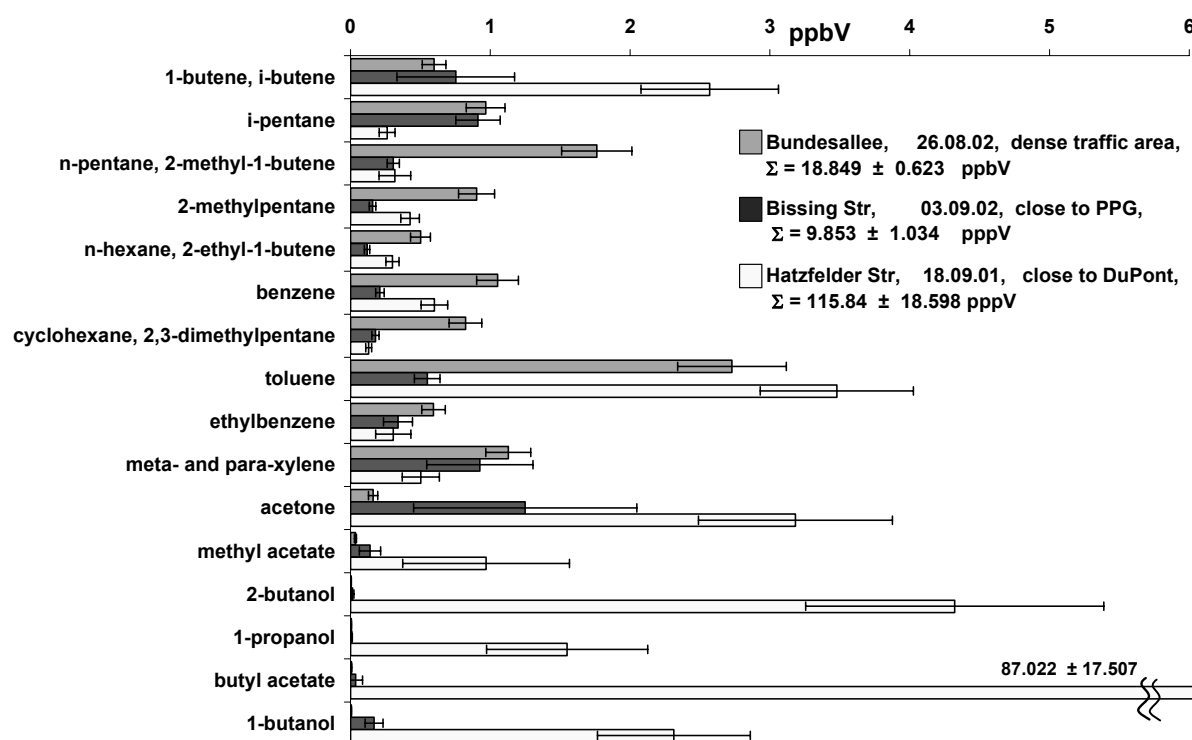


Figure 3.1: Mixing ratios (ppbV) of some abundant compounds at sites under the influence of different emission sources

As observed in figure 3.1, for the sampling point relevant for traffic (Bundesallee) toluene has the highest mixing ratio. The values of other important compounds like xylenes, benzene and other aliphatic hydrocarbons fall in the same mixing ratio range whereas, except for acetone, no oxygenated VOCs are important here. For the sample collected close to the PPG varnish factory (Bissing Str.) the most important compounds are xylenes, toluene and acetone. On

the contrary to traffic also some others oxygenated compounds like 1-butanol, methyl acetate and butyl acetate show high mixing ratios. In the case of the measurement performed close to the DuPont coatings factory (Hatzfelder Str.) butyl acetate exhibits a very high mixing ratio of more than 87 ppbV. Also others oxygenated compounds and toluene show a large abundance.

A comparison of the obtained NMVOC mixing ratios with the results from other urban studies is difficult because of differences in the measured species, sampling sites, sampling periods and the city characteristics. Nevertheless, as it can be observed from the table 3.2, where the average mixing ratios (ppbV) of some measured species were compared with other urban centres, the results from this study agrees with other studies. The mixing ratios measured in Wuppertal during the time period 2002-2004 correspond with the results from prior measurements carried out in Wuppertal in 1995 and 1998 (Gomes, 2002; Schmitz *et al.* 1997). Comparing with other cities, particularly Leipzig (Knobloch *et al.*,1997), Rome (Brocco *et al.*, 1997) and Milan (Ciccioli, 1993) the mixing ratios observed in Wuppertal during the present work were relatively low.

Table 3.2: Average mixing ratios (ppbV) of some selected compounds from various European studies

	<i>n-butane</i>	<i>i-pentane</i>	<i>trans-pentene</i>	<i>cis-pentene</i>	<i>benzene</i>	<i>toluene</i>
Wuppertal 2001-2003^a	0.41	1.20	0.20	0.13	0.99	3.09
Wuppertal 1998^b	1.66	1.12	0.23	0.40	0.64	1.06
Wuppertal 1995^c	1.39	2.74	0.02	0.01	0.65	1.37
Leipzig^d	8.90	10.30	0.10	0.10	10.00	21.67
Berlin (residential)^e	1.86	2.48	0.10	0.05	0.70	1.88
Berlin (street side)^e	3.11	6.04	0.19	0.10	1.49	4.49
Hamburg^f	7.80	6.40	-	-	3.20	8.20
Copenhagen^g	-	-	0.20	0.10	3.40	10.20
Vienna^h	4.90	6.90	-	-	6.00	10.90
Romeⁱ	14.93	25.21	2.09	1.05	11.11	26.46
Milan^j	-	24.23	1.43	0.59	12.24	22.40
Athens^k	2.10	11.70	-	-	5.00	14.30
Edinburgh^l	3.44	1.49	0.09	0.04	0.70	1.28
Leeds^l	5.15	2.40	0.21	0.10	1.04	2.00
London Eltham^l	3.23	2.57	0.13	0.08	1.06	2.16
Dublin^m	4.16	2.86	0.29	0.17	1.92	3.76

^a this study; ^b Gomes, 2002; ^c Schmitz *et al.*, 1997; ^d Knobloch *et al.*,1997; ^e Thijsse *et al.*, 1999; ^f Bruckmann *et al.*, 1988; ^g Christensen *et al.*, 1999; ^h Lanzerstoffer and Puxbaum, 1990; ⁱ Brocco *et al.*, 1997; ^j Ciccioli, 1993; ^k Moschonas and Glavas, 1996; ^l Derwent *et al.*, 2000; ^m Broderick and Marnane, 2002

In the case of oxygenated compounds the number of the available field data is much smaller than for hydrocarbons. There are some measurements of ketones in the atmosphere and far fewer of alcohols and esters (Finlayson-Pitts and Pitts, 2000). Table 3.3 presents the comparison of the results of oxygenated species measured in Wuppertal with the results from other studies.

Table 3.3: Overview of average mixing ratios (ppbV) of some selected oxygenated compounds from various studies

	<i>methanol</i>	<i>ethanol</i>	<i>i-</i> <i>butanol</i>	<i>ethyl</i> <i>acetate</i>	<i>propyl</i> <i>acetate</i>	<i>butyl</i> <i>acetate</i>	<i>acetone</i>	<i>2-</i> <i>butanone</i>
Wuppertal 2001-2003 ^a	0.17	0.78	0.13	0.05	0.06	3.14	1.79	0.05
Milan, Italy ^b	-	-	0.20	-	-	-	-	-
Grenoble, France ^c	-	2.20	-	-	-	-	-	-
Creteil, France ^c	-	2.96	-	-	-	-	-	-
Porto Alegre, Brazil ^d	-	10.30	-	-	-	-	5.30	0.71
Rio de Janeiro, Brazil ^e	14.00	66.40	-	-	-	-	-	-
Sao Paulo, Brazil ^e	19.60	36.20	-	-	-	-	-	-
Los Angeles, USA ^f	16.70	17.70	-	-	-	-	-	-
Hamilton, Kanada ^g	-	-	0.40	0.03	0.06	0.03	2.28	0.44
Alabama, USA (rural) ^h	11.00	1.20	-	-	-	-	4.20	0.49
Wank, Germany (remote) ⁱ	2.26	0.24	-	-	-	-	1.71 ¹	0.19
Arctic ^j	-	-	-	-	-	-	1.30	-

¹ acetone and propanal

^a this study; ^b Ciccioli, 1993; ^c Mond *et al.*, 2003; ^d Grosjean *et al.*, 1998; ^e de Paula Pereira *et al.*, 1999;

^f Lonneman *et al.*, 1997; ^g Aiello *et al.*, 2000; ^h Goldan *et al.*, ⁱ Leibrock and Slemr, 1997; ^j Yokouchi *et al.*, 1994

As observed, the average mixing ratios obtained from the present study are in the lower level of all mixing ratios measured. Only in the case of butyl acetate, the average value of 3.14 ppbV is much higher than the values from other measurements, what can be explained by the very high mixing ratios of this compounds measured close to the solvent factories in Wuppertal.

The total NMVOC mixing ratios calculated as a sum of 23 measured alkanes, 28 alkenes and alkynes, 14 aromatic hydrocarbons, 18 oxygenated compounds and 19 unidentified species varied during the measurements from 6.58 to 159.61 ppbV, with the average value of 27.90 ppbV.

3.2 Mixing ratios relative to benzene

Due to the fact that the absolute concentrations measured at different sampling sites cannot directly be compare because of different dilution factors, the normalisation to benzene is commonly used. Benzene is considered as a compound emitted exclusively from the road traffic since it is one of the most abundant traffic exhaust component and is officially prohibited from using as solvent in European Union countries (Directive 89/677/EEC, Wickert *et al.*, 1999). According to this for further evaluation and data discussion the NMVOC concentrations were recalculated from the ppbV and $\mu\text{g}/\text{m}^3$ units to ppbC/ppbC benzene.

As an example the ratio between toluene and benzene is discussed. The ratio between these two compounds is similar for all the measurement sites, which can be observed in figure 3.2. Measurements carried out at typical traffic sites like traffic tunnel and free-way as well as

down-wind from the city centre and at residential and industrial areas produced the same ratio of about 4.00 ppbC/ppbC. Because the Kiesberg Tunnel represents only traffic emissions and the other measurement sites have the same ratio as obtained in tunnel it can be concluded that for all these sites the toluene emission from the traffic is dominant. The only exception is one site, on Hatzfelder Str. in 2001, in the direct neighbourhood of the DuPont solvents factory. For this site the toluene/benzene ratio has a higher value, which points to other than traffic emission sources, very likely emissions from solvent production.

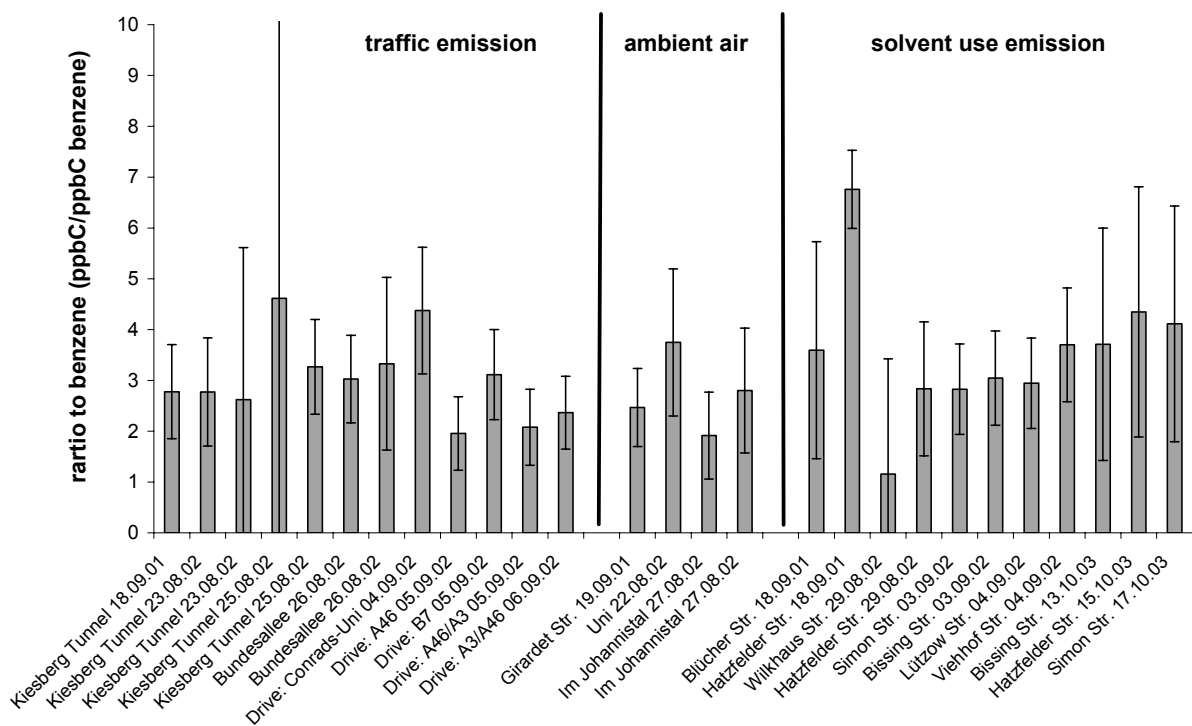


Figure 3.2: Toluene profile relative to benzene (ppbC/ppbC) for different measurement sites in Wuppertal

Similar relations between the ratios to benzene at different sites were found for many other hydrocarbons. No correlation to benzene was obtained for the oxygenated compounds.

Figure 3.3 shows a correlation plot between toluene and benzene obtained from the values measured during three campaigns performed at traffic sites in Wuppertal.

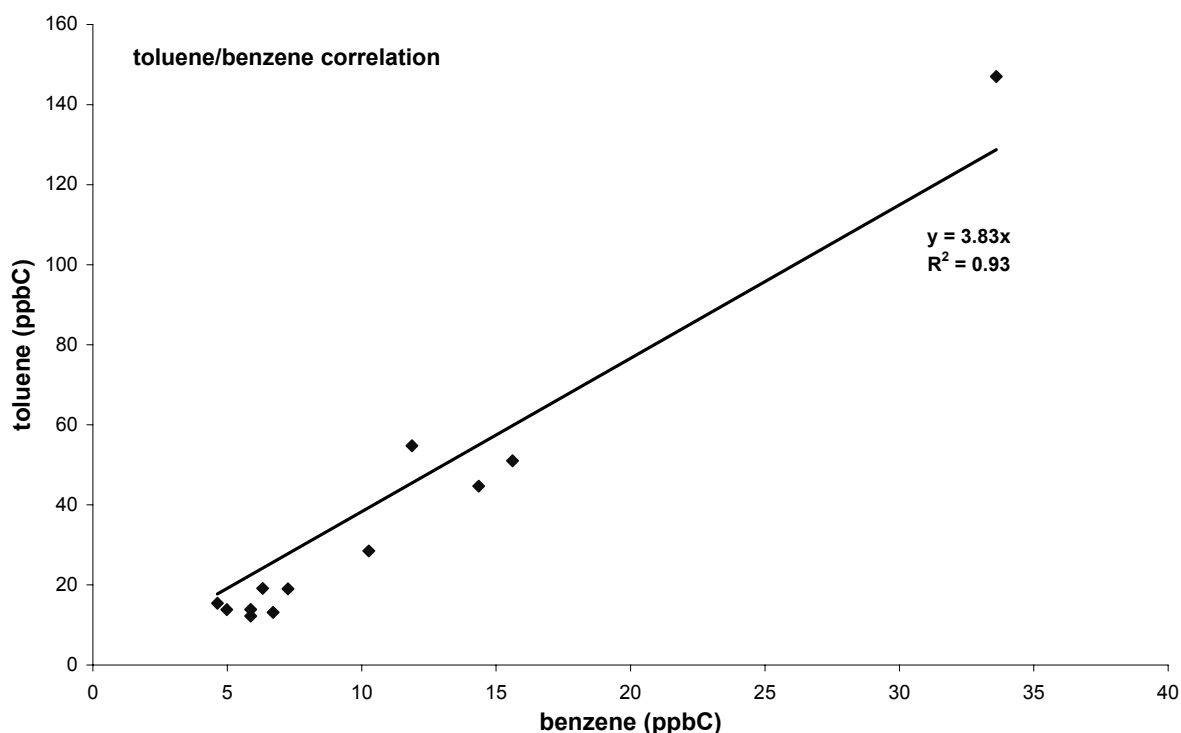


Figure 3.3: Correlation plot between toluene and benzene for the measurements performed at traffic sites

Figure 3.3 presents a good correlation between the measured values of toluene and benzene. The obtained toluene/benzene ratio of about (3.83 ± 0.22) ppbC/ppbC is significantly higher than previously measured ratios in typical traffic areas. For example, the ratio obtained from the measurements performed in Kiesberg Tunnel in Wuppertal in 1997 and 1998 was of about 2.40 ppbC/ppbC (Kurtenbach *et al.*, 2002). This is in agreement with other tunnel, city and dynamometer studies, where typically toluene/benzene ratios of 1.50 up to 2.50 ppbC/ppbC were measured (Conner *et al.*, 1995; Derwent *et al.*, 1995; Brocco *et al.*, 1997; Staehelin *et al.*, 1998; Schmitz *et al.*, 2000). The new measured value can be explained by an over proportional decrease of benzene emission compared with other aromatic compounds, because in year 2000 new European regulations on the benzene content in gasoline have been implemented (Directive 98/70/EC). On the basis of these regulations the benzene content in gasoline was reduced from 5 to 1% (V/V). A corresponding downward trend in the concentrations of aromatic compounds has been recently reported (Kristensson *et al.*, 2004; Reimann *et al.*, 2004; Stemmler *et al.*, 2005).

3.3 A composition of the NMVOC-mix

From the NMVOC profiles (ppbC/ppbC benzene) the average percentage composition of the hydrocarbons mix for all measurement points from Wuppertal was calculated. The results are presented in table 3.4, which also shows a comparison with other studies.

Table 3.4: Percentage composition of NMVOC-mix in wt% of the city air of Wuppertal in comparison with other cities

	NMVOC composition (%)			
	alkanes	alkenes and alkynes	aromatic hydrocarbons	oxygenated compounds
Wuppertal 2001-2003 ^a	32	16	37	15 ¹
Wuppertal 1998 ^b	46	9	42	3 ²
Wuppertal 1995 ^c	56	15	29	n. m.
Berlin (residential) ^d	46	10	26	18 ³
Berlin (street side) ^d	45	12	33	10 ³
Hamburg ^e	42	12	47	n. m.
Vienna ^f	42	11	47	n. m.
Rome ^g	35	7	33	23 ⁴
Milan ^h	30	5	44	15 ⁴
Madrid ⁱ	34	8	35	20 ⁴
Athens ^j	30	4	66	n. m.
Krakow ^k	36	19	44	n. m.

¹ alcohols, ketones, esters; ² phenols, cresols, aldehydes; ³ carbonyls; ⁴ alcohols, aldehydes, ketones, free acids; n.m. – not measured

^a this study; ^b Kurtenbach *et al.*, 2002; ^c Schmitz *et al.*, 1997; ^d Thijsse *et al.*, 1999; ^e Bruckmann *et al.*, 1988;

^f Lanzerstorfer and Puxbaum, 1990; ^g Brocco *et al.*, 1997; Ciccio *et al.*, 1999; ^h Ciccio, 1993; ⁱ Ciccio *et al.*, 1999;

^j Moschonas and Glavas, 1996; ^k Juszkiewicz *et al.*, 1997

As the table 3.4 shows the highest contribution comes from the aromatic hydrocarbons and the second highest from the alkanes. The composition of the hydrocarbons mix is in agreement with the results from measurements carried out in Wuppertal in 1998 and with the results from other studies.

Figures 3.4, 3.5, 3.6 and 3.7 show the distribution of different compounds in the main classes of hydrocarbons, namely alkanes, alkenes and alkynes, aromatic hydrocarbons and oxygenated compounds.

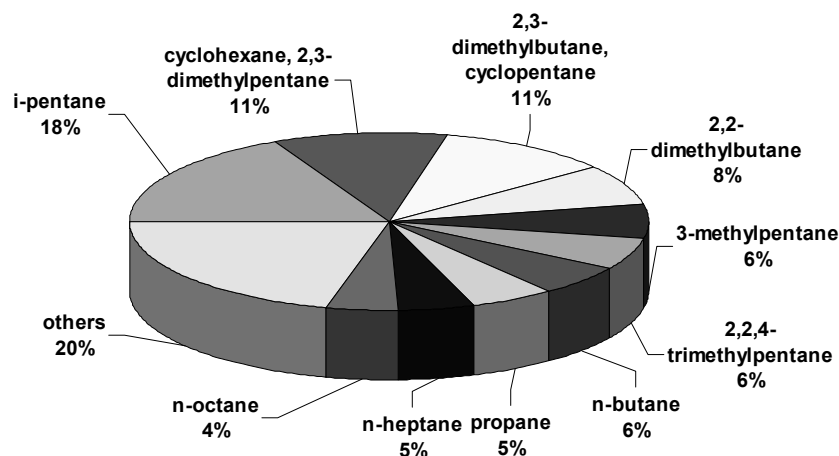


Figure 3.4: Percent contribution (% ppbC/ppbC benzene) of the compounds from the group of alkanes for the city air of Wuppertal from the campaigns 2001-2003

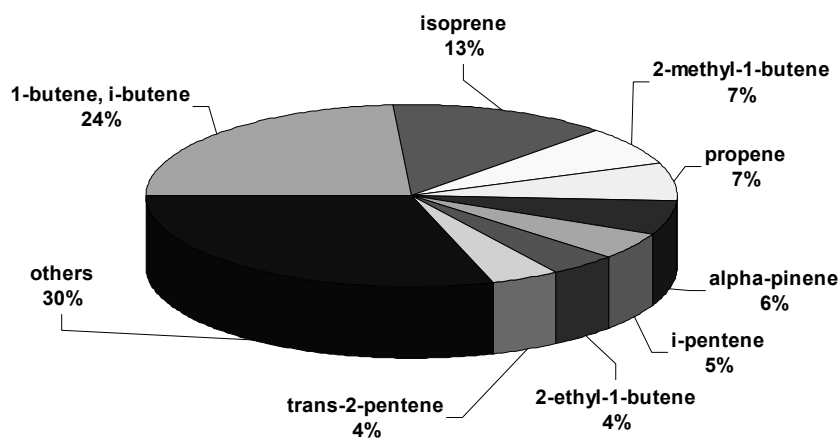


Figure 3.5: Percent contribution (% ppbC/ppbC benzene) of the compounds from the group of alkenes and alkynes for the city air of Wuppertal from the campaigns 2001-2003

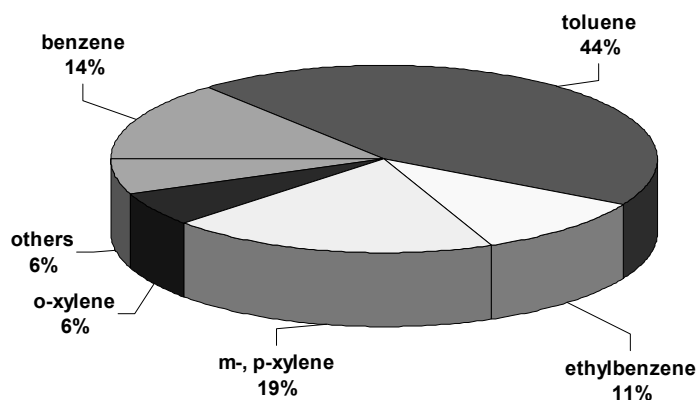


Figure 3.6: Percent contribution (% ppbC/ppbC benzene) of the compounds from the group of aromatic hydrocarbons for the city air of Wuppertal from the campaigns 2001-2003

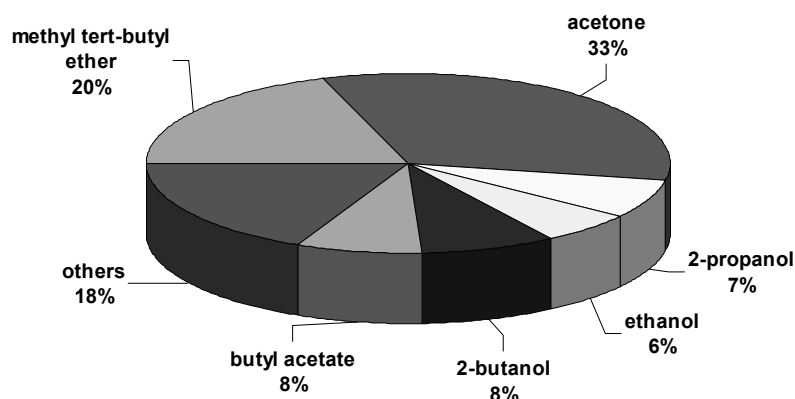


Figure 3.7: Percent contribution (% ppbC/ppbC benzene) of the compounds from the groups of oxygenated compounds for the city air of Wuppertal from the campaigns 2001-2003

As observed from the figures above, among the alkanes i-pentane, among alkenes and alkynes 1-butene, i-butene, among the aromatic hydrocarbons toluene and among the oxygenated compounds acetone have the highest percental contribution, respectively.

3.4 NMVOC/NO_x ratios

The ratio between total NMVOC and NO_x (ppbC/ppbV) plays a very important role in atmospheric chemistry, particularly in the tropospheric ozone production (Carter *et al.*, 1995; Derwent *et al.*, 1996; Jenkin and Hayman, 1999; Andersson-Sköld and Holmberg, 2000). From the measured data the NMVOC/NO_x ratios were calculated separately for the measurements performed at typical traffic sites, namely in Kiesberg Tunnel and during the drives at free-ways and for the measurements performed in the city. For the traffic sites (figure 3.8) the NMVOC/NO_x ratio of (0.56 ± 0.06) ppbC/ppbV was calculated. This value is in agreement with the results from previous study performed in Kiesberg Tunnel (Kurtenbach *et al.*, 2002) where ratios from 0.64 up to 1.92 ppbC/ppbV were calculated during week days.

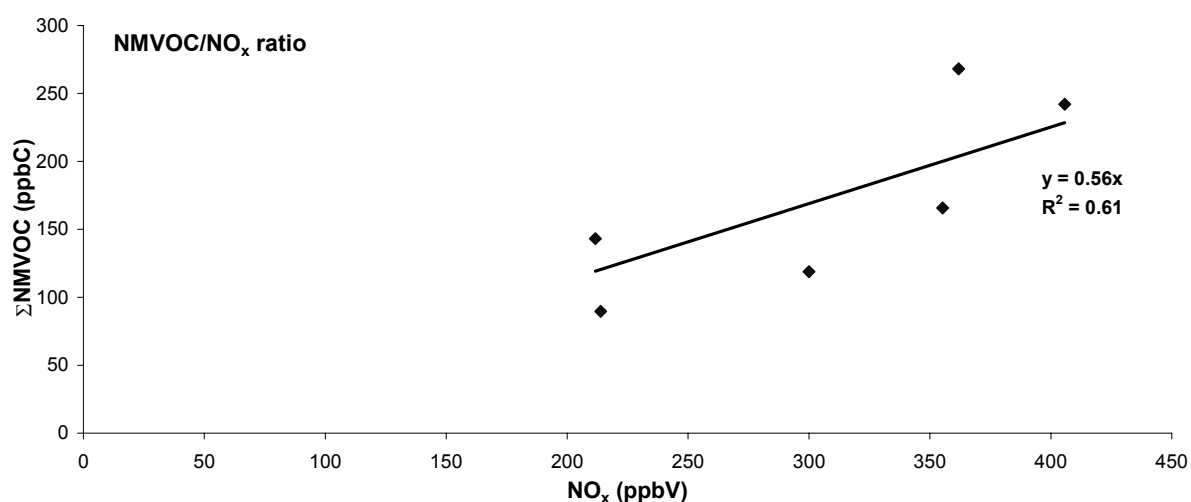


Figure 3.8: Correlation plot between the sum of the total measured NMVOC (ppbC) and NO_x (ppbV) for the measurements performed in the Kiesberg Tunnel and during the free-ways drives

For the measurements performed at the various location in the city of Wuppertal the total NMVOC does not correlate well with the NO_x data. The ratios show quite broad intervals, from 1.76 up to 7.93 ppbC/ppbV. This can be explained by the fact that all these measurements were carried out at different sites with different emission characteristic. The average NMVOC/NO_x ratio obtained from these measurements was (3.74 ± 2.15) ppbC/ppbV.

Table 3.5 presents a comparison of the NMVOC/NO_x ratios of the present studies with literature data.

Table 3.5: Comparison of NMVOC/NO_x ratios (ppbC/ppbV) found in the present study and in the previous results

location	characterisation	ΣNMVOC/NO _x	references
Wuppertal 2001-2003	traffic tunnel, free-way	0.6	this study
Wuppertal 2001-2003	urban	1.8 – 7.9	this study
Wuppertal 1997-1998	traffic tunnel	0.6 – 4.4	Kurtenbach <i>et al.</i> , 2002; Gomes, 2002
Wuppertal 1998	urban	2.4 – 4-8	Kurtenbach <i>et al.</i> , 2002; Gomes, 2002
Wuppertal 1995	urban	5.4 – 7.5	Schmitz <i>et al.</i> , 1997
German cities	urban	3.5 – 7.4	Bruckman <i>et al.</i> , 1980; Klemp <i>et al.</i> , 1997, Kern <i>et al.</i> , 1998
Menz	rural area	12.0	Kurtenbach <i>et al.</i> , 2002; Gomes, 2002

From table 3.5 can be seen that the values obtained in the present studies are comparable with previous results obtained in Wuppertal and also in other German cites.

Chapter 4

CHEMICAL MASS BALANCE MODELLING

4.1 Theory, assumptions and requirements of CMB modelling

4.1.1 Technique description

An assessment of the contribution of emission categories to the observed NMVOC concentrations was made by using the Chemical Mass Balance (CMB) modelling technique, version 8 from the US Environmental Protection Agency (Watson *et al.*, 1998). The CMB model is one of several receptor models applied to air resources management, which are based on measured mass concentrations and the use of appropriate mass balances. The model has been used since more than 30 years (Winchester and Nifong, 1971; Miller, 1972; Friedlander, 1973) and is a standard approach for apportioning measured concentrations of pollutants to their various sources.

The CMB model uses an effective variance least squares solution to a set of linear equations, which expressed each measured concentration c_i of species i as a linear sum of products of source profile abundances x_{ij} and contributions s_j of source j (Watson *et al.*, 1998; Watson *et al.*, 2001). In other words, the method uses source specific ratios between the emission rates of a certain set of compounds and aims to recognise these fingerprints, also called source profiles, in the concentration profiles measured at receptor points. The mass concentration c_i at the receptor point is expressed by the following mass balance equation:

$$c_i = \sum_{j=1}^k x_{ij} s_j + e_i, \quad i = 1, \dots, p \quad [4.1]$$

with c_i : ambient mass concentration of species i at the receptor point in $\mu\text{g}/\text{m}^3$,
 x_{ij} : fraction of species i in the emission from source j ,

- s_j : mass contribution of source j to the receptor point in $\mu\text{g}/\text{m}^3$, s_j is given by $s_j = \sum c_{ij}$ (sum over i) and can be understood as sum of partial mass concentrations c_{ij} of all species in the NMVOC emission from source j ,
- e_i : measurement error of concentration c_i at the receptor point for species i in $\mu\text{g}/\text{m}^3$,
- k : number of pollution sources,
- p : number of chemical species.

The CMB 8 used for the purpose of this study applies the effective variance weighted solution for the least square equation. This method uses all available chemical species, not only traces species, and analytically estimates the uncertainty of the source contribution based on the precision of both the ambient concentrations and source profiles. The effective variance weighted solution gives greater influence to the chemical species with higher precision in both the source and receptor measurements than to species with lower precision (Watson *et al.*, 1998).

The fundamental principle of the receptor models is that mass conservation can be assumed and the composition of source emissions remains constant over the ambient and source sampling period. Therefore, the ratios between components emitted by a single source are identical to the ratios between the resulting concentrations at the receptor points. This is based on the assumption that the species undergo no chemical transformations and there is no deposition during the transport from the source to the receptor. Other assumptions required by the model are i) all sources which may significantly contribute to the receptor have been identified and their emissions have been characterised, ii) the number of source categories is less than or equal the number of chemical species, which are being measured, iii) source profiles are linearly independent, i.e. sufficiently different from each other, iv) measurement errors are random, uncorrelated and normally distributed.

These assumptions are fairly restrictive and difficult to be fulfilled in practice. However, the CMB model tolerates some deviations, which increase the final uncertainties of the source contribution estimations (Watson *et al.*, 1998).

4.1.2 Input data for the CMB model

As input to the CMB model serves:

- NMVOC emission source profiles, so-called source fingerprints, which are the sets $\{x_{ij}\}$ of the fractional amounts x_{ij} of the chemical species i in the NMVOC emissions from source j ,
- the total NMVOC mass $\sum c_i$ (sum over i) at a receptor point and the concentrations c_i of the individual compounds for which the contributions from all emission sources have to be considered,

- realistic uncertainties e_i for source and receptor values, which are used to weight the relative importance of input data to model solutions and to estimate uncertainty of the source contributions.

Because the purpose of this study is to provide more information about the contribution of road traffic and solvent use to the total NMVOC emission only these two source categories were included in the CMB analysis.

As has already mentioned above, in the CMB analysis of emissions by a first approximation it is assumed that the relative mass contribution of a compound i to the total mass emitted by source j remains constant during the dispersion process, chemical transformations and depositions are excluded. Under this condition, the emission profiles or fingerprints for a particular emission sources j , understood as sets of fractional amounts x_{ij} of the chemical species i within the emission of source j , are calculated by dividing the partial concentration c_{ij} (in $\mu\text{g}/\text{m}^3$) of the individual compound i for the emission source j by the sum of $\sum c_{ij}$ (sum over all species i); in equation 4.1 this sum is defined as s_j . The following equation explains this relation:

$$x_{ij} = \frac{c_{ij}}{\sum_{i=1}^p c_{ij}}, \quad i = 1, \dots, p \quad [4.2]$$

with x_{ij} : fraction of species i in the emission from the particular source j ,
 c_{ij} : partial mass concentration of species i for the NMVOC emission source j in $\mu\text{g}/\text{m}^3$,
 p : number of chemical species.

In practice, the source emission profiles $\{x_{ij}\}$ can be determined by a detailed chemical analysis of the emission source j or by ambient measurements at sites located close to the particular source. Generally, in ambient measurement the partial concentration c_{ij} are not directly assessable because of overlapping of emissions from all sources ($c_i = \sum c_{ij}$, sum over j). However, the measurements near a emission source j can be used to derive the particular emission profiles provided that the NMVOC concentrations are determined only, or at least approximately, by this source ($c_i \rightarrow c_{ij}$).

In the present work the concentrations profiles were measured at different sites. It has been assumed, that the concentration profiles measured at sites dominated by traffic emissions like traffic tunnels, free-ways, street intersections etc. are determined only by traffic emission ($c_i \rightarrow c_{i,traffic}$) and provide the traffic emission profile.

The same assumption was made for the concentration profiles measured near a particular solvent factory, but down-wind from this emission source. In this case it has been assumed that the concentration profile is exclusively originating from solvent emissions ($c_i \rightarrow c_{i,solvent}$)

and provide a solvent use emission profile at least for the emission type of the particular factory. In reality even close to solvent factories an influence of traffic emissions on the measured c_i had to be expected. Only those concentration profiles for particular solvent sources, which significantly differed from concentration profiles obtained from measurements in traffic areas had been taken as profiles of solvent emission after some corrections for the background concentrations.

The $\{x_{ij}\}$ can also be calculated from speciated emission data of an emission inventory. However, this provides not an experimentally based approach, but can be used for comparison with data achieved by measurements. Such a comparison between experimentally determined emission profiles and the calculated profiles offers a test method for the quality of the emission inventory for certain source categories.

In the present work all profiles measured at the receptor points contained the concentrations of 102 NMVOC species. From about 190 NMVOCs peaks detected in GC-FID signals, the following compounds were selected for further investigation and CMB analysis:

- 65 hydrocarbons in the range of C₃-C₁₀ from the hydrocarbon groups: alkanes, alkenes, alkynes and aromatics,
- 18 oxygenated compounds in the range of C₁-C₆ including alcohols, ketones and esters and also methyl *tert*-butyl ether (MTBE),
- 19 hydrocarbon compounds with known carbon number but unidentified structure; these species were selected on basis of their abundance and variation (compounds with average concentration above 0.3 µg/m³ and significant variation) and because of their high significance to the source profiles diversification.

The convention has been used in this work that the sum over the relative mass distribution of the measured compounds i in the fingerprint of source j is normalised to unity, $\sum x_{ij} = 1$ (sum over i).

4.2 Results

4.2.1 Traffic emission profiles

As already mentioned in chapter 2.4.1 (Measurement sites in Wuppertal, Road traffic) the measurements of the source profiles from the traffic emission were carried out in a traffic tunnel (Kiesberg Tunnel), at a downtown street intersection and during driving in the city centre of Wuppertal and on the free-ways around Wuppertal. The way how the measured concentration profiles were recalculated to emission profiles is explained in the previous subchapter (chapter 4.1.2: Input data for the CMB model). All profiles from the measurements at sites dominated by traffic emission have been compared for establishing

similarities. Figure 4.1 presents the concentration distributions of the analysed compounds for all sites dominated by traffic emission.

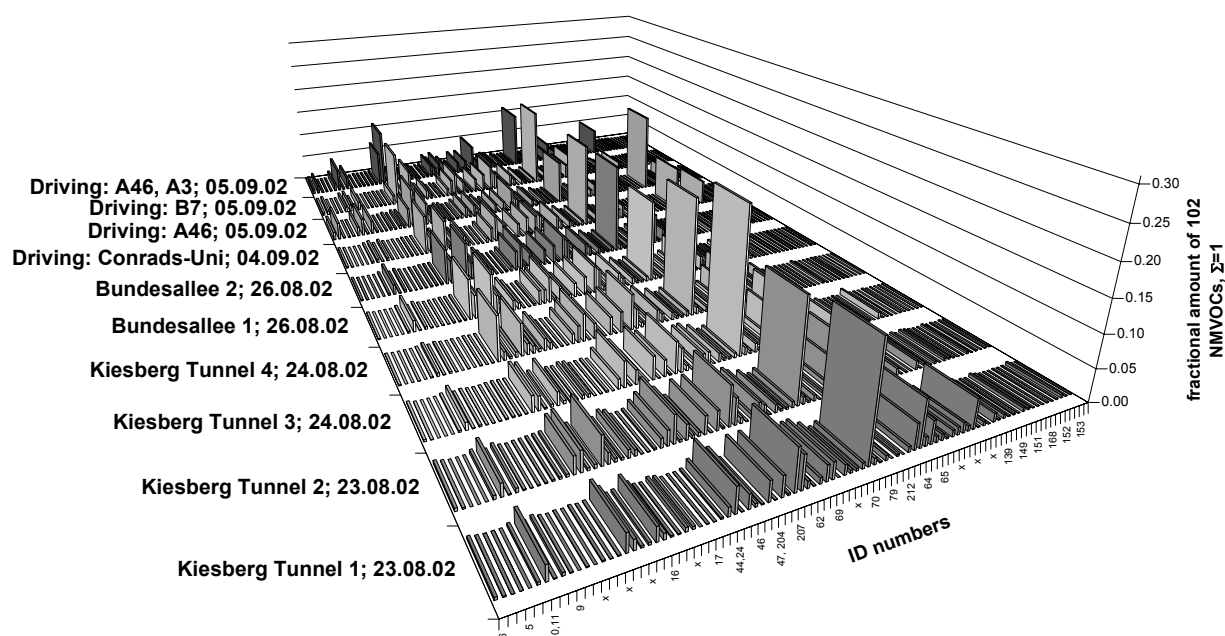


Figure 4.1: Emission profiles as relative mass distribution of 102 compounds at different sites dominated by traffic emission

All ten measured profiles dominated by traffic were found to be very similar; they all show the highest contribution from toluene, about 18%, and the importance of benzene, meta- and para-xylene, 2-methylpentane, iso-pentane, 1-butene and iso-butene.

According to the good agreement between these profiles, they have been averaged to obtain only *one* traffic emission profile. This profile represents all characteristic traffic conditions and was used in the CMB analysis. The traffic fingerprint, including the uncertainties, can be seen in table E.1 in Annex E, the graphical presentation is shown in figure 4.2.

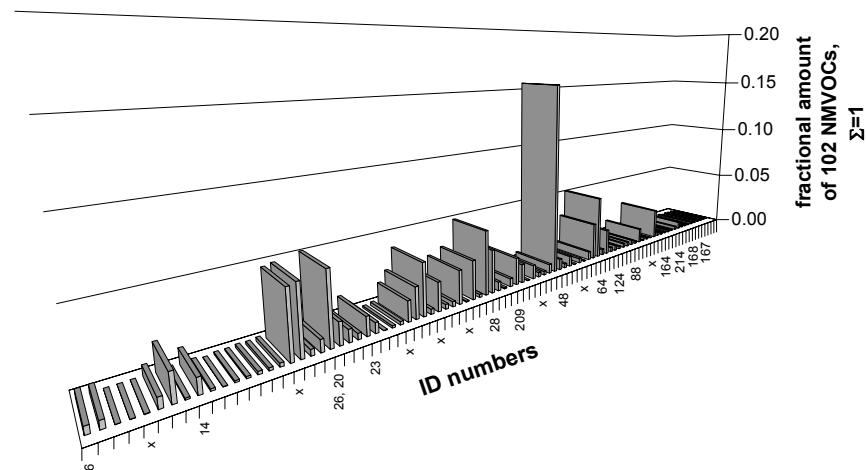


Figure 4.2: Average emission profile of road traffic

4.2.2 Solvent use emission profiles

To obtain relevant solvent emission profiles measurements were performed around various solvents factories and workshops in Wuppertal (chapter 2.4.2: Measurement sites in Wuppertal, Solvent use). In the beginning of the investigation, the measurements carried out for the solvent sector sources did not give satisfying results. The profiles differed not significantly from the traffic profile. This was mainly caused by the large influence of traffic emission at the sites where the measurements were performed. Accordingly, in order to split up the traffic emission and the emission from solvent use parallel NMVOC measurements up-wind and down-wind from solvent factories were carried out. Together with these measurements SF_6 was released as gaseous tracer at the point located up-wind from the factory and measured down-wind, providing information about the transport direction of the contaminated plume. The emission profiles for solvent use were finally obtained by subtracting the background concentration profiles normalised to benzene from the profiles measured down-wind from the factories. In EU countries benzene can be used as a traffic marker by which traffic and solvent emissions can be separated, because since more than 20 years the use of benzene as a solvent has been banned (Directive 89/677/EEC).

Eventually, solvent emission profiles were obtained by recalculating the measured concentration profiles according to the equation shown in chapter 4.1.2 (Input data for the CMB model). The solvent use fingerprints, including the uncertainties, can be seen in table E.2 in Annex E, they are graphically presented in figure 4.3.

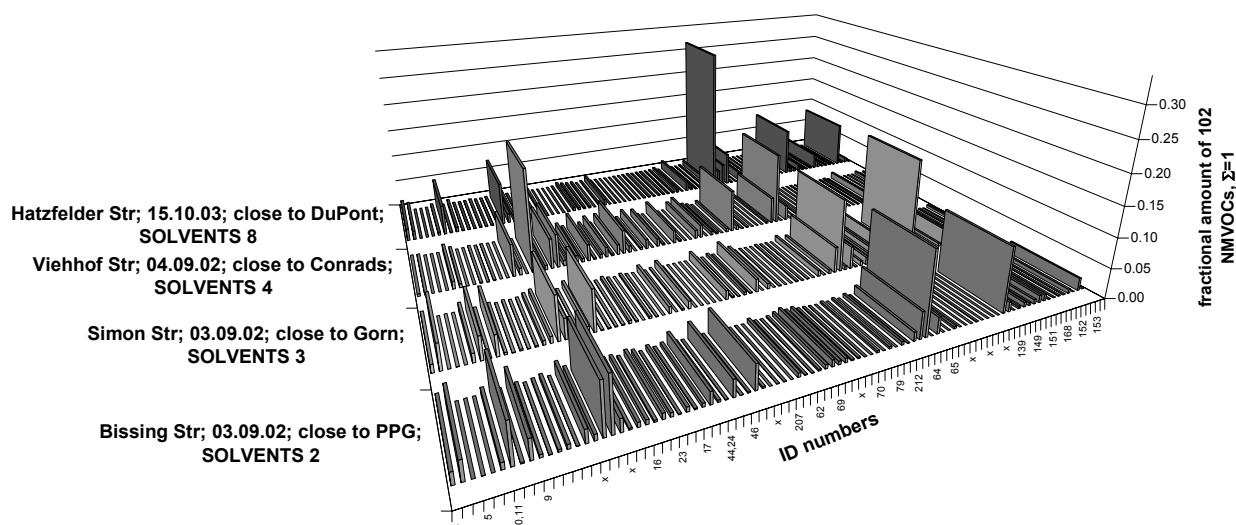


Figure 4.3: Emission profiles as relative mass distribution of 102 compounds for sites points strongly influenced by emission sources of solvent use

It is observed, that the presented solvent fingerprints exhibit much higher contributions from oxygenated compounds than in the case of traffic. For example, the measurements performed close to the DuPont factory (measurements on 15.10.03) show a relative mass contribution of butyl acetate of about 10%. Also ethanol and acetone contribute significantly to the total mass. From the hydrocarbons the xylenes and also toluene are important markers for the emission of solvents. However, the solvent profiles obtained at the different receptor points differ significantly from each other, which does not allow the average to *one* solvent emission profile like in the case of the traffic profile. Accordingly, *four* different solvent use emission profiles were applied in the CMB analysis.

4.2.3 Receptors

CMB analysis with the emission profiles from traffic and solvent use has been applied to the NMVOCs concentrations measured at the different receptor points in Wuppertal. The measurements were performed down-wind from the city centre, in residential areas, in areas close to the factories and workshop producing or using solvents and in dense traffic area. The location of all receptor points and the sites of solvent sources from the factories which were investigated are shown on map 4.1 and in more details on maps C.1-C.5 in Annex C. The characteristics of particular receptor points, with specification of different receptor areas, are presented in table 4.1. The concentrations of individual compounds measured at particular receptor points are presented in tables E.3-E.7 in Annex E.

The CMB analysis assumes that the source profiles are constant over the ambient and source sampling period, which excludes the degradation of individual compounds during the transport time from source to receptor. The transport time from sources to receptors did not exceed 40 min which has been calculated by the prevailing wind speeds during the

experiments. In 40 min the degradation of the investigated compounds by reactions with OH radicals does not exceed 15%, more reactive hydrocarbons like isoprene can undergo a degradation of about 20%. Since the error of measurements of the individual compounds is about 20%, the degradation of species transported from sources to receptor points can be neglected.

Table 4.1: Receptor points for CMB analysis

receptor points	CMB ID	characteristic	sampling time		wind sector	Σ NMVOC	
						($\mu\text{g}/\text{m}^3$)	\pm
residential areas, down-wind from the city centre							
Girardet Str.	GIRAR	Down-wind from the city centre of Wuppertal	19.09.01	11:10-12:10	SE-E	34.349	2.726
Uni	UNI	Down-wind from the city centre of Wuppertal	22.08.02	15:06-16:06	N-NW	35.993	2.594
Im Johannistal	JOTAL1	Residential area outside from the city centre	27.08.02	15:55-17:05	W-NNW	39.871	1.903
Im Johannistal	JOTAL2	Residential area outside from the city centre	27.08.02	17:12-18:24	W-NNW	27.435	1.336
dense traffic areas							
Bundesallee	BUNDA1	City centre of Wuppertal, dense traffic intersection	26.08.02	15:35-16:35	N-NE	73.627	2.328
Bundesallee	BUNDA2	City centre of Wuppertal, dense traffic intersection	26.08.02	16:40-17:40	N-NE	52.809	4.453
Märkisch Str.	MARKIS	Close to free-way A46	15.10.03	13:08-14:08	S-SE	84.287	8.466
areas close to solvent factories and workshops							
Wilkhaus Str.	WILKHA	Industrial area, close to DuPont solvent factory	29.08.02	13:06-14:10	NW	21.561	3.688
Hatzfelder Str.	HATZEN	Industrial area, close to DuPont solvent factory	29.08.02	14:55-15:55	W-NW	55.124	3.742
Hatzfelder Str.	HATZEM	Industrial area, close to DuPont solvent factory	15.10.03	12:55-14:00	S-SE	68.189	5.642
Bissing Str.	BISSIN	Industrial area, close to PPG solvent factory	03.09.02	12:52-13:52	E	37.593	3.159
Lützow Str.	LUTZOW	Industrial area, close to PPG solvent factory	04.09.02	14:29-15:30	SW	28.281	1.511
Bissing Str.	BISSIM	Industrial area, close to PPG solvent factory, down-wind from the object	13.10.03	13:06-14:06	E-SE	32.872	2.470
Yorck Str.	YOREK	Industrial area, close to PPG solvent factory, up-wind from the object	13.10.03	13:06-14:06	E-SE	24.609	1.959
Simon Str.	SIMONS	Industrial area, close to Gorn solvent workshop	03.09.02	10:35-11:40	N	28.252	2.973
Simon Str.	SIMONB	Industrial area, close to Gorn solvent workshop	17.10.03	09:45-10:45	NE	124.128	10.398
Simon Str.	SIMONM	Industrial area, close to Gorn solvent workshop	17.10.03	09:45-10:55	NE	88.706	10.966
Viehhof Str.	VIEHOF	Industrial area, close to Conrads solvent factory	04.09.02	16:17-17:17	SW	56.989	3.008



Map 4.1 Location of the receptor points (+) and sites of the investigated solvent factories and workshops (▲):
 D: DuPont Performance Coating GmbH, P: PPG Industries Lacke GmbH, B: Bayer AG, C: Dr. Alfred Conrads Lackfabrik Nachf. KG, G: Karosserbau Gorn GmbH
 1: GIRAR, 2: UNI, 3: JOTAL – receptor points located down-wind from the city centre
 4: BUNDA, 5: MARKIS – receptor point located at dense traffic areas
 6: WILKHA, 7: HATZEN, 8: HATZEM, 9: BISSIN, 10: LUTZOW, 11: BISSIM, 12: YOREK,
 13: SIMONS, 14: SIMONB, 15: SIMONM, 16: VIEHOF – receptor points located at areas close to solvent factories and workshops

4.2.4 Outcome of the CMB analysis

The CMB model delivers contributions from each source type to the total mass of the ambient NMVOCs and the contributions of the individual species at the receptor points and their uncertainties. Additionally, each CMB analysis provides a set of performance parameters like reduced χ^2 , R^2 , percent mass accounted, degrees of freedom and other parameters describing ratios between measured and calculated species concentrations. These performance parameters provide information about the quality of the CMB apportionment analysis (Watson *et al.*, 1998).

The CMB analysis has been executed with 102 NMVOCs. All measured receptor profiles were analysed using *one* average fingerprint for traffic and *four* selected different fingerprints

for solvent use emissions. However, some of the solvent fingerprints did not fit to the concentration profiles of a particular receptor point; negative contributions were obtained. The results of all performances are shown in table 4.2. The positive contributions using different solvent emission fingerprints are marked in table 4.2.

Table 4.2: Results of the CMB analysis, comparability of particular emission profiles to the concentration profiles measured at different receptor points

receptor points (CMB IDs)	source fingerprints (CMB IDs)	TRAFFIC1	SOLVENTS2	SOLVENTS3	SOLVENTS4	SOLVENTS8
		average traffic emission profile	solvent emission profile for PPG factory	solvent emission profile for Gorn workshop	solvent emission profile for Conrads factory	solvent emission profile for DuPont factory
GIRAR	source contributions	positive	negative	negative	negative	positive
UNI	source contributions	positive	negative	positive	negative	negative
JOTAL1	source contributions	positive	positive	negative	positive	negative
JOTAL2	source contributions	positive	negative	negative	positive	negative
BUNDA1	source contributions	positive	negative	negative	negative	negative
BUNDA2	source contributions	positive	negative	negative	negative	negative
MARKIS	source contributions	positive	negative	negative	negative	positive
WILKHA	source contributions	positive	negative	positive	negative	negative
HATZEN	source contributions	positive	negative	positive	negative	negative
HATZEM	source contributions	positive	negative	negative	negative	positive
BISSIN	source contributions	positive	positive	negative	negative	negative
LUTZOW	source contributions	positive	positive	negative	negative	negative
BISSIM	source contributions	positive	positive	negative	negative	negative
YOREK	source contributions	positive	positive	negative	negative	negative
SIMONS	source contributions	positive	negative	positive	negative	negative
SIMONB	source contributions	positive	negative	negative	negative	positive
SIMONM	source contributions	positive	negative	negative	negative	positive
VIEHOF	source contributions	positive	negative	negative	positive	negative

In a second step the CMB analysis was executed only with those profiles which gave positive contributions. Table 4.3 presents the results of these CMB analyses. Shown are: i) the emission profiles applied in particular cases, ii) contributions of traffic and solvent use emissions to the total NMVOC concentrations as result of the CMB analysis, iii) the total NMVOC mass concentration calculated by the model and the measured values at the receptor points. Additionally, the error limits, performance parameters as R^2 , reduced χ^2 and percent mass accounted by the model (% mass) are given.

Table 4.3: Results of the CMB analysis for receptor points measured in Wuppertal

receptor points (CMB IDs)	source fingerprints used (CMB IDs)	source contributions ($\mu\text{g}/\text{m}^3$)		total NMVOC ($\mu\text{g}/\text{m}^3$)		performance parameters		
		traffic	solvent use	CMB	measured	R ²	χ^2	% mass
residential areas, down-wind from the city centre								
GIRAR	TRAFFIC1, SOLVENTS8	17.016±0.913	1.717±0.393	18.733±0.866	34.349±2.726	0.64	3.01	54.5
UNI	TRAFFIC1, SOLVENTS3	29.176±1.648	3.274±0.949	32.450±1.369	35.993±2.594	0.83	1.29	90.2
JOTAL1	TRAFFIC1, SOLVENTS2, SOLVENTS4	27.567±1.416	3.239±0.639	30.807±1.261	39.871±1.903	0.79	1.79	77.3
JOTAL2	TRAFFIC1, SOLVENTS4	23.323±1.008	1.041±0.329	24.364±0.953	27.435±1.336	0.76	2.39	88.8
dense traffic areas								
BUNDA1	TRAFFIC1	69.417±2.328	0.000	69.417±2.328	73.672±2.328	0.89	1.22	94.2
BUNDA2	TRAFFIC1	46.314±2.215	0.000	46.314±2.215	52.809±4.453	0.88	0.63	87.7
MARKIS	TRAFFIC1, SOLVENTS8	36.968±2.209	0.662±0.247	37.630±2.203	84.287±8.466	0.54	2.80	44.6
areas close to solvent factories and workshops								
WILKHA	TRAFFIC1, SOLVENTS3	12.695±1.242	3.998±0.816	16.693±0.986	21.561±3.688	0.81	0.77	77.4
HATZEN	TRAFFIC1, SOLVENTS3	39.721±2.379	4.654±1.507	44.375±2.033	55.124±3.742	0.79	1.41	80.5
HATZEM	TRAFFIC1, SOLVENTS8	8.407±0.642	63.014±3.882	71.420±3.802	68.189±5.642	0.91	0.59	104.7
BISSIN	TRAFFIC1, SOLVENTS2	12.644±0.837	24.893±1.714	37.537±1.532	37.593±3.159	0.99	0.07	99.9
LUTZOW	TRAFFIC1, SOLVENTS2	16.867±0.897	7.493±0.854	24.361±0.915	28.281±1.511	0.84	1.57	86.1
BISSIM	TRAFFIC1, SOLVENTS2	6.134±0.646	10.949±1.333	17.083±1.231	32.873±2.470	0.54	2.43	52.0
YOREK	TRAFFIC1, SOLVENTS2	5.416±0.487	8.125±0.912	13.541±0.800	24.609±1.959	0.56	3.41	55.0
SIMONS	TRAFFIC1, SOLVENTS3	10.662±0.662	17.718±1.112	28.380±1.010	28.252±2.973	1.00	0.04	100.5
SIMONB	TRAFFIC1, SOLVENTS8	39.367±2.909	28.007±3.639	67.374±3.653	124.128±10.938	0.68	2.00	54.3
SIMONM	TRAFFIC1, SOLVENTS8	49.719±2.930	4.926±1.798	54.644±3.080	88.706±10.96	0.70	1.55	61.6
VIEHOF	TRAFFIC1, SOLVENTS4	33.278±1.791	23.097±2.042	56.375±1.900	56.989±3.008	0.96	0.41	98.9

The results for particular receptor points are graphically presented in figure 4.4. Plotted are the measured total NMVOC concentrations (presented as points with error limits) and the results from the CMB model for the concentrations caused by traffic and solvent use emissions (as bars) which add to the total NMVOC concentrations and can be compared with the experimental data.

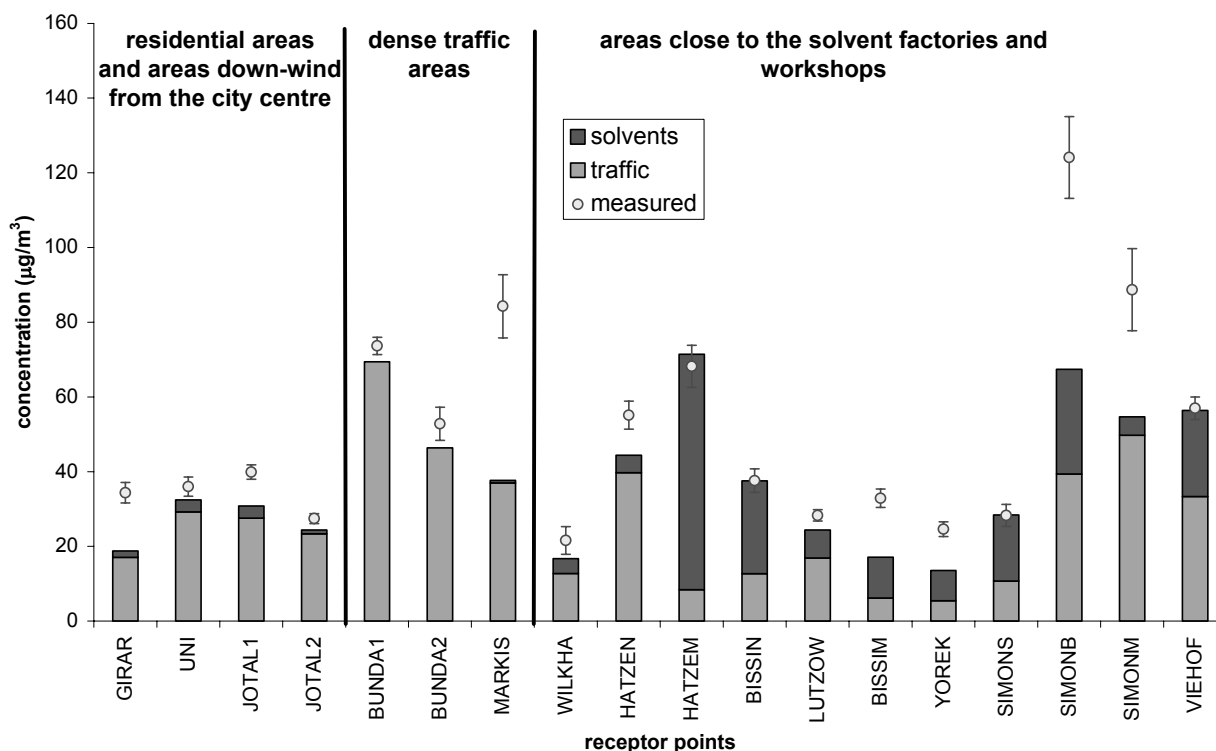


Figure 4.4: The measured total concentrations of NMVOC and the concentrations reproduced by the CMB model for traffic and solvent use emissions at different receptor points in Wuppertal

As has already been mentioned, the CMB model delivers contributions from each source type not only to the total ambient NMVOC mass at receptor points but also to the distribution of individual species. The detailed results of CMB analysis presenting contributions of the investigated sources to the concentrations of individual compounds for all receptor points are presented in tables F.1–F.18 in Annex F. As an example, figures 4.5 and 4.6 show the contributions of traffic emission and solvent use emission to the individual NMVOC concentrations at two receptor points. Plotted are CMB fits for the site UNI where traffic has the main influence and for the site HATZEM where the emission from solvent use dominates.

As expected, figure 4.5 shows, that at receptor point UNI traffic emission determines mainly the contribution of the majority of the compounds. The mass distribution presents a typical traffic profile with toluene and benzene as leading compounds. For most of the compounds, the measured concentrations are quite well reproduced by the model. In the case of receptor point HATZEM (figure 4.6), which is located in close neighbourhood to the DuPont solvent factory, solvent emission determines the NMVOC concentrations. At this site oxygenated compounds show a larger abundance. Their measured concentrations are almost by 100% attributed to the solvent emission.

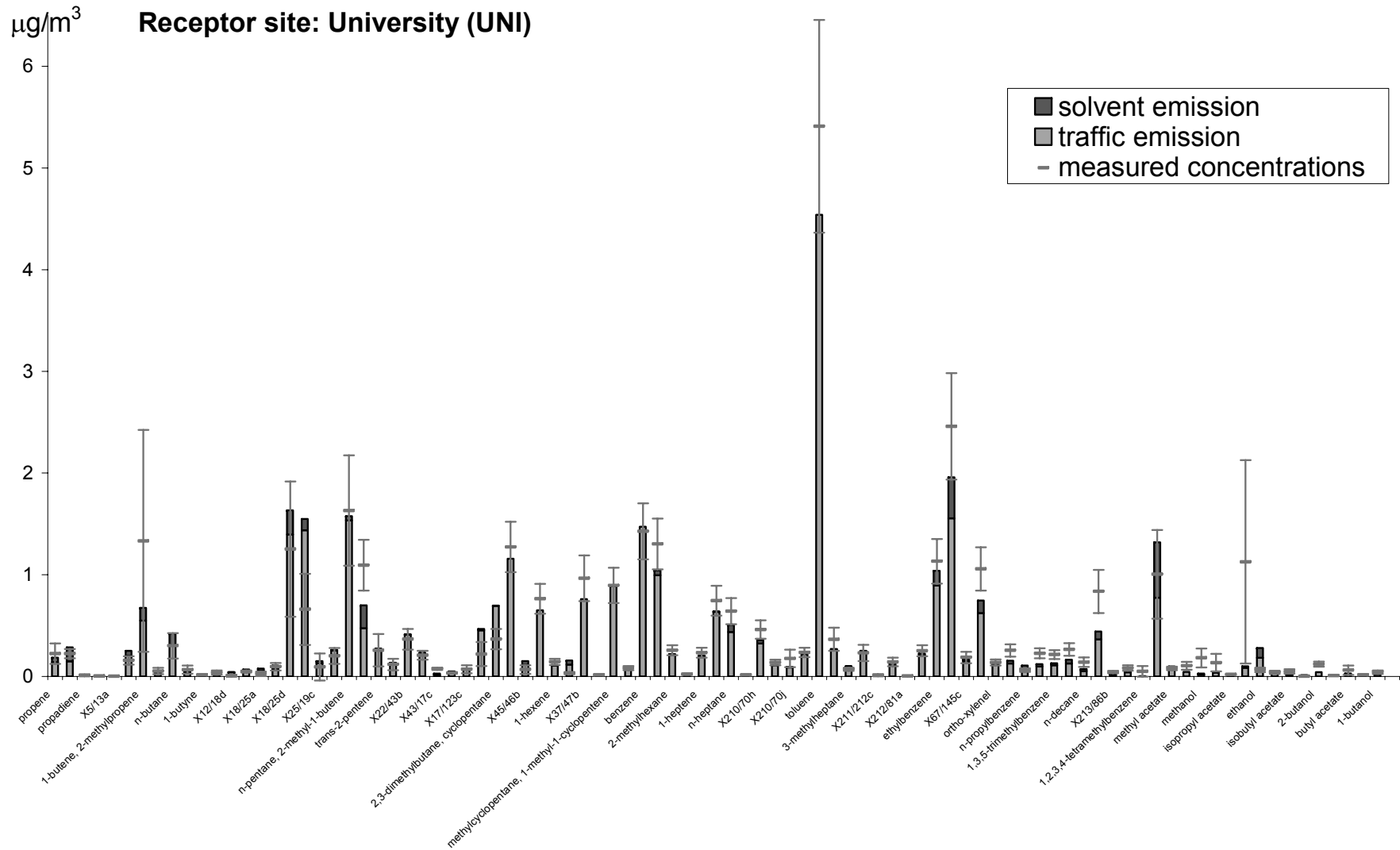


Figure 4.5: Contribution from traffic and solvent use emissions to the individual NMVOC concentrations calculated by the CMB model and the measured values at the receptor point UNI, down-wind from the city centre

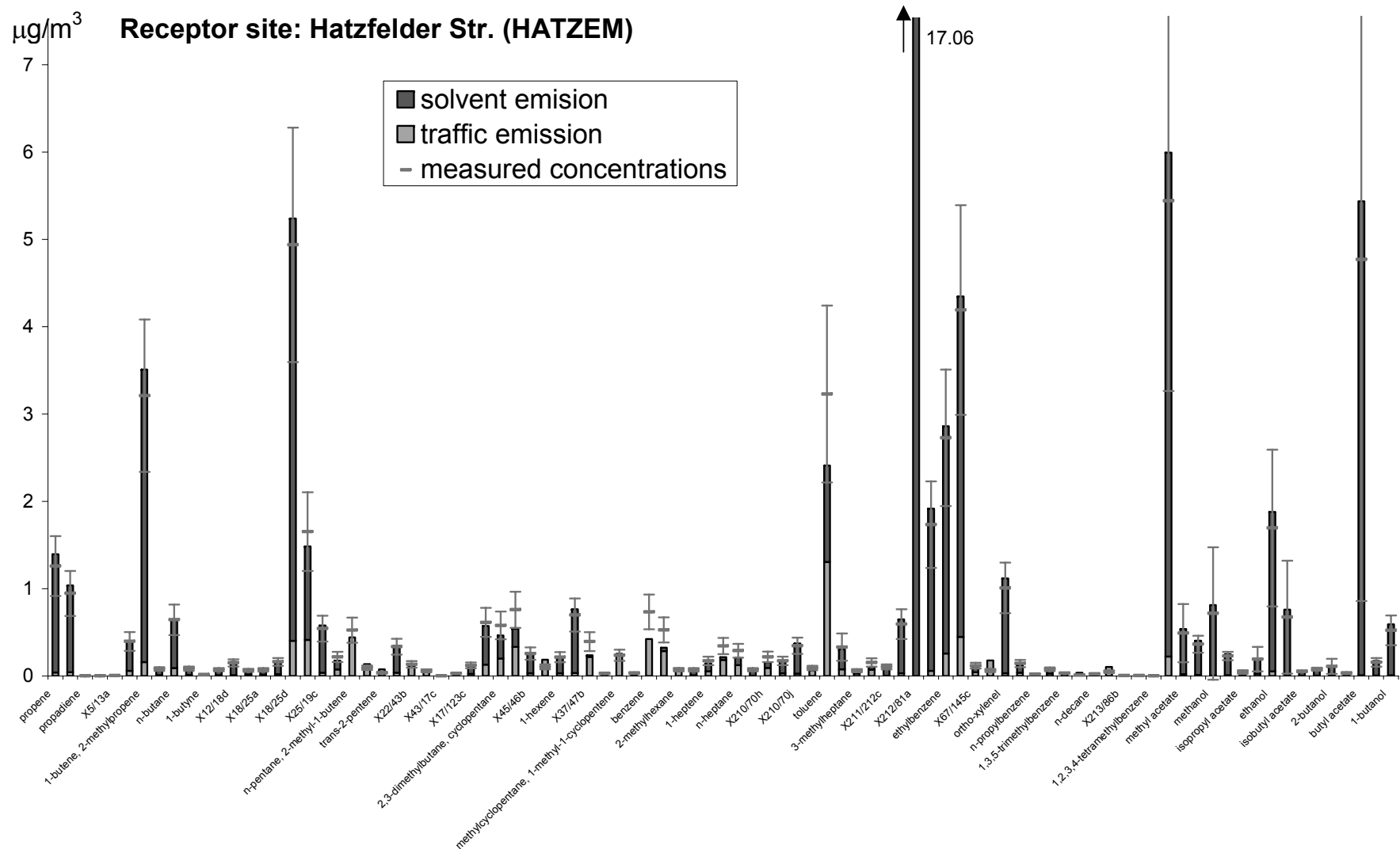


Figure 4.6: Contribution from traffic and solvent use emissions to the individual NMVOC concentrations calculated by the CMB model and the measured values at the receptor point HATZEM, close to the DuPont solvents factory

4.3 Evaluation of the results and discussion

4.3.1 Comparison of the emission profiles from the present work with literature data

In this chapter the emission profiles obtained from the measurements in Wuppertal and used as input to the CMB analysis are compared with the results from other studies.

Traffic emission profile

The average road traffic profile measured in Wuppertal was compared with profiles measured in Tegel Tunnel, Berlin (Thijssse *et al.*, 1999), close to a busy road in Munich (Kern *et al.*, 1998), in a tunnel-like underpass in Atlanta (Conner *et al.*, 1995) and in Caldecott Tunnel, San Francisco Bay area (Fujita *et al.*, 1994). These studies give the best opportunity for a comparison because a large number of identical NMVOCs have been measured in the different studies. The profiles have been normalised using only those compounds which are included in the studies from Wuppertal and Berlin. The results of the comparison are presented in figures 4.7 and 4.8.

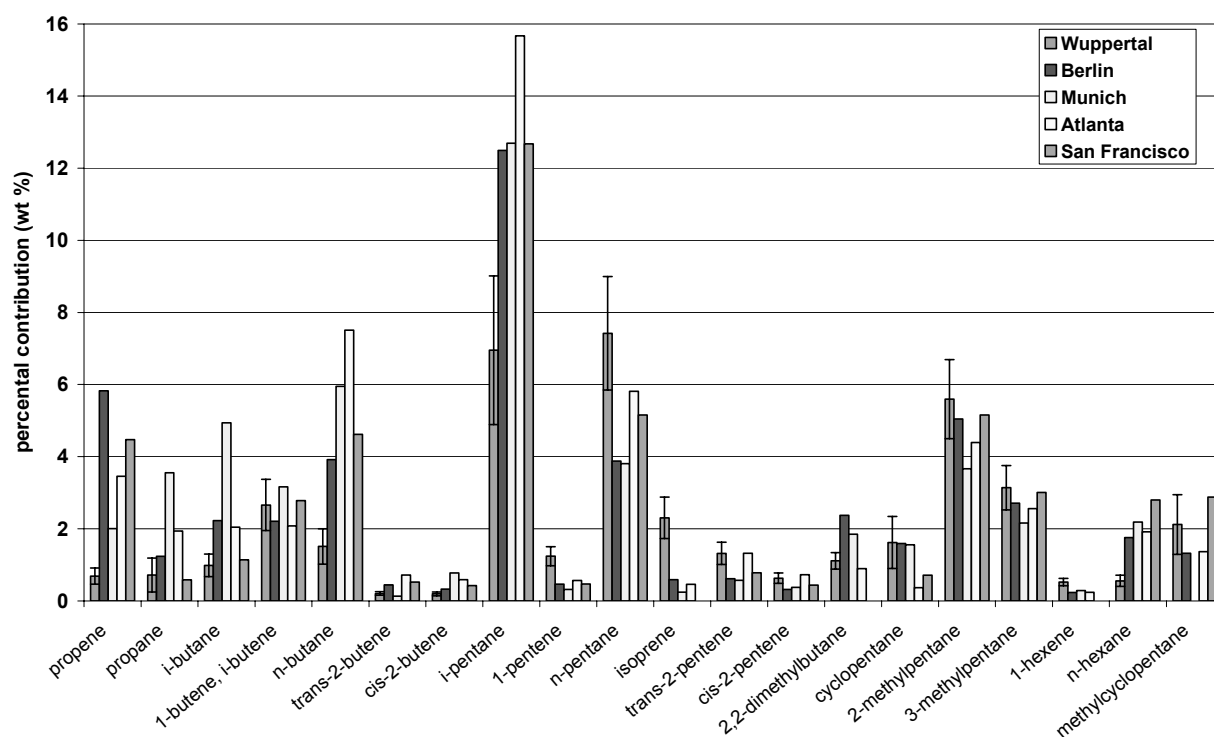


Figure 4.7: Comparison of the road traffic emission profile from Wuppertal with the results from other studies

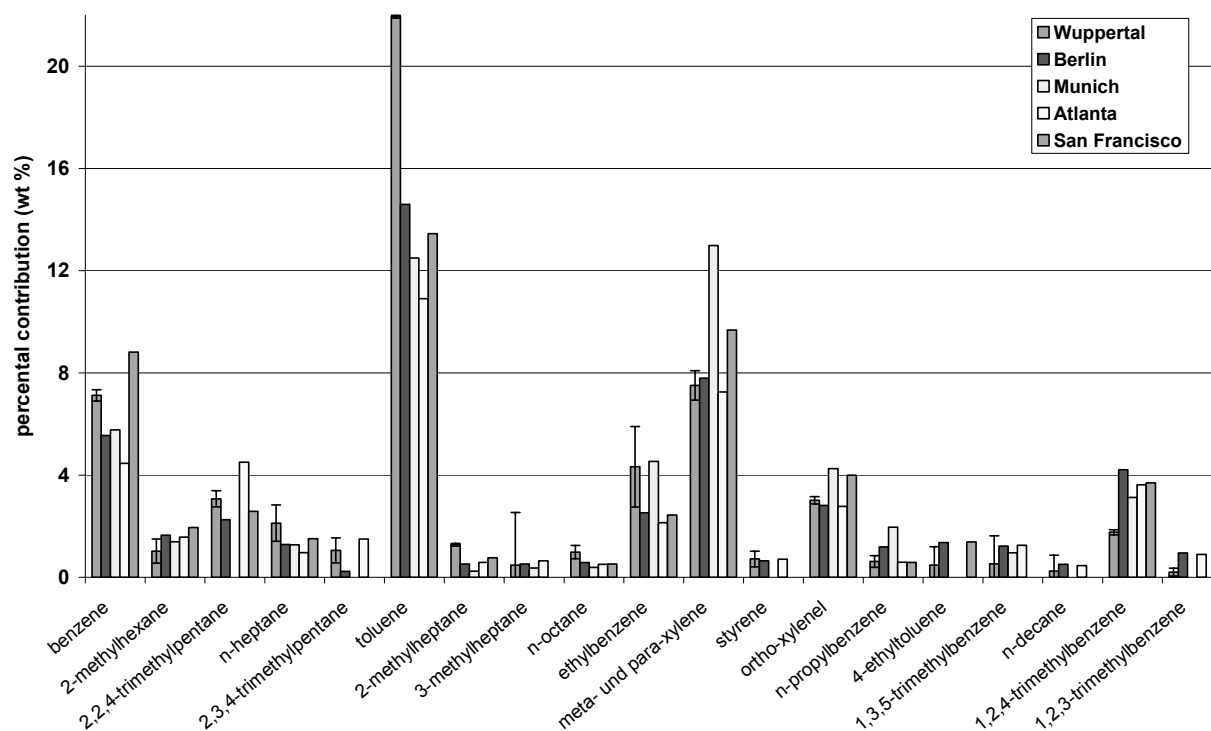


Figure 4.8: Comparison of the road traffic emission profile from Wuppertal with the results from other studies; continuation of the profile in figure 4.7

As observed in figures 4.7 and 4.8 the average profile obtained for Wuppertal agrees well with the other profiles, only a few larger deviations can be seen. Compounds like propene, *n*-butane, *i*-pentane, *n*-hexane and 1,2,4-trimethylbenzene show lower contributions in comparison with the other profiles, whereas toluene and isoprene are considerably more abundant in Wuppertal. These differences can be due to differences of traffic conditions for the particular profiles. It has also to be considered that there exist a larger time difference between the studies. The traffic fingerprint from Wuppertal presents all traffic situations, “stop and go” as well as “warm” driving conditions and free-way cycle, whereas all the other profiles represent hot, stabilised traffic emissions. Also the difference in fuel composition between Europe and the US and the years of the particular measurements might cause some deviations.

Solvent use emission profiles

Solvent use emission profiles measured in Wuppertal were compared with a solvent profile derived from data of emission calculations for the solvent sector in Germany (Theloke *et al.*, 2000). The comparison was limited to those compounds covered by the measurements in Wuppertal, namely C₃-C₁₀ hydrocarbons, alcohols, esters and ketones. The emissions reported in the inventory are specified only to several individual compounds, whereas the

more significant part of the emission is represented as a total of petroleum distillates defined as “Spezialbenzin”, “Testbenzin” and “Solvent Naphta”. These market names epitomise the hydrocarbon mixtures with rough content specifications. The ratios between particular components in these mixtures can be different for different producers making the detailed compound specification impossible. Accordingly, only a limited number of individual compounds could be directly compared and all others were grouped under aliphatic and aromatic hydrocarbons.

All solvent emission profiles measured in Wuppertal represent sources, which are relevant to the production and application of paints and varnishes. Hence, the four profiles obtained from the city measurements were compared both with the calculated emission profile of total solvent use and the profile of paint applications. The results of the comparison are presented in figure 4.9.

As observed in figure 4.9 the solvent profiles measured in Wuppertal are comparable with the profiles obtained from the emission inventory (Theloke *et al.*, 2000). Comparing with the total solvent emission, profiles of Wuppertal solvent factories show higher contributions of the hydrocarbons propane, i-pentane, cyclohexane, heptane, octane and the oxygenated hydrocarbon acetone, whereas the contributions of other oxygenated species like ethanol, i-propanol, n-, i-butanol, ethyl acetate and i-butyl acetate are significantly lower. The contributions of the sum of all other not specified aliphatic and aromatic hydrocarbons agree reasonably well. In the case of the calculated paint application emission profile, a significant difference to profiles measured in Wuppertal are observed for all specified individual aliphatic hydrocarbons. According to the emission inventory these compounds do not contribute to the emission from paint applications, but they can clearly be recognised in the profiles measured in Wuppertal. In contrary, some of the measured oxygenated species show lower contributions than the calculated equivalents. In general, among all solvent profiles measured in Wuppertal the DuPont fingerprint shows the best compatibility with the calculated emission profile for paint applications.

The differences between solvent profiles measured in Wuppertal and calculated from production and consumption of solvent related goods can be due to various unknown factors. Higher contributions of some individual aliphatic hydrocarbons in the profiles measured in Wuppertal can be due to the influence of some non-solvents sources on the measured profiles. However, they can also originate from the emission of unspecified hydrocarbon mixtures defined as “Spezialbenzin” and “Testbenzin” whose contribution is presented in inventory profiles as the sum of aliphatic and aromatic hydrocarbons.

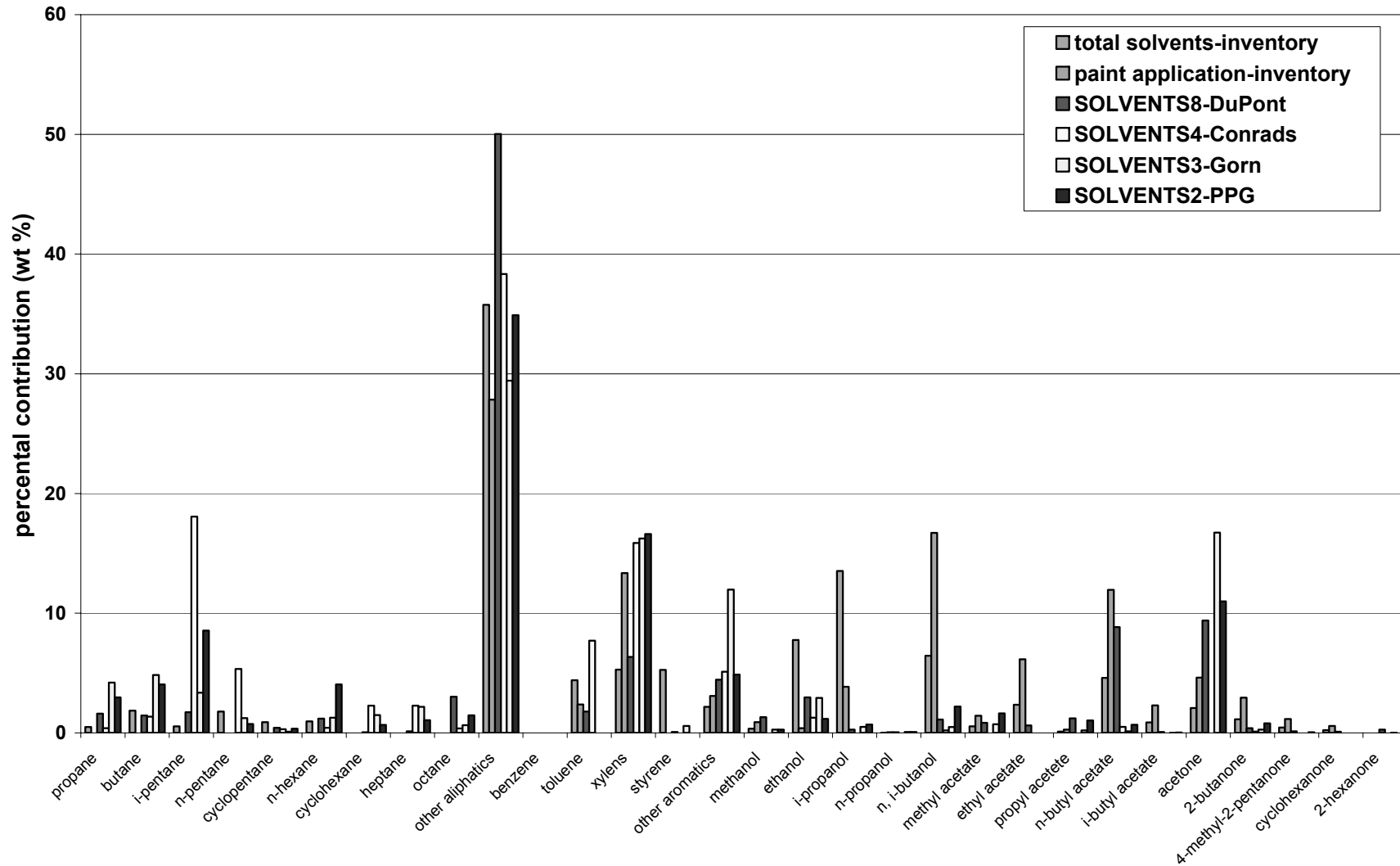


Figure 4.9: Comparison of solvent use emission profiles measured in Wuppertal with the results of speciated emission calculations for Germany (Theloke *et al.*, 2000)

Lower contributions of oxygenated compounds in the measured profiles may indicate that the emission of these compounds are overestimated in the emission inventory or the processes and applications responsible for the emission of these particular compounds were of less importance in the emission sources of Wuppertal, however, the last argument seems to be unlikely. The profile based on the data of the emission inventory assumes that a certain fraction from the solvent application is always emitted into the atmosphere, which also may create a larger uncertainty in the speciation of the data from the inventory.

Nevertheless, it seems to be reasonable to assume that the profiles obtained from the measurements performed in Wuppertal near several very different solvent factories and workshops represent quite well the solvent emission sector which is related to production and application of paints.

4.3.2 Discussion of the CMB results

In this chapter the CMB modelling results will be discussed and evaluated. The final results of the model calculation of the contribution of the traffic and solvent emissions to the NMVOC concentrations at different receptor points are presented in table 4.3 in chapter 4.2.4 (Outcomes from the CMB analysis) and in tables F.1-F.18 in Annex F.

As observed in figure 4.4, presented also in chapter 4.3.4, the contributions of source categories vary in location. According to expectations, for the receptor points located in the city centre and in areas with high traffic densities, the contribution from traffic emission is much higher than the contribution from solvent use and dominates the profiles.

For measurements performed at a busy traffic intersection in the city centre of Wuppertal (BUNDA1, BUNDA2, table 4.1, map 4.1) none of solvent fingerprints could be fitted to the measured concentration profiles. CMB analysis was performed only with traffic fingerprint (table 4.3, figure 4.4). According to the modelling results, traffic emission covered about 90% of total NMVOC concentrations at this site, the remaining 10% were not explained by the investigated emission sources.

For the receptor point located close to free-way A46 (MARKIS, table 4.1, map 4.1) the CMB analysis was performed with the traffic profile and solvent profile obtained from the measurements close to the DuPont factory (SOLVENTS8). During the measurements the receptor point was located down-wind from the free-way and up-wind from the factory. The modelling results indicate traffic as a major emission source for this point, whereas the contribution from the DuPont factory was less than 1%. More than 50% of NMVOC concentrations for MARKIS site could not be explained with the two investigated emission sources.

On average, for receptor points located in dense traffic areas more than 99% of the apportioned concentrations come from traffic emission. As example, a share diagram at one of the receptor points in a dense traffic area is presented by figure 4.10.

Receptor site: **Bundesallee (BUNDA1)**
Date: 26.08.02

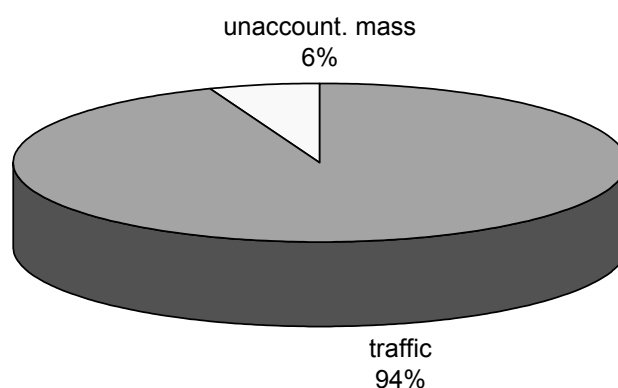


Figure 4.10: Contribution of traffic and solvent use emissions to the total NMVOC concentration measured at a street intersection in the city centre of Wuppertal

In the case of receptor points located outside of the city centre and in residential areas the contribution of traffic emission was similar as in the city centre.

For the receptor point located down-wind from the city centre, on the northern border of downtown (GIRAR, table 4.1, maps 4.1 and C.1 in Annex C), the CMB analysis was performed with the traffic fingerprint and solvent fingerprint obtained from the measurements close to the DuPont factory (SOLVENTS8). None of remaining solvent profiles fitted to the apportioned concentrations. The detected influence of the DuPont solvent factory on the NMVOC concentrations at the receptor site GIRAR can be due to the wind direction from east during the measurements. The particular receptor point is located westerly from the DuPont factory. Apportioned solvent contribution amounted to about 5% and traffic contributed to about 50% of the total NMVOC concentrations. About 45% of the NMVOC concentrations could not be explained with investigated emission sources.

The receptor point placed in the area of the University was located down-wind from the city centre, on the southern border of downtown (UNI, table 4.1, maps 4.1 and C.1 in Annex C). Wind direction during the measurements was in N-NW sector. For this point the CMB analysis was performed with the traffic profile and the solvent profile measured around Gorn workshop (SOLVENTS3). Other solvent profiles did not fit to the concentration profile of this site. The contribution of solvent use emission was about 9%, whereas traffic contributed to about 81% of the total NMVOC concentration. 10% of the measured concentration at this site remained unaccounted. The observed contribution of a solvent emission source may indicate influences by emissions from the Gorn workshop and other small workshops located up-wind of the receptor point.

Another receptor point (JOTAL1, JOTAL2, table 4.1, maps 4.1 and C.1 in Annex C) was located in a residential area, down-wind from the city centre. Wind direction during the measurements was from W-NNW sector. In the case of a first experiment, the CMB analysis was performed with traffic fingerprint and the solvents profiles of Conrads factory

(SOLVENTS4) and PPG factory (SOLVENTS2). The Conrads factory is located north-westerly and the PPG factory westerly from this receptor point. The remaining solvent profiles did not fit at all to the concentration profile at this site. The calculated contribution of solvents was about 8%, whereas traffic contributed to about 69% of total NMVOC concentration. 23% of measured concentration at this site remained unaccounted. During a second experiment performed at the same site, wind speed was significantly lower and, at the same time, the local traffic had increased. According to this, the results from the CMB analysis changed. The modelling was performed with the traffic emission profile and solvent profile for the Conrads factory (SOLVENTS4). The others solvent profiles did not fit to the apportioned concentrations at this site. The contribution of solvent was about 4%, whereas traffic contributed with about 85% to the total NMVOC concentration. 11% of the measured concentration at this site remained unaccounted.

On average, for the receptor points located down-wind from the city centre the relative contributions of traffic and solvents to the total concentration at the sites were about 91 and 9%, respectively. Figure 4.11 presents the contribution diagrams of selected receptor points located down-wind from the city centre.

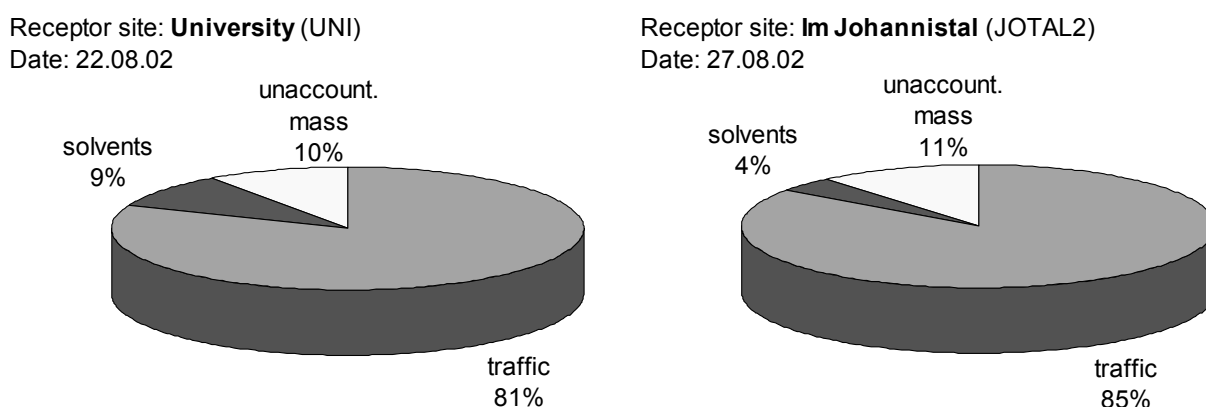


Figure 4.11: Contribution of traffic and solvent use emissions to the total NMVOC concentrations measured in residential areas, down-wind from the city centre of Wuppertal

Larger influences of the solvent use emissions on the total NMVOC concentration were found for the receptor points located in areas with solvents industry (solvents factories and workshops).

For the receptor point located close to the DuPont solvent factory (WILKHA, HATZEN, HATZEM, table 4.1, maps 4.1 and C.2 in Annex C) only in the case of the measurements performed at the HATZEM receptor point, a significant influence of the factory could be calculated. This point was placed exactly down-wind from the factory. The contribution of solvent emission was about 88%, whereas traffic contributed only to about 11% to the total NMVOC concentration (table 4.3, figures 4.4 and 4.12). For two remaining receptor points the DuPont solvent fingerprint could not be identified in the concentration profiles at these

sites. In addition, the CMB analysis was performed at these sites with the traffic emission profile and the solvent emission profile from the Gorn workshop (SOLVENTS3). The calculated contribution of solvent emission was about 19 and 8% for the receptor points WILKHA and HATZEN, respectively (table 4.3, figure 4.4). The detected contribution of solvent emission profile representing a car workshop can indicate the influence of emissions from some small workshops located up-wind from these receptor points.

For all receptor points located around the PPG solvent factory (BISSIN, LUTZOW, BISSIM, YOREK, table 4.1, maps 4.1 and C.3 in Annex C) the CMB analyses were performed with the traffic emission profile and the solvent emission profile from the PPG factory. According to the location and wind direction the contribution of the emission from the solvent factory to the measured NMVOC concentrations varied from 26 to 66% (table 4.3, figure 4.4).

As an example, the contributions of traffic and solvent use emissions at two receptor points located close to solvent factories DuPont (site: HATZEM) and PPG (site: LUTZOW) are presented by figure 4.12

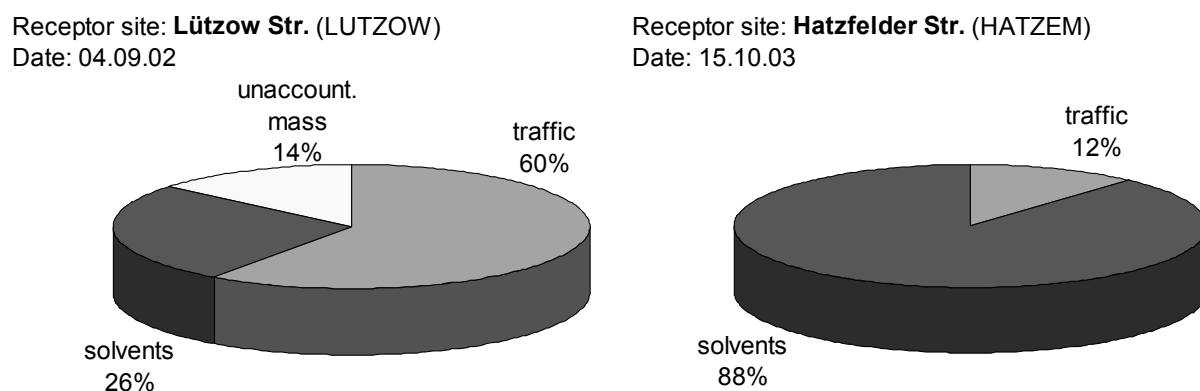


Figure 4.12: Contribution of traffic and solvent use emissions to the total NMVOC concentrations measured close to the solvent factories in Wuppertal

In the case of the measurements performed close to the Gorn workshop (SIMONS, SIMONB, SIMONM, table 4.1, maps 4.1 and C.4 in Annex C) only for the measurements performed at the SIMONS receptor point, a significant influence of the workshop could be calculated. The contribution of the solvent use emission was about 63%, whereas traffic contributed by about 37% to the total NMVOC concentration (table 4.3, figure 4.4). For two remaining receptor points located close to the Gorn workshop (SIMONB, SIMONM) the solvent fingerprint attributed to the workshop could not be identified in the concentration profiles, but for these two receptors the CMB analyses were performed with solvent emission profile of the DuPont solvent factory (SOLVENTS8).

For the receptor point located close the Conrads solvent factory (VIEHOF, table 4.1, maps 4.1 and C.5 in Annex C) the CMB analysis was performed with the traffic emission profile and the solvent emission profile from the Conrads factory. The contribution of the emission from the solvent factory to the measured NMVOC concentrations was 41% (table 4.3, figure 4.4), whereas traffic contributed with 58% to the total NMVOC concentration.

On average, for receptor points located in close neighbourhood of solvent factories and workshops the relative contributions of traffic and solvents to the total concentrations were about 55 and 45%, respectively.

The results from the CMB analysis for different receptor points show that the concentrations reproduced by the CMB model do not cover the measured concentrations very well. On average (77.0 ± 19.5) % of the measured total NMVOC concentration were accounted by the CMB analysis (table 4.3). It can be concluded that some other important NMVOC source categories like evaporative losses of motor fuel, natural gas leakage, other than traffic fuel combustion, biogenic emission and other solvent relevant sources (wood conservation, domestic use of solvents, dry cleaning) are missing in the CMB analysis. For a full characterisation of the NMVOC emission situation considerations of all important sources are required.

For comparison, the CMB analysis for receptor points located in Wuppertal was also performed with solvent use emission profiles taken from the emission calculations of Theloke *et al.* (2000). Besides the traffic profile obtained from the measurements performed in Wuppertal (chapter 4.2.1: Traffic emission source profiles), three calculated solvent profiles were applied. The profile representing the total solvent use emission (figure 4.9), the profile for paint application (figure 4.9) and the profile for domestic solvent use were applied. All profiles were limited to 30 variables (individual compounds and groups of compounds; figure 4.9) according to limitations of the compound speciation of the emission inventory.

However, such modelling tasks did not give satisfying results. In general, the calculated solvent profiles based on the data from the emission inventory could not be recognised in the measured concentrations at the receptor points. For the receptor points GIRAR and UNI (table 4.1, maps 4.1 and C.1 in Annex C) only minor contributions from the calculated profile of total solvent use to the concentrations measured at the receptor points were found. For these two sites located down-wind from the city centre the relative contributions of traffic and solvents to the total concentrations were about 98 and 2%, respectively.

But, the CMB analysis using the calculated solvent emission profiles gave some reasonable results for two receptor points located close to solvents factories, namely the site HATZEM (table 4.1) located close to the DuPont factory and the site BISSIM (table 4.1) located close to the PPG factory. In this case the calculated solvent profile based on the data from the inventory for paint application agreed reasonably well with the measured concentrations. For

these two points located in industrial areas the relative contributions of traffic and solvents to the total concentrations were about 92 and 8%, respectively.

The calculated profile from emission data for domestic solvent use could not be apportioned at any of the investigated receptor points in Wuppertal. In general, the CMB performance parameters obtained from the apportionment analysis executed with the calculated solvent emission profiles were quite poor, which may indicate larger errors of the speciated emission data taken from the inventory.

4.3.3 CMB results from Wuppertal in comparison with other studies

The present results obtained from the CMB analysis were compared with two other German studies, namely from Berlin (Thijsse and van Oss, 1997; Thijsse *et al.*, 1999) and from Augsburg (Mannscheck, 2000; Slemr *et al.*, 2002). These studies differ in terms of the chemical compounds used in the calculation and the applied source profiles. No oxygenated compounds were analysed in the studies of Berlin and Augsburg what obstructs a direct comparison. In Berlin the contribution of solvent use emissions has completely been neglected. Nevertheless, all studies came to the similar conclusion, that the emissions from road traffic together with evaporative losses of fuel still dominate the NMVOC composition in urban air (table 4.4).

Table 4.4: Percentage contributions of different emission sources to the total NMVOC concentrations calculated from the CMB analysis for various German cities

emission sources	Wuppertal ^a			Berlin ^b			Augsburg ^c
	dense traffic areas ¹	residential areas and areas down-wind from the city centre ¹	industrial areas ^{1,2}	street sides	residential areas	rural back-ground	areas down-wind from the city centre
traffic exhaust	99%	91%	55%	89%	83%	60%	19%
fuel evaporation	-	-	-	6%	7%	7%	29%
natural gas	-	-	-	5%	10%	33%	-
household	-	-	-	-	-	-	22%
solvent use	1%	9%	45%	-	-	-	5%
trade and industry	-	-	-	-	-	-	24%

^a this study; ^b Thijsse and van Oss, 1997; ^c Mannscheck, 2000

¹ average from the results for various receptor points; ² areas close to the solvent factories

In addition to the mentioned German CMB studies also many others NMVOC apportionment analyses, mostly from United States, reported at least qualitatively similar results (Watson *et al.*, 2001 and references therein). The results of these studies varied with the total apportionment fraction, the calculation method, the chemical compounds used in calculations and the source profiles applied. But even so, they show qualitatively similar source contributions to the NMVOC composition. Vehicle exhaust and gasoline evaporation contribute with 50% or more to the ambient NMVOC concentrations for most of these

studies. The relative contributions from motor vehicle emissions were significantly larger from CMB modelling than the numbers given in the national emissions inventories. The contributions from coating and solvent applications derived from CMB analysis were, like in the case for Germany, much lower than the proportions attributed to these sources in the national emission inventories.

The solvent emission profiles obtained from the measurements performed at industrial sites in Wuppertal do not cover the whole solvent use emissions, since some important solvent sectors like domestic solvent use, printing industry, dry cleaning and others were not investigated. In spite of this, it can be assumed that the solvent profiles applied in the CMB analysis represent the most important emission sector of production and application of paints and varnishes. According to the emission inventories and information about solvent production and consumption (Theloke *et al.*, 2000; Dore *et al.*, 2001; EEA, 2003c; Theloke, 2004), the paint application sector is responsible for about 40% of the total solvent use emission in Europe as well as in Germany (figure 1.2 in chapter 1.1.2: Emission sources of NMVOC).

The CMB modelling performed for the purpose of this study provided estimated contributions of traffic and investigated solvent use emissions to the ambient air concentrations of NMVOC in the city of Wuppertal. A *maximum* contribution of solvent emission, understood as emission of the paint application sector, apportioned by the CMB analysis to the receptor points down-wind from the city centre of Wuppertal, yielded about 9%. It is assumed that these receptor points are representative for the whole city. Using the ratio between the paint application sector and the total solvent use emission of 0.4 the results of the CMB analysis support that the remaining solvent sectors contribute *at the most* 14% to the NMVOC concentrations in Wuppertal. Such an estimated contribution of other solvent sources can partly explain the unaccounted NMVOC mass obtained from the CMB analysis performed only with traffic and paint applications source profiles. Therefore, it is concluded that the *maximum* contribution of solvent use to the total NMVOC emission in the whole urban area of Wuppertal is around 23%. The lower limit of the solvent use contribution has been taken from the lowest apportionment by CMB solvent contribution at the receptor points located down-wind from the city centre, which yielded about 4%.

Wuppertal can be considered as a German city with a typical share of traffic, industry and domestic activities. Accordingly, these estimations can be taken for the whole country. These results are in strong disagreement with the German Emission Inventory which states, that at present (reference year 2000) about 62% of the total NMVOC emissions originate from solvent use and only 18% from road traffic (UBA, 2001; Theloke *et al.*, 2001).

4.4 Conclusions

The inconsistency of the German Emission Inventory data, which assign about 62% (in year 2000) of the total German NMVOC emissions to the solvent use sector with the real-world situation, is clearly demonstrated by the results of the present work. This finding is supported by two other German experimental studies which were previously carried out in Berlin and Augsburg. Some shortcomings of the previous studies with respect to an incomplete cover of the oxygenated species were resolved in the present work.

The results from the CMB analysis with the application of source profiles and receptor concentrations obtained from city measurements in Wuppertal showed that road traffic rather than solvent use dominates the NMVOC emission. The contribution of traffic emission was dominant at all investigated points located down-wind from the city centre, with a relative contribution on average of about 90%. In dense traffic areas the traffic emission is responsible for almost 100% of the NMVOC concentrations. Significant contribution from solvent emissions could only be observed in the close vicinity of solvent factories, where the impact of investigated solvent sources accounted on average for about 45% of the measured NMVOC concentrations.

The maximal contribution of solvent use to the NMVOC emission, estimated on the basis of experimentally obtained results, amounts to about 23% for the whole city area of Wuppertal. This value is an approximation, but it can be considered as an upper limit for the solvent use contribution to the total NMVOC emission. Accordingly, it can be concluded that the contribution of solvent use to the NMVOC concentration in German cities falls in the range of a few to about 20%.

The CMB analysis performed with the solvent emission profiles calculated from production and consumption of solvents and solvent related goods used as input data for the German Emission Inventory, where the contribution from solvent use dominates, strongly disagrees with the NMVOC concentrations measured in Wuppertal. Calculated emission profiles could either not be apportioned to the measured NMVOC concentrations or the apportionment gave much smaller contributions of the solvent emission. The fact that the calculated solvent profiles do not fit to the measured NMVOC concentrations very likely indicates some major flaws in the manner in which solvent use emissions have been calculated.

The presented results raise some serious doubts as to whether the trends predicted by the European Emission Inventories, in particular in the German Inventory, where the relative contribution from the solvent sector has increased to 62% and is still increasing, whereas the emissions from traffic have significantly decreased and are still decreasing, reflect the reality. All experimentally based findings so far show that traffic emissions still dominate the NMVOC fingerprint in the ambient air of European cities.

Although the CMB analysis may have severe limitations, the discrepancies between the results of the present work and the German Emission Inventory exceed by far these limitations. Any abatement strategy based on erroneous inventories can never be verified for its efficiency.

The outcome of the present work will hopefully initiate further studies for improving the NMVOC emission inventories in Europe.

Chapter 5

SUMMARY

The objectives of this study were to measure the NMVOC concentrations in the city air of Wuppertal in order to obtain more information about the relative importance of road traffic and solvent use to the total NMVOC emission in the city.

Besides a number of hydrocarbons from the groups of alkanes, alkenes, alkynes and aromatic hydrocarbons also oxygenated species such as alcohols, esters and ketones were included in the measurements. The NMVOC concentrations in ambient air were measured by means of GC/FID analysis with cryo focussing as an enrichment system and adsorption tubes as sampling device. As adsorption material a combination of Carbotrap and Carbosieve SIII was used. To improve the chromatographic separation hydrocarbons and oxygenated species were analysed separately by applying two different gas chromatographs. Hydrocarbons were analysed by the GC-FID instrument equipped with a non-polar capillary column, whereas for oxygenated species a polar capillary column was used. Preparatory tests in the laboratory showed that these methods are suited for measurements of hydrocarbons and oxygenated species under ambient concentrations.

During three campaigns performed in September 2001, August/September 2002 and October 2003 NMVOC concentrations were measured at different sites in Wuppertal. Measurements were carried out by a car equipped with the hydrocarbon sampling system and automatic analysers for monitoring carbon monoxide, carbon dioxide, nitrogen oxides and sulphur hexafluoride. In addition, a small station for the registration of meteorological parameters was operated during the measurements.

The experimental results show that among the alkanes 2-methylpentane and i-pentane, among the alkenes and alkynes i-butene and 1-butene, among the aromatic hydrocarbons

toluene followed by m- and p-xylene and among the oxygenated compounds butyl acetate and acetone have the largest abundance. The total NMVOC concentrations calculated as a sum of 23 measured alkanes, 28 alkenes and alkynes, 14 aromatic hydrocarbons, 18 oxygenated compounds and 19 unidentified species varied during the measurements from 8.31 to 993.58 $\mu\text{g}/\text{m}^3$, with an average value of 95.67 $\mu\text{g}/\text{m}^3$. The average percentage compositions of the NMVOC-mix in wt% was calculated for all measurement points in Wuppertal. The percental contribution of alkanes, alkenes and alkynes, aromatic hydrocarbons and oxygenated compounds were 32, 16, 37 and 15%, respectively, which agrees with the results from other urban studies.

From the measured data the NMVOC/NO_x ratios were calculated separately for the measurements performed at typical traffic sites, namely in the Kiesberg Tunnel and during drives on the free-ways. Ratios were also measured at various locations in the city. For the traffic sites an average ratio of (0.56 ± 0.06) ppbC/ppbV was obtained. For the measurements performed at various locations in the city the ratios varied from 1.76 up to 7.93 ppbC/ppbV. These results agree well with the results from other studies in urban areas. The obtained toluene/benzene ratio of about (3.83 ± 0.22) ppbC/ppbC is significantly higher than the previously reported ratios of 1.50 up to 2.50 ppbC/ppbC measured in traffic areas. This can be explained by a strong decrease in the benzene emissions compared to the other aromatic compounds since the year 2000, when, due to new European regulations, the benzene content in gasoline was significantly reduced.

An assessment of the contribution of the two emission sources road traffic and solvent use to the observed NMVOC concentrations was made by applying the Chemical Mass Balance (CMB) modelling technique version 8 from the US EPA (Watson *et al.*, 1998). The method uses source specific ratios between the emission rates of a certain set of compounds and aims at recognising these fingerprints, or source profiles, in the NMVOC concentration profiles measured at receptor points.

More than 100 compounds were measured and used for the CMB calculations. Apportionment analyses were performed for several receptor points located down-wind from the city centre, in residential areas, in dense traffic areas and in industrial areas.

The required emission profiles of both investigated sources were recalculated from the concentration profiles measured at sites representative for particular sources.

The profiles for traffic were obtained from the measurements performed in a traffic tunnel, at a down-town street intersection and during drives through the city and on free-ways. It was assumed that concentrations measured at these sites are dominated by emissions from traffic and deliver the traffic emission profile. Solvent emission profiles were obtained from NMVOC measurements at sites down-wind but close to different solvent factories and workshops. These profiles were corrected by subtracting the background concentration profile. With this correction finally the solvent use emission profiles were obtained. All measured profiles at sites dominated by traffic emissions were found to be very similar and

were averaged to one traffic emission profile which was used in the CMB analysis. In the case of the solvent use emission four different profiles obtained from the sites close to four different solvent factories had to be used in the CMB model calculation because they exhibited large differences and could be not averaged to one profile.

The solvent emission profiles contained much higher contributions of oxygenated compounds than in the case of traffic. Butyl acetate, 2-butanol and acetone contributed significantly to the total mass. For hydrocarbons the xylenes and also toluene showed a larger abundance. These profiles, however, do not cover the whole solvent use emissions. Some important solvent sectors like domestic solvent use, the printing industry, dry cleaning and others were not covered by the present work. However, it can be assumed that the solvent profiles applied in the CMB analysis represent the most important emission sector of production and application of paints and varnishes which contributes 40% to the total emissions from solvent use according to the German Emission Inventory.

The results of the CMB analysis showed that road traffic rather than solvent use mainly contributes to the ambient NMVOC concentrations. The contribution of traffic emission was dominant at all investigated sites located down-wind from the city centre, with a relative contribution on average of about 90%. At dense traffic areas the traffic emission was responsible for almost 100% of the NMVOC concentrations. A significant influence of solvent emissions could only be observed in the close vicinity of solvent factories, where the impact of the investigated solvent sources amounted on average to about 45% of the measured NMVOC concentrations.

At the most the solvent emissions, understood as emissions from the paint application sector, apportioned by the CMB analysis to the receptor points down-wind from the city centre of Wuppertal, contribute about 9% to the total NMVOC concentrations. Accordingly, it could be concluded that the maximal contribution of the total solvent use emission to the NMVOC amounts to about 23% in the whole city area. These results have led to the conclusion that the contribution of solvent use to the NMVOC concentration in German cities, which are comparable to Wuppertal, falls in the range of a few to about 20%.

The CMB analysis performed with the solvent emission profiles calculated from production and consumption of solvents and solvent related goods used as input data for the German Emission Inventory, where the contribution from solvent use dominates, strongly disagrees with the NMVOC concentrations measured in Wuppertal. Calculated emission profiles could not be apportioned to the measured NMVOC concentrations or the apportionment gave much smaller contributions of the solvent emission. The fact that the calculated solvent profiles do not fit to the measured NMVOC concentrations very likely indicates some major disagreements between the calculated and effective solvent use emissions.

In conclusion, the proportions between traffic and solvent use emissions found in the present work strongly disagree with the German Emission Inventory which states, that at present (reference year 2000) about 62% of the total NMVOC emissions originate from solvent use and only 18% from road traffic. This disagreement is supported by the results of two other previous experimental studies carried out in Berlin and Augsburg.

Annex A: Abbreviations

ARTEMIS	Assessment and Reliability of Transport Emission Models and Inventory Systems
BV	Breakthrough Volume
CMB	Chemical Mass Balance
CMB ID	Identification name used in CMB modelling
CORINAIR	Co-ordination of information on air emission (the European air emission inventory system)
DBU	Deutsche Bundesstiftung Umwelt
DIN	Deutsches Institut für Normung e.V.
DOAS	Differential Optical Absorption Spectrometry
EC	European Commission
ECD	Electron Capture Detector
EEA	European Environmental Agency
EEC	European Economic Community
EMEP	Co-operative programme for monitoring and evaluation of the long-range transmissions of air pollutants in Europe
EPA	Environmental Protection Agency of the United States of America
EU-15	Germany, United Kingdom, France, Italy, Spain, Netherlands, Greece, Belgium, Portugal, Sweden, Austria, Denmark, Finland, Ireland and Luxembourg
EU-31	31 European Environmental Agency member countries: Austria, Belgium, Denmark, Finland, France, Germany, Greece, Ireland, Italy, Luxembourg, Netherlands, Portugal, Spain, Sweden, United Kingdom, Czech Republic, Cyprus, Estonia, Hungary, Latvia, Lithuania, Malta, Poland, Slovenia, Slovak Republic, Bulgaria, Romania, Turkey, Iceland, Liechtenstein, Norway
FID	Flame Ionisation Detector
FTIR	Fourier Transform Infrared Spectroscopy
GC	Gas Chromatography
GC-FID	Gas Chromatograph with Flame Ionisation Detector
HP GC	Hewlett-Packard Gas Chromatograph
ID No.	Identification Number
LUA	Landesumweltamt (North-Rhine Westfalia, Germany)
MS	Mass Spectroscopy
NDIR	Dual Wavelength Infrared
NMVOG	Non-Methane Volatile Organic Compound
NO _x	Oxides of nitrogen (NO + NO ₂)
NPL	National Physical Laboratory (United Kingdom)
PA	Peak Area
PAN	Peroxyacetyl Nitrate
RF	Response Factor
RR	Recovery Rate
SNAP	Selected Nomenclature for Air Pollution; the hierarchical structure of emission sources according to CORINAIR nomenclature

SSV	Save Sampling Volume
UBA	Umweltbundesamt (Federal Environmental Agency of Germany)
UV	Ultraviolet
VOC	Volatile Organic Compound
VUV	Vacuum Ultraviolet

Annex B: Gas mixtures

Table B.1: NPL standard gas mixture; hydrocarbons mixture delivered from National Physics Laboratory, cylinder number A003597

	compounds	ID No.	molecular weight (g/mol)	mixing ratio (ppb)	uncertainty (ppb)
1	<i>ethene</i>	2	28.05	22.03	0.44
2	<i>ethyne</i>	1	26.04	46.86	0.94
3	<i>ethane</i>	3	30.07	42.18	0.84
4	<i>propene</i>	6	42.08	21.19	0.42
5	<i>propane</i>	7	44.10	18.69	0.37
6	<i>propyne</i>	5	40.07	13.05	0.26
7	<i>i-butane</i>	13	58.12	6.22	0.12
8	<i>1-butene</i>	10	56.11	20.73	0.41
9	<i>i-butene</i>	11	56.11	20.86	0.42
10	<i>1,3-butadiene</i>	8	54.09	28.15	0.56
11	<i>n-butane</i>	14	58.12	9.72	0.19
12	<i>trans-2-butene</i>	9	56.11	7.03	0.14
13	<i>cis-2-butene</i>	12	56.11	13.90	0.28
14	<i>i-pentane</i>	18	72.15	7.19	0.14
15	<i>n-pentane</i>	26	72.15	5.75	0.12
16	<i>isoprene</i>	16	68.12	15.12	0.30
17	<i>trans-2-pentene</i>	21	70.14	24.13	0.48
18	<i>cis-2-pentene</i>	22	70.14	12.42	0.25
19	<i>2-methylpentane</i>	45	86.18	9.24	0.18
20	<i>3-methylpentane</i>	46	86.18	14.32	0.29
21	<i>n-hexane</i>	47	86.18	16.26	0.33
22	<i>benzene</i>	28	78.11	27.85	0.56
23	<i>cyclohexane</i>	42	84.16	24.61	0.49
24	<i>n-heptane</i>	61	100.21	12.42	0.25
25	<i>toluene</i>	48	92.14	21.46	0.43
26	<i>ethylbenzene</i>	64	106.17	8.81	0.18
27	<i>m-xylene</i>	66	106.17	10.92	0.22
28	<i>o-xylene</i>	65	106.17	7.20	0.14
29	<i>1,3,5-trimethylbenzene</i>	88	120.20	6.47	0.13
30	<i>1,2,4-trimethylbenzene</i>	87	120.20	5.51	0.11

Table B.2.a: RM2 gas mixture; hydrocarbons mixture in synthetic air prepared on 25.02.2002, cylinder number 1949A

	compounds	ID No.	molecular weight (g/mol)	mixing ratio (ppb)	uncertainty (ppb)
1	<i>ethene</i>	2	28.05	40.779	6.860
2	<i>ethyne</i>	1	26.04	40.682	10.761
3	<i>ethane</i>	3	30.07	40.256	8.238
4	<i>propene</i>	6	42.08	31.424	4.391
5	<i>propane</i>	7	44.10	41.184	4.674
6	<i>i-butane</i>	13	58.12	43.324	3.700
7	<i>i-butene</i>	11	56.11	38.681	3.492
8	<i>n-butane</i>	14	58.12	40.132	3.265
9	<i>trans-2-butene</i>	9	56.11	30.461	4.029
10	<i>cis-2-butene</i>	12	56.11	31.714	2.604
11	<i>i-pentane</i>	25	72.15	24.901	2.341
12	<i>1-pentene</i>	19	70.14	3.515	0.708
13	<i>n-pentane</i>	26	70.14	40.739	3.108
14	<i>isoprene</i>	16	68.12	5.920	0.973
15	<i>trans-2-pentene</i>	21	70.14	7.194	1.193
16	<i>cis-2-pentene</i>	22	70.14	3.316	0.475
17	<i>2,2-dimethylbutane</i>	43	86.18	46.467	3.837
18	<i>cyclopentene</i>	17	68.12	7.702	0.795
19	<i>methyl tert-butyl ether</i>	123	88.19	22.497	1.145
20	<i>2,3-dimethylbutane</i>	44	86.18	47.895	4.044
21	<i>cyclopentane</i>	24	70.14	26.029	2.198
22	<i>2-methylpentane</i>	45	86.18	47.523	15.561
23	<i>3-methylpentane</i>	46	86.18	37.508	2.613
24	<i>1-hexene</i>	37	84.16	13.197	0.986
25	<i>n-hexane</i>	47	84.16	22.277	1.443
26	<i>2-ethyl-1-butene</i>	204	84.16	47.338	3.067
27	<i>2,3-dimethyl-1,3-butadiene</i>	205	82.15	20.951	1.590
28	<i>methylcyclopentane</i>	41	84.16	51.133	3.514
29	<i>1-methyl-1-cyclopentene</i>	206	82.15	11.499	0.790
30	<i>2,3-dimethyl-2-butene</i>	207	84.16	20.617	1.364
31	<i>benzene</i>	28	78.11	41.695	3.679
32	<i>cyclohexane,</i>	42	84.16	44.281	2.803
33	<i>2,3-dimethylpentane</i>	58	84.16	35.904	2.272
34	<i>1,3-cyclohexadiene</i>	208	80.13	41.481	2.625
35	<i>2-methylhexane</i>	62	100.21	55.298	5.411
36	<i>cyclohexene</i>	30	82.15	36.360	3.258
37	<i>1-heptene</i>	209	98.19	34.388	3.600
38	<i>i-octane</i>	69	114.23	59.528	5.775
39	<i>n-heptane</i>	61	100.21	37.058	3.735
40	<i>1,4-cyclohexadiene</i>	210	80.13	29.600	3.528
41	<i>2,3,4-trimethylpentane</i>	70	100.21	65.097	8.032
42	<i>toluene</i>	48	92.14	27.136	2.911
43	<i>2-methylheptane</i>	78	114.23	52.356	3.136
44	<i>3-methylheptane</i>	79	114.23	59.389	4.318
45	<i>4-methylheptane</i>	80	114.23	63.078	4.472
46	<i>1-methyl-1-cyclohexene</i>	211	96.17	44.003	3.120
47	<i>1-octene</i>	212	112.21	57.959	4.314
48	<i>n-octane</i>	81	114.23	49.471	2.785

Table B.2.b: RM2 gas mixture; hydrocarbons mixture in synthetic air prepared on 25.02.2002, cylinder number 1949A

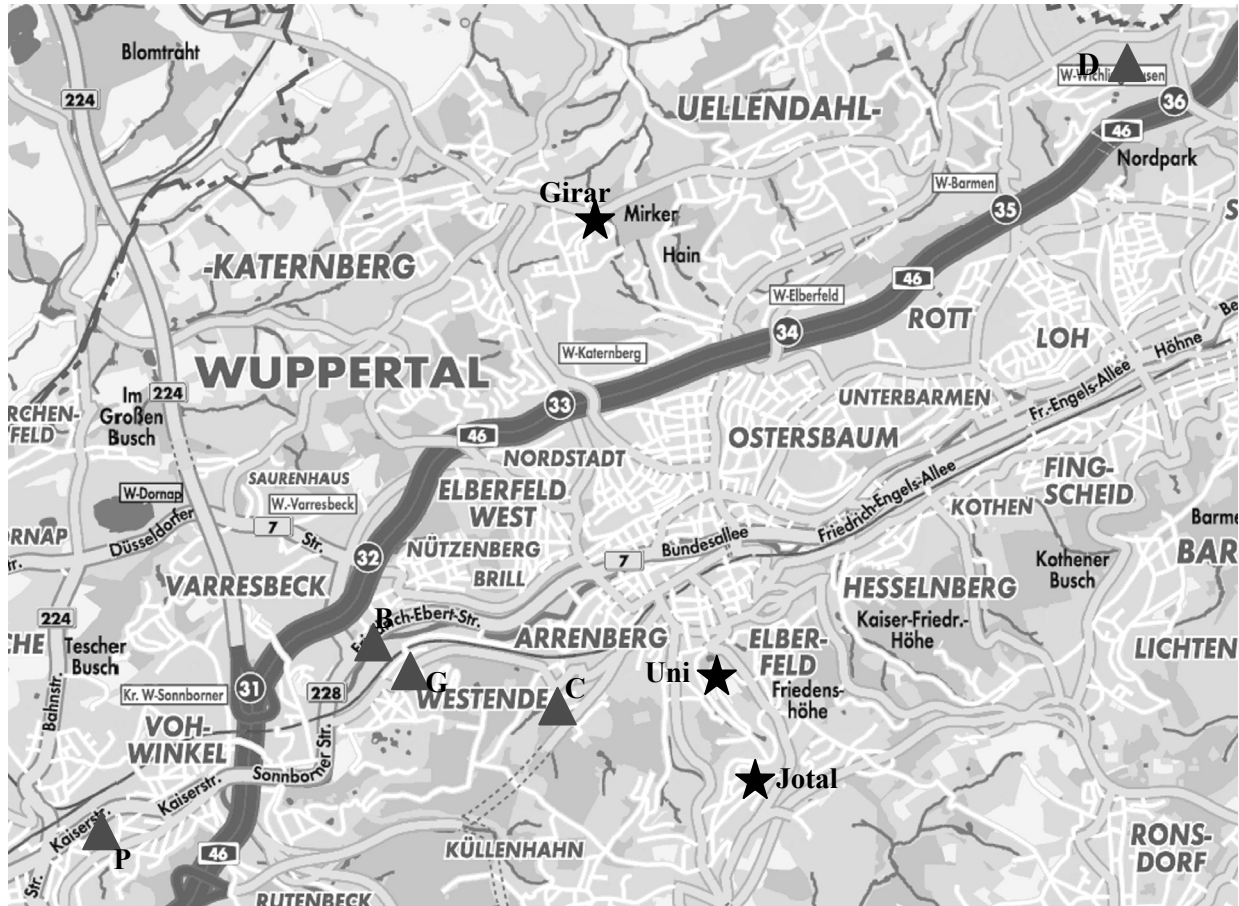
	compounds	ID No.	molecular weight (g/mol)	mixing ratio (ppb)	uncertainty (ppb)
49	<i>ethylbenzene</i>	64	106.17	30.717	2.524
50	<i>meta-xylene</i>	67	106.17	31.090	3.347
51	<i>para-xylene</i>	66	106.17	29.871	3.216
52	<i>styrene</i>	145	104.15	57.661	11.848
53	<i>ortho-xylene</i>	65	106.17	34.625	4.248
54	<i>alpha-pinene</i>	124	136.24	102.444	9.128
55	<i>n-propylbenzene</i>	85	120.20	32.335	1.907
56	<i>4-ethyltoluene</i>	91	120.20	24.322	2.128
57	<i>1,3,5-trimethylbenzene</i>	88	120.20	38.263	6.871
58	<i>n-decane</i>	120	142.28	18.803	3.414
59	<i>1,2,4-trimethylbenzene</i>	87	120.20	23.647	6.342
60	<i>tetr-butylbenzene</i>	213	120.20	38.285	10.267
61	<i>1,2,3-trimethylbenzene</i>	86	120.20	24.366	12.829
62	<i>1,2,3,4-tetramethylbenzene</i>	115	134.22	16.911	2.341

Table B.3: OXY gas mixture; oxygenated compound mixture in synthetic air prepared on 18.02.2002, cylinder number A003607

	compounds	ID No.	molecular weight (g/mol)	mixing ratio (ppb)	uncertainty (ppb)
1	<i>acetone</i>	139	58.08	95.874	28.654
2	<i>methyl acetate</i>	164	74.08	69.008	36.524
3	<i>ethyl acetate</i>	165	88.11	65.911	18.367
4	<i>methanol</i>	149	32.04	220.823	34.453
5	<i>2-butanone</i>	159	72.11	95.848	18.728
6	<i>isopropyl acetate</i>	215	102.13	3.335	1.550
7	<i>2-propanol</i>	151	60.10	31.471	7.818
8	<i>ethanol</i>	150	46.07	40.918	16.828
9	<i>propyl acetate</i>	166	102.13	43.426	2.626
10	<i>isobutyl acetate</i>	168	116.16	37.873	4.647
11	<i>4-methyl-2-pentanone</i>	160	100.16	34.486	7.250
12	<i>2-butanol</i>	214	74.12	23.490	9.045
13	<i>1-propanol</i>	152	60.10	23.350	9.218
14	<i>butyl acetate</i>	167	116.16	6.203	1.995
15	<i>2-hexanone</i>	216	100.16	9.413	4.105
16	<i>1-butanol</i>	153	74.12	16.493	6.440
17	<i>cyclohexanone</i>	161	98.14	11.182	5.446

Annex C: Locations of sampling points

Map C.1: Locations of the investigated solvent factories and workshops against locations of receptor points



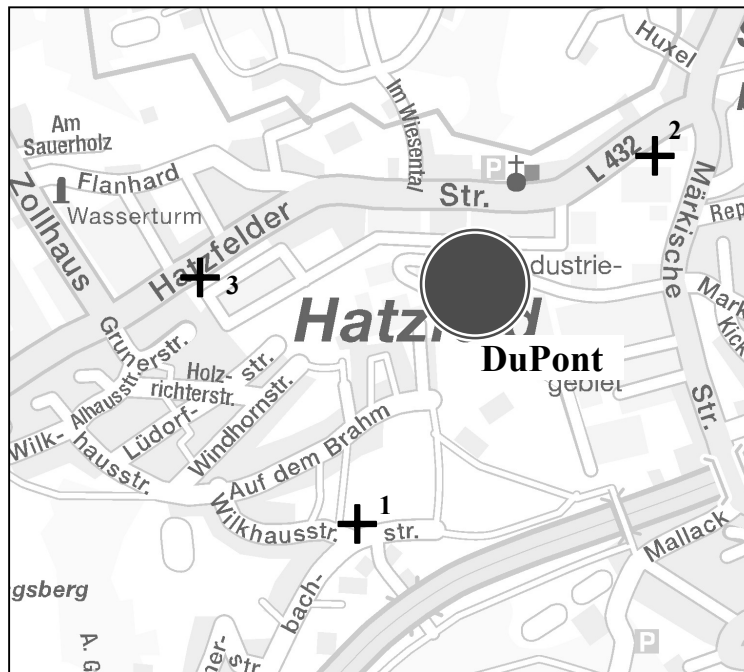
σ Solvent factories and workshops:

- D: DuPont Performance Coatings GmbH
- P: PPG Industries Lacke GmbH
- B: Bayer AG
- C: Dr. Alfred Conrads Lackfabrick Nachf, KG
- G: Karosseriebau Gorn GmbH

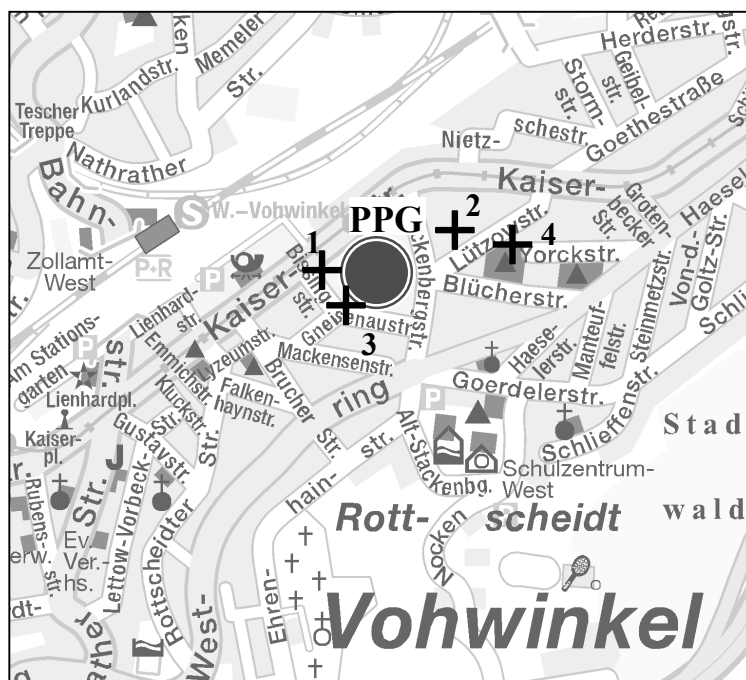
H Receptor points down-wind from the city centre:

- GIRAR: Girardet Str.
- UNI: Universität
- JOTAL: Im Johannistal

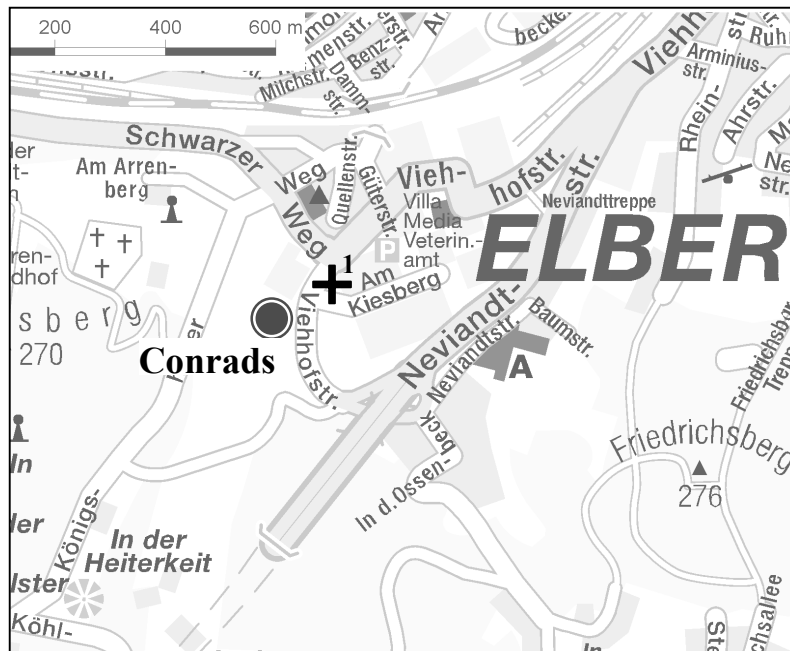
Map C.2: Locations of the measurement points around the DuPont Performance Coatings GmbH solvent factory (1: WILKHA, 2: HATZEN, 3: HATZEM)



Map C.3: Locations of the measurement points around the PPG Industries Lacke GmbH solvent factory (1: BISSIM, 2: LUTZOW, 3: BISSIM, 4: YOREK)



Map C.4: Location of the measurement point close to the Dr. Alfred Conrads Lackfabrick Nachf, KG solvent factory (1: VIEHOF)



Map C.5: Locations of the measurement points around the Karosseriebau Gorn GmbH workshop (1: SIMONS; 2: SIMONB, 3: SIMONM)



Annex D: Measurement resultsTable D.1.a: Overview of NMVOC mixing ratios (ppbC)¹ measured during the study carried out in Wuppertal

compounds	maximum	minimum	average	st. dev. ²	median
<i>propene</i>	3.180	0.169	1.035	0.751	0.701
<i>propane</i>	4.583	0.018	1.275	1.351	0.839
<i>propadiene</i>	0.272	0.003	0.023	0.050	0.006
<i>propyne</i>	0.164	0.002	0.033	0.046	0.020
<i>2-methylpropane</i>	2.958	0.070	0.945	0.758	0.688
<i>1-butene, i-butene</i>	10.278	1.115	3.443	2.121	2.848
<i>1,3-butadiene</i>	0.497	0.058	0.179	0.114	0.145
<i>n-butane</i>	4.643	0.105	1.633	1.382	1.132
<i>trans-2-butene</i>	0.910	0.088	0.273	0.212	0.195
<i>1-butyne</i>	0.189	0.004	0.033	0.034	0.027
<i>cis-2-butene</i>	0.764	0.064	0.226	0.192	0.146
<i>3-methyl-1-butene</i>	1.601	0.079	0.278	0.291	0.197
<i>2-methylbutane (i-pentane)</i>	27.426	1.119	5.985	6.139	4.092
<i>1-pentene</i>	9.134	0.147	1.014	1.672	0.653
<i>n-pentane, 2-methyl-1-butene</i>	48.814	0.476	5.642	8.955	3.187
<i>2-methyl-1,3-butadiene</i>	7.315	0.203	2.020	1.708	1.606
<i>trans-2-pentene</i>	10.650	0.063	0.984	1.990	0.407
<i>cis-2-pentene</i>	5.132	0.038	0.641	0.956	0.384
<i>2,2-dimethylbutane</i>	6.071	0.053	0.794	1.143	0.571
<i>cyclopentene</i>	1.463	0.026	0.222	0.280	0.118
<i>methyl tert-butyl ether</i>	5.950	0.049	1.367	1.295	0.906
<i>2,3-dimethylbutane, cyclopentane</i>	27.890	0.379	3.275	5.130	2.102
<i>2-methylpentane</i>	40.209	0.552	4.706	7.271	2.865
<i>3-methylpentane</i>	22.823	0.178	2.638	4.116	1.644
<i>1-hexene</i>	3.513	0.117	0.471	0.607	0.362
<i>n-hexane, 2-ethyl-1-butene</i>	22.480	0.483	3.134	4.154	2.302
<i>2,3-dimethyl-1,3-butadiene</i>	1.544	0.004	0.141	0.296	0.053
<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	31.436	0.327	3.478	5.725	2.131
<i>2,3-dimethyl-2-butene</i>	3.157	0.040	0.312	0.566	0.177
<i>benzene</i>	33.607	0.957	5.926	6.455	4.493
<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	32.377	0.545	4.434	5.872	2.742
<i>2-methylhexane</i>	6.887	0.107	0.834	1.265	0.439
<i>cyclohexene</i>	0.633	0.020	0.107	0.117	0.079
<i>1-heptene</i>	6.057	0.133	0.803	1.073	0.548
<i>2,2,4-trimethylpentane</i>	23.131	0.317	2.574	4.163	1.570
<i>n-heptane</i>	12.900	0.338	1.919	2.369	1.139
<i>1,4-cyclohexadiene</i>	0.256	0.006	0.077	0.064	0.062
<i>2,3,4-trimethylpentane</i>	8.790	0.064	0.950	1.616	0.474
<i>toluene</i>	147.015	2.689	21.629	28.012	13.859
<i>2-methylheptane</i>	9.063	0.213	1.255	1.670	0.721
<i>3-methylheptane</i>	3.000	0.053	0.384	0.573	0.211
<i>4-methylheptane, 1-methyl-1-cyclohexene</i>	11.670	0.138	1.261	2.156	0.665
<i>1-octene</i>	2.953	0.141	0.721	0.681	0.492
<i>n-octane</i>	8.481	0.221	1.443	1.789	0.732
<i>ethylbenzene</i>	17.365	0.396	4.330	3.978	2.909
<i>meta- and para-xylene</i>	24.379	0.537	7.572	6.162	5.576
<i>styrene</i>	2.740	0.004	0.509	0.644	0.297
<i>ortho-xylene</i>	8.365	0.092	2.266	2.088	1.777
<i>alpha-pinene</i>	6.818	0.016	0.862	1.537	0.232
<i>n-propylbenzene</i>	2.096	0.009	0.439	0.503	0.297

Table D.1.b: Overview of NMVOC mixing ratios (ppbC)¹ measured during the study carried out in Wuppertal

compounds	maximum	minimum	average	st. dev. ²	median
<i>4-ethyltoluene</i>	1.594	0.002	0.340	0.426	0.190
<i>1,3,5-trimethylbenzene</i>	1.935	0.002	0.357	0.519	0.148
<i>n-decane</i>	1.204	0.006	0.178	0.228	0.120
<i>1,2,4-trimethylbenzene, tetrabutylbenzene</i>	7.193	0.008	1.185	1.728	0.635
<i>1,2,3-trimethylbenzene</i>	0.969	0.005	0.128	0.201	0.054
<i>1,2,3,4-tetramethylbenzene</i>	0.092	0.002	0.011	0.016	0.010
<i>acetone</i>	52.175	0.216	5.397	9.869	1.833
<i>methyl acetate</i>	3.674	0.015	0.480	0.821	0.257
<i>ethyl acetate</i>	1.540	0.004	0.204	0.335	0.020
<i>methanol</i>	1.003	0.004	0.167	0.264	0.050
<i>2-butanone</i>	1.672	0.003	0.193	0.312	0.082
<i>isopropyl acetate</i>	2.478	0.005	0.150	0.452	0.054
<i>2-propanol</i>	2.529	0.032	0.443	0.557	0.255
<i>ethanol</i>	24.934	0.006	1.554	4.726	0.212
<i>propyl acetate</i>	2.440	0.020	0.298	0.519	0.082
<i>isobutyl acetate</i>	1.683	0.002	0.129	0.315	0.047
<i>4-methyl-2-pentanone</i>	1.054	0.003	0.081	0.203	0.013
<i>2-butanol</i>	27.165	0.010	2.490	6.299	0.127
<i>1-propanol</i>	4.649	0.004	0.191	0.859	0.018
<i>butyl acetate</i>	522.129	0.015	18.829	96.815	0.078
<i>2-hexanone</i>	0.616	0.005	0.082	0.155	0.022
<i>1-butanol</i>	9.253	0.011	0.500	1.713	0.073
<i>cyclohexanone</i>	0.841	0.003	0.090	0.151	0.067
Σ NMVOC	857.546	38.224	156.758	181.212	103.326

¹ volume mixing ratio multiplied with carbon number; ² st.dev. – standard deviation

Table D.2.a: Overview of NMVOC concentrations ($\mu\text{g}/\text{m}^3$)¹ measured during the study carried out in Wuppertal

compounds	maximum	minimum	average	st. dev. ²	median
<i>propene</i>	1.824	0.097	0.594	0.431	0.402
<i>propane</i>	2.756	0.011	0.766	0.812	0.504
<i>propadiene</i>	0.149	0.002	0.012	0.028	0.004
<i>propyne</i>	0.090	0.001	0.018	0.025	0.011
<i>2-methylpropane</i>	1.758	0.042	0.562	0.451	0.409
<i>1-butene, i-butene</i>	5.897	0.640	1.976	1.217	1.634
<i>1,3-butadiene</i>	0.275	0.032	0.099	0.063	0.080
<i>n-butane</i>	2.759	0.062	0.971	0.821	0.673
<i>trans-2-butene</i>	0.522	0.050	0.157	0.122	0.112
<i>1-butyne</i>	0.104	0.002	0.018	0.019	0.015
<i>cis-2-butene</i>	0.438	0.037	0.130	0.110	0.084
<i>3-methyl-1-butene</i>	0.919	0.045	0.159	0.167	0.113
<i>2-methylbutane (i-pentane)</i>	16.187	0.661	3.532	3.623	2.415
<i>1-pentene</i>	5.240	0.084	0.582	0.959	0.374
<i>n-pentane, 2-methyl-1-butene</i>	28.007	0.273	3.237	5.138	1.828
<i>2-methyl-1,3-butadiene</i>	3.397	0.094	0.938	0.793	0.746
<i>trans-2-pentene</i>	6.110	0.036	0.565	1.142	0.233
<i>cis-2-pentene</i>	2.945	0.022	0.368	0.549	0.221
<i>2,2-dimethylbutane</i>	3.567	0.031	0.467	0.671	0.335
<i>cyclopentene</i>	0.815	0.015	0.124	0.156	0.066
<i>methyl tert-butyl ether</i>	4.293	0.035	0.986	0.934	0.653
<i>2,3-dimethylbutane, cyclopentane</i>	13.335	0.181	1.566	2.453	1.005
<i>2-methylpentane</i>	23.621	0.325	2.765	4.271	1.683
<i>3-methylpentane</i>	13.408	0.105	1.550	2.418	0.966
<i>1-hexene</i>	2.015	0.067	0.270	0.348	0.207
<i>n-hexane, 2-ethyl-1-butene</i>	12.896	0.277	1.814	2.375	1.321
<i>2,3-dimethyl-1,3-butadiene</i>	0.864	0.002	0.079	0.166	0.030
<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	17.818	0.186	1.972	3.245	1.208
<i>2,3-dimethyl-2-butene</i>	1.811	0.023	0.179	0.325	0.101
<i>benzene</i>	17.894	0.510	3.155	3.437	2.392
<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	17.145	0.289	2.348	3.110	1.452
<i>2-methylhexane</i>	4.033	0.063	0.488	0.741	0.257
<i>cyclohexene</i>	0.354	0.011	0.060	0.065	0.044
<i>1-heptene</i>	3.475	0.076	0.460	0.616	0.314
<i>2,2,4-trimethylpentane</i>	13.509	0.185	1.503	2.431	0.917
<i>n-heptane</i>	7.553	0.198	1.124	1.387	0.667
<i>1,4-cyclohexadiene</i>	0.140	0.003	0.042	0.035	0.034
<i>2,3,4-trimethylpentane</i>	4.503	0.033	0.487	0.828	0.243
<i>toluene</i>	79.147	1.447	11.644	15.081	7.461
<i>2-methylheptane</i>	5.293	0.124	0.733	0.976	0.421
<i>3-methylheptane</i>	1.752	0.031	0.224	0.334	0.123
<i>4-methylheptane, 1-methyl-1-cyclohexene</i>	5.907	0.070	0.638	1.091	0.337
<i>1-octene</i>	1.694	0.081	0.414	0.391	0.282
<i>n-octane</i>	4.953	0.129	0.843	1.045	0.428
<i>ethylbenzene</i>	9.426	0.215	2.350	2.159	1.579
<i>meta- and para-xylene</i>	12.912	0.284	4.011	3.264	2.953
<i>styrene</i>	1.563	0.000	0.289	0.368	0.169
<i>ortho-xylene</i>	4.303	0.047	1.171	1.073	0.914
<i>alpha-pinene</i>	3.395	0.009	0.430	0.765	0.117
<i>n-propylbenzene</i>	1.100	0.005	0.231	0.264	0.156
<i>4-ethyltoluene</i>	0.865	0.001	0.184	0.231	0.103

Table D.2.b: Overview of NMVOC concentrations ($\mu\text{g}/\text{m}^3$)¹ measured during the study carried out in Wuppertal

compounds	maximum	minimum	average	st. dev. ²	median
<i>1,3,5-trimethylbenzene</i>	0.970	0.000	0.179	0.261	0.074
<i>n-decane</i>	0.797	0.004	0.118	0.151	0.080
<i>1,2,4-trimethylbenzene, tetrabutylbenzene</i>	4.051	0.005	0.667	0.973	0.357
<i>1,2,3-trimethylbenzene</i>	0.606	0.000	0.080	0.126	0.033
<i>1,2,3,4-tetramethylbenzene</i>	0.053	0.001	0.005	0.010	0.002
<i>acetone</i>	41.313	0.171	4.273	7.815	1.451
<i>methyl acetate</i>	3.711	0.015	0.485	0.829	0.260
<i>ethyl acetate</i>	1.388	0.003	0.183	0.302	0.018
<i>methanol</i>	1.315	0.006	0.219	0.347	0.065
<i>2-butanone</i>	1.232	0.003	0.142	0.230	0.061
<i>isopropyl acetate</i>	2.070	0.004	0.125	0.378	0.045
<i>2-propanol</i>	2.072	0.026	0.363	0.456	0.209
<i>ethanol</i>	23.491	0.006	1.464	4.453	0.200
<i>propyl acetate</i>	2.039	0.017	0.249	0.433	0.068
<i>isobutyl acetate</i>	1.332	0.001	0.102	0.249	0.037
<i>4-methyl-2-pentanone</i>	0.720	0.002	0.055	0.139	0.009
<i>2-butanol</i>	20.588	0.008	1.887	4.774	0.097
<i>1-propanol</i>	3.809	0.003	0.156	0.704	0.014
<i>butyl acetate</i>	413.433	0.012	14.909	76.660	0.061
<i>2-hexanone</i>	0.421	0.004	0.056	0.106	0.015
<i>1-butanol</i>	7.013	0.008	0.379	1.299	0.055
<i>cyclohexanone</i>	0.563	0.002	0.060	0.101	0.045
Σ NMVOC	993.580	8.131	95.667	191.491	47.408

¹ concentrations calculated for the normal conditions (273.15 K and 1 atm); ² st.dev – standard deviation

Annex E: Source profiles and receptor concentrations

Table E.1.a: Average source fingerprint of road traffic (CMB ID: TRAFFIC1)

	compounds	carbon number	ID number	species code for CMB	mass fraction	±
1	<i>propene</i>	3	6	6C	0.0049	0.0016
2	<i>propane</i>	3	7	7C	0.0051	0.0033
3	<i>propadiene</i>	3	4	4C	0.0002	0.0002
4	<i>propyne</i>	3	5	5C	0.0001	0.0002
5	<i>X5/13a</i> ¹	3/4	<i>x13</i>	X13C	0.0003	0.0002
6	<i>2-methylpropane</i>	4	13	13C	0.0070	0.0022
7	<i>1-butene, 2-methylpropene</i>	4	10,11	10,11C	0.0189	0.0051
8	<i>1,3-butadiene</i>	4	8	8C	0.0012	0.0003
9	<i>n-butane</i>	4	14	14C	0.0107	0.0035
10	<i>trans-2-butene</i>	4	9	9C	0.0015	0.0004
11	<i>1-butyne</i>	4	203	203C	0.0002	0.0001
12	<i>cis-2-butene</i>	4	12	12C	0.0014	0.0004
13	<i>X12/18d</i> ¹	4/5	<i>x32</i>	X32C	0.0014	0.0005
14	<i>3-methyl-1-butene</i>	5	18	18C	0.0021	0.0004
15	<i>X18/25a</i> ¹	5	<i>x34</i>	X34C	0.0019	0.0007
16	<i>X18/25b</i> ¹	5	<i>x35</i>	X35C	0.0025	0.0007
17	<i>X18/25d</i> ¹	5	<i>x37</i>	X37C	0.0479	0.0114
18	<i>2-methylbutane</i>	5	25	25C	0.0493	0.0146
19	<i>X25/19c</i> ¹	5	<i>x41</i>	X41C	0.0045	0.0009
20	<i>1-pentene</i>	5	19	19C	0.0088	0.0019
21	<i>n-pentane, 2-methyl-1-butene</i>	5	26, 20	26,20C	0.0526	0.0112
22	<i>2-methyl-1,3-butadiene</i>	6	16	16C	0.0163	0.0041
23	<i>trans-2-pentene</i>	5	21	21C	0.0093	0.0022
24	<i>cis-2-pentene</i>	5	22	22C	0.0045	0.0010
25	<i>X22/43b</i> ¹	5/6	<i>x52</i>	X52C	0.0141	0.0019
26	<i>2,2-dimethylbutane</i>	6	43	43C	0.0079	0.0016
27	<i>X43/17c</i> ¹	5/6	<i>x60</i>	X60C	0.0004	0.0001
28	<i>cyclopentene</i>	5	17	17C	0.0015	0.0004
29	<i>X17/123c</i> ¹	5/6	<i>x66</i>	X66C	0.0027	0.0010
30	<i>methyl tert-butyl ether</i>	5	123	123C	0.0156	0.0039
31	<i>2,3-dimethylbutane, cyclopentane</i>	6	44,24	44,24C	0.0238	0.0051
32	<i>2-methylpentane</i>	6	45	45C	0.0397	0.0078
33	<i>X45/46b</i> ¹	6	<i>x71</i>	X71C	0.0039	0.0014
34	<i>3-methylpentane</i>	6	46	46C	0.0223	0.0044
35	<i>1-hexene</i>	6	37	37C	0.0037	0.0007
36	<i>n-hexane, 2-ethyl-1-butene</i>	6	47, 204	47,204C	0.0040	0.0011
37	<i>X37/47b</i> ¹	6	<i>x77</i>	X77C	0.0261	0.0051
38	<i>2,3-dimethyl-1,3-butadiene</i>	6	205	205C	0.0007	0.0003
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	6	41, 206	41,206C	0.0304	0.0059
40	<i>2,3-dimethyl-2-butene</i>	6	207	207C	0.0024	0.0005
41	<i>benzene</i>	6	28	28C	0.0505	0.0097
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	6, 7	42, 58, 208	42,58C	0.0341	0.0068
43	<i>2-methylhexane</i>	7	62	62C	0.0073	0.0015
44	<i>cyclohexene</i>	6	30	30C	0.0009	0.0002
45	<i>1-heptene</i>	7	209	209C	0.0065	0.0013
46	<i>2,2,4-trimethylpentane</i>	8	69	69C	0.0218	0.0043

Table E.1.b: Average source fingerprint of road traffic (CMB ID: TRAFFIC1)

	compounds	carbon number	ID number	species code for CMB	mass fraction	±
47	<i>n</i> -heptane	7	61	61C	0.0150	0.0031
48	<i>1,4</i> -cyclohexadiene	6	210	210C	0.0004	0.0001
49	<i>X210/70h</i> ¹	7	<i>x122</i>	X122C	0.0112	0.0023
50	<i>X210/70i</i> ¹	7	<i>x123</i>	X123C	0.0038	0.0008
51	<i>X210/70j</i> ¹	7	<i>x124</i>	X124C	0.0031	0.0006
52	<i>2,3,4</i> -trimethylpentane	8	70	70C	0.0075	0.0016
53	toluene	7	48	48C	0.1556	0.0315
54	<i>2</i> -methylheptane	8	78	78C	0.0091	0.0018
55	<i>3</i> -methylheptane	8	79	79C	0.0034	0.0007
56	<i>4</i> -methylheptane, <i>1</i> -methyl- <i>1</i> -cyclohexene	8, 7	80, 211	80211C	0.0086	0.0019
57	<i>X211/212c</i> ¹	8	<i>x137</i>	X137C	0.0002	0.0001
58	<i>1</i> -octene	8	212	212C	0.0037	0.0008
59	<i>X212/81a</i> ¹	8	<i>x140</i>	X140C	0.0001	0.0000
60	<i>n</i> -octane	8	81	81C	0.0070	0.0014
61	ethylbenzene	8	64	64C	0.0307	0.0066
62	<i>meta</i> - and <i>para</i> -xylene	8	66,67	66,67C	0.0533	0.0117
63	styrene	8	145	145C	0.0051	0.0016
64	<i>ortho</i> -xylene	8	65	65C	0.0214	0.0050
65	<i>alpha</i> -pinene	10	124	124C	0.0039	0.0016
66	<i>n</i> -propylbenzene	9	85	85C	0.0044	0.0013
67	<i>4</i> -ethyltoluene	9	91	91C	0.0022	0.0007
68	<i>X67/145c</i> ¹	8	<i>x163</i>	X163C	0.0034	0.0011
69	<i>X88/120c</i> ¹	9	<i>x166</i>	X166C	0.0038	0.0013
70	<i>1,3,5</i> -trimethylbenzene	9	88	88C	0.0044	0.0016
71	<i>n</i> -decane	10	120	120C	0.0018	0.0008
72	<i>1,2,4</i> -trimethylbenzene, <i>tetr</i> -butylbenzene	9	87, 213	87213C	0.0125	0.0048
73	<i>X213/86b</i> ¹	9/10	193	X193C	0.0004	0.0001
74	<i>1,2,3</i> -trimethylbenzene	9	86	86C	0.0014	0.0006
75	<i>1,2,3,4</i> -tetramethylbenzene	10	115	115C	0.0001	0.0000
76	acetone	3	139	139C	0.0266	0.0163
77	methyl acetate	3	164	164C	0.0026	0.0009
78	ethyl acetate	4	165	165C	0.0016	0.0007
79	methanol	1	149	149C	0.0007	0.0002
80	<i>2</i> -butanone	4	159	159C	0.0013	0.0005
81	isopropyl acetate	5	214	214C	0.0007	0.0005
82	<i>2</i> -propanol	3	151	151C	0.0029	0.0011
83	ethanol	2	150	150C	0.0063	0.0050
84	propyl acetate	5	166	166C	0.0012	0.0011
85	isobutyl acetate	6	168	168C	0.0005	0.0001
86	<i>4</i> -methyl- <i>2</i> -pentanone	6	160	160C	0.0005	0.0008
87	<i>2</i> -butanol	4	215	215C	0.0015	0.0008
88	<i>1</i> -propanol	3	152	152C	0.0003	0.0001
89	butyl acetate	6	167	167C	0.0009	0.0005
90	<i>2</i> -hexanone	6	216	216C	0.0005	0.0005
91	<i>1</i> -butanol	4	153	153C	0.0008	0.0003
92	cyclohexanone	6	161	161C	0.0007	0.0002
				Σ	1.0000	

¹ names of unknown compounds; the names are attributed according to the location of the unidentified peak at the chromatogram, for example name *X18/25b* means that the particular compound is the second unidentified peak located between known compounds with ID numbers 18 and 25

Table E.2.a: Source fingerprints of solvent use, four profiles obtained from measurements of emission from different solvent factories and workshops

	ID number ¹	SOLVENTS2 ²		SOLVENTS3 ²		SOLVENTS4 ²		SOLVENTS8 ²	
		mass fraction	±	mass fraction	±	mass fraction	±	mass fraction	±
1	6	0.0131	0.0037	0.0176	0.0029	0.0042	0.0007	0.0215	0.0061
2	7	0.0418	0.0085	0.0289	0.0052	0.0039	0.0010	0.0158	0.0045
3	4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	5	0.0005	0.0001	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000
5	x13	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
6	13	0.0144	0.0030	0.0098	0.0017	0.0134	0.0021	0.0054	0.0015
7	10,11	0.0377	0.0120	0.0606	0.0342	0.0064	0.0011	0.0532	0.0151
8	8	0.0011	0.0004	0.0018	0.0004	0.0000	0.0000	0.0011	0.0003
9	14	0.0336	0.0063	0.0298	0.0050	0.0000	0.0000	0.0088	0.0025
10	9	0.0035	0.0011	0.0044	0.0013	0.0019	0.0003	0.0012	0.0003
11	203	0.0005	0.0001	0.0007	0.0002	0.0001	0.0000	0.0002	0.0001
12	12	0.0029	0.0008	0.0034	0.0010	0.0011	0.0002	0.0009	0.0003
13	x32	0.0009	0.0013	0.0067	0.0031	0.0000	0.0000	0.0024	0.0007
14	18	0.0021	0.0004	0.0007	0.0003	0.0000	0.0000	0.0006	0.0002
15	x34	0.0069	0.0066	0.0196	0.0162	0.0557	0.0097	0.0008	0.0002
16	x35	0.0108	0.0050	0.0089	0.0045	0.0120	0.0018	0.0023	0.0006
17	x37	0.0718	0.0128	0.0780	0.0224	0.0000	0.0000	0.0768	0.0218
18	25	0.0334	0.0110	0.0834	0.0161	0.1770	0.0716	0.0170	0.0048
19	x41	0.0063	0.0011	0.0196	0.0279	0.0050	0.0013	0.0086	0.0025
20	19	0.0014	0.0003	0.0028	0.0005	0.0075	0.0037	0.0016	0.0005
21	26, 20	0.0124	0.0026	0.0073	0.0012	0.0524	0.0155	0.0000	0.0000
22	16	0.0682	0.0146	0.0070	0.0015	0.0579	0.0178	0.0000	0.0000
23	21	0.0014	0.0003	0.0028	0.0005	0.0098	0.0035	0.0000	0.0000
24	22	0.0015	0.0003	0.0093	0.0034	0.0078	0.0020	0.0049	0.0014
25	x52	0.0015	0.0003	0.0063	0.0014	0.0136	0.0051	0.0000	0.0000
26	43	0.0014	0.0003	0.0010	0.0003	0.0063	0.0016	0.0000	0.0000
27	x60	0.0052	0.0025	0.0075	0.0082	0.0285	0.0080	0.0000	0.0000
28	17	0.0019	0.0003	0.0018	0.0003	0.0025	0.0026	0.0001	0.0000
29	x66	0.0000	0.0000	0.0058	0.0014	0.0074	0.0015	0.0015	0.0004
30	123	0.0037	0.0028	0.0191	0.0066	0.0176	0.0035	0.0070	0.0020
31	44,24	0.0010	0.0005	0.0034	0.0008	0.0031	0.0009	0.0042	0.0012
32	45	0.0000	0.0000	0.0012	0.0002	0.0179	0.0032	0.0033	0.0009
33	x71	0.0112	0.0030	0.0267	0.0138	0.0415	0.0075	0.0036	0.0010
34	46	0.0000	0.0000	0.0004	0.0001	0.0113	0.0020	0.0000	0.0000
35	37	0.0022	0.0004	0.0017	0.0004	0.0000	0.0000	0.0029	0.0008
36	47, 204	0.0127	0.0023	0.0395	0.0065	0.0042	0.0007	0.0116	0.0033
37	x77	0.0000	0.0000	0.0025	0.0005	0.0164	0.0027	0.0003	0.0001
38	205	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001
39	41, 206	0.0001	0.0000	0.0004	0.0001	0.0136	0.0031	0.0000	0.0000
40	207	0.0003	0.0001	0.0004	0.0001	0.0027	0.0005	0.0000	0.0000
41	28	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42	42, 58, 208	0.0148	0.0031	0.0066	0.0011	0.0224	0.0040	0.0006	0.0002
43	62	0.0024	0.0004	0.0011	0.0002	0.0027	0.0004	0.0000	0.0000
44	30	0.0002	0.0002	0.0004	0.0003	0.0000	0.0000	0.0010	0.0003
45	209	0.0050	0.0009	0.0026	0.0006	0.0000	0.0000	0.0014	0.0004
46	69	0.0012	0.0003	0.0062	0.0016	0.0150	0.0023	0.0005	0.0001
47	61	0.0217	0.0052	0.0104	0.0031	0.0224	0.0035	0.0013	0.0004
48	210	0.0002	0.0000	0.0055	0.0034	0.0000	0.0000	0.0012	0.0003
49	x122	0.0092	0.0020	0.0069	0.0014	0.0063	0.0010	0.0010	0.0003
50	x123	0.0002	0.0001	0.0023	0.0006	0.0032	0.0005	0.0022	0.0006
51	x124	0.0008	0.0002	0.0019	0.0009	0.0000	0.0000	0.0055	0.0016

Table E.2.b: Source fingerprints of solvent use, four profiles obtained from measurements of emission from different solvent factories and workshops

	ID number ¹	SOLVENTS2 ²		SOLVENTS3 ²		SOLVENTS4 ²		SOLVENTS8 ²	
		mass fraction	±	mass fraction	±	mass fraction	±	mass fraction	±
52	70	0.0000	0.0000	0.0005	0.0001	0.0065	0.0010	0.0000	0.0000
53	48	0.0000	0.0000	0.0000	0.0000	0.0755	0.0116	0.0175	0.0057
54	78	0.0017	0.0004	0.0032	0.0006	0.0076	0.0013	0.0036	0.0017
55	79	0.0003	0.0001	0.0002	0.0000	0.0007	0.0001	0.0002	0.0001
56	80, 211	0.0005	0.0001	0.0034	0.0006	0.0019	0.0003	0.0005	0.0002
57	<i>x137</i>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0018	0.0005
58	212	0.0097	0.0023	0.0056	0.0013	0.0001	0.0001	0.0098	0.0029
59	<i>x140</i>	0.0002	0.0002	0.0002	0.0002	0.0001	0.0001	0.2707	0.0807
60	81	0.0065	0.0014	0.0144	0.0025	0.0037	0.0006	0.0295	0.0088
61	64	0.0436	0.0083	0.0438	0.0139	0.0472	0.0076	0.0413	0.0123
62	66,67	0.1234	0.0237	0.1357	0.0569	0.1282	0.0243	0.0619	0.0184
63	145	0.0058	0.0021	0.0000	0.0000	0.0000	0.0000	0.0008	0.0002
64	65	0.0380	0.0079	0.0264	0.0131	0.0272	0.0062	0.0000	0.0000
65	124	0.0014	0.0006	0.0000	0.0000	0.0000	0.0000	0.0172	0.0051
66	85	0.0082	0.0025	0.0000	0.0000	0.0000	0.0000	0.0014	0.0004
67	91	0.0133	0.0028	0.0033	0.0020	0.0021	0.0005	0.0000	0.0000
68	<i>x163</i>	0.0066	0.0024	0.0000	0.0000	0.0000	0.0000	0.0005	0.0001
69	<i>x166</i>	0.0062	0.0029	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
70	88	0.0109	0.0053	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
71	120	0.0063	0.0035	0.0008	0.0005	0.0000	0.0000	0.0000	0.0000
72	87, 213	0.0239	0.0142	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
73	193	0.0037	0.0010	0.0002	0.0001	0.0006	0.0001	0.0000	0.0000
74	86	0.0022	0.0017	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
75	115	0.0003	0.0003	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000
76	139	0.1662	0.1476	0.1072	0.0690	0.0000	0.0000	0.0916	0.0374
77	164	0.0071	0.0023	0.0160	0.0087	0.0000	0.0000	0.0082	0.0056
78	165	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0062	0.0017
79	149	0.0027	0.0036	0.0026	0.0010	0.0000	0.0000	0.0128	0.0136
80	159	0.0027	0.0012	0.0079	0.0048	0.0011	0.0006	0.0038	0.0009
81	214	0.0012	0.0007	0.0048	0.0055	0.0028	0.0006	0.0006	0.0003
82	151	0.0050	0.0012	0.0070	0.0061	0.0000	0.0000	0.0027	0.0020
83	150	0.0292	0.0068	0.0114	0.0030	0.0126	0.0028	0.0290	0.0156
84	166	0.0021	0.0016	0.0102	0.0126	0.0000	0.0000	0.0119	0.0114
85	168	0.0002	0.0001	0.0005	0.0003	0.0000	0.0000	0.0008	0.0002
86	160	0.0000	0.0000	0.0006	0.0005	0.0000	0.0000	0.0013	0.0003
87	215	0.0000	0.0000	0.0011	0.0007	0.0000	0.0000	0.0016	0.0013
88	152	0.0008	0.0002	0.0008	0.0002	0.0000	0.0000	0.0005	0.0002
89	167	0.0014	0.0007	0.0067	0.0089	0.0050	0.0053	0.0862	0.0710
90	216	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0027	0.0009
91	153	0.0049	0.0036	0.0205	0.0079	0.0022	0.0005	0.0093	0.0031
92	161	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0009
	Σ	1.0000		1.0000		1.0000		1.0000	

¹ compounds name, carbon number, and species code for CMB according to table E.1

² CMB ID names:

SOLVENTS2: source profile of PPG Industries Lacke GmbH factory
SOLVENTS3: source profile of Karosseriebau Gorn GmbH workshop
SOLVENTS4: source profile of Dr. Alfred Conrads Lackfabrick Nachf, KG factory
SOLVENTS8: source profile of DuPont Performance Coatings GmbH factory

Table E.3.a: NMVOC concentrations measured at different receptor points, four concentration profiles obtained from measurements at residential areas and areas down-wind from the city centre

	ID number ¹	GIRAR ²		UNI ²		JOTAL1 ²		JOTAL2 ²	
		concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm
1	6	0.354	0.055	0.224	0.101	0.338	0.122	0.219	0.036
2	7	0.093	0.017	0.224	0.046	0.634	0.322	0.024	0.005
3	4	0.003	0.001	0.012	0.009	0.007	0.002	0.002	0.002
4	5	0.006	0.002	0.004	0.005	0.011	0.008	0.011	0.002
5	x13	0.106	0.065	0.002	0.003	0.011	0.007	0.002	0.002
6	13	0.155	0.031	0.158	0.042	0.264	0.087	0.042	0.012
7	10,11	2.892	1.070	1.334	1.091	0.798	0.298	0.648	0.125
8	8	0.103	0.018	0.054	0.031	0.052	0.010	0.040	0.007
9	14	0.087	0.013	0.302	0.124	0.883	0.364	0.062	0.013
10	9	0.079	0.038	0.068	0.041	0.128	0.051	0.052	0.020
11	203	0.003	0.005	0.016	0.003	0.006	0.001	0.009	0.001
12	12	0.042	0.008	0.039	0.020	0.097	0.035	0.040	0.006
13	x32	0.023	0.032	0.007	0.010	0.166	0.035	0.050	0.010
14	18	0.049	0.015	0.049	0.010	0.111	0.021	0.067	0.010
15	x34	0.123	0.076	0.026	0.021	0.207	0.035	0.134	0.024
16	x35	0.230	0.064	0.096	0.036	0.202	0.047	0.155	0.025
17	x37	1.984	0.355	1.253	0.666	1.577	0.260	0.916	0.131
18	25	2.561	0.400	0.661	0.350	3.792	1.016	0.891	0.172
19	x41	0.121	0.019	0.093	0.133	0.229	0.062	0.082	0.019
20	19	0.110	0.033	0.202	0.077	0.423	0.118	0.084	0.013
21	26, 20	0.324	0.185	1.632	0.542	3.110	0.719	1.109	0.432
22	16	0.214	0.088	1.094	0.250	1.178	0.222	0.386	0.110
23	21	0.037	0.017	0.258	0.158	0.445	0.118	0.061	0.012
24	22	0.054	0.011	0.119	0.056	0.200	0.047	0.068	0.017
25	x52	0.131	0.051	0.366	0.102	0.631	0.168	0.194	0.058
26	43	0.047	0.011	0.209	0.044	0.386	0.081	0.200	0.091
27	x60	0.036	0.013	0.075	0.107	0.041	0.011	0.032	0.010
28	17	0.054	0.011	0.034	0.008	0.067	0.027	0.015	0.002
29	x66	0.003	0.003	0.071	0.039	0.067	0.027	0.189	0.037
30	123	0.644	0.112	0.221	0.118	0.592	0.206	0.268	0.267
31	44,24	1.062	0.372	0.367	0.524	0.895	0.141	0.471	0.403
32	45	0.325	0.051	1.273	0.248	1.427	0.300	1.161	0.305
33	x71	0.173	0.055	0.068	0.042	0.330	0.058	0.133	0.019
34	46	0.241	0.053	0.765	0.147	0.785	0.169	0.635	0.173
35	37	0.112	0.018	0.144	0.030	0.115	0.032	0.094	0.017
36	47, 204	0.044	0.063	0.034	0.049	2.479	0.483	0.003	0.003
37	x77	0.323	0.052	0.966	0.225	1.070	0.188	1.664	0.357
38	205	0.019	0.007	0.016	0.006	0.006	0.001	0.004	0.005
39	41, 206	0.207	0.050	0.896	0.174	0.960	0.190	0.640	0.206
40	207	0.050	0.029	0.082	0.020	0.045	0.008	0.040	0.013
41	28	0.580	0.090	1.428	0.276	1.921	0.442	1.505	0.352
42	42, 58, 208	1.269	0.196	1.302	0.250	1.372	0.271	1.133	0.265
43	62	0.083	0.014	0.258	0.050	0.205	0.042	0.210	0.038
44	30	0.011	0.004	0.023	0.006	0.019	0.010	0.014	0.003
45	209	0.105	0.029	0.235	0.048	0.172	0.029	0.188	0.034
46	69	0.319	0.093	0.746	0.148	0.534	0.127	0.575	0.107
47	61	0.268	0.041	0.643	0.128	0.451	0.079	0.508	0.083
48	210	0.014	0.002	0.016	0.004	0.039	0.007	0.054	0.009
49	x122	0.161	0.029	0.462	0.091	0.377	0.073	0.324	0.065
50	x123	0.054	0.016	0.138	0.029	0.092	0.019	0.084	0.012
51	x124	0.079	0.068	0.178	0.086	0.099	0.045	0.086	0.013

Table E.3.b: NMVOC concentrations measured at different receptor points, four concentration profiles obtained from measurements at residential areas and areas down-wind from the city centre

	ID number ¹	GIRAR ²		UNI ²		JOTAL1 ²		JOTAL2 ²	
		concentr. µg/m ³	±	concentr. µg/m ³	±	concentr. µg/m ³	±	concentr. µg/m ³	±
52	70	0.063	0.012	0.237	0.046	0.127	0.021	0.178	0.027
53	48	1.447	0.224	5.410	1.046	3.717	0.744	4.260	0.724
54	78	0.124	0.019	0.366	0.114	0.257	0.041	0.288	0.046
55	79	0.031	0.006	0.071	0.017	0.090	0.022	0.092	0.017
56	80, 211	0.070	0.011	0.232	0.080	0.174	0.030	0.190	0.034
57	x137	0.118	0.024	0.012	0.011	0.003	0.000	0.004	0.004
58	212	0.149	0.037	0.143	0.043	0.104	0.017	0.107	0.015
59	x140	0.099	0.028	0.005	0.005	0.005	0.005	0.005	0.005
60	81	0.129	0.025	0.253	0.054	0.206	0.035	0.217	0.038
61	64	0.215	0.051	1.133	0.219	0.844	0.126	1.081	0.186
62	66,67	0.291	0.095	2.460	0.522	1.468	0.221	1.987	0.342
63	145	0.007	0.005	0.188	0.056	0.081	0.052	0.103	0.024
64	65	0.075	0.027	1.058	0.214	0.607	0.127	0.959	0.165
65	124	0.011	0.005	0.137	0.030	0.137	0.020	0.110	0.031
66	85	0.005	0.005	0.256	0.060	0.079	0.050	0.186	0.041
67	91	0.017	0.005	0.063	0.016	0.047	0.007	0.093	0.016
68	x163	0.001	0.002	0.228	0.049	0.058	0.050	0.126	0.030
69	x166	0.005	0.005	0.216	0.044	0.048	0.041	0.069	0.015
70	88	0.005	0.005	0.266	0.061	0.105	0.056	0.180	0.047
71	120	0.004	0.006	0.141	0.048	0.075	0.043	0.219	0.052
72	87, 213	0.005	0.003	0.837	0.212	0.156	0.067	0.369	0.101
73	193	0.005	0.005	0.043	0.011	0.037	0.020	0.078	0.017
74	86	0.005	0.005	0.083	0.026	0.013	0.004	0.026	0.009
75	115	0.003	0.001	0.051	0.053	0.005	0.005	0.003	0.005
76	139	3.397	1.011	1.006	0.436	0.318	0.078	0.171	0.035
77	164	0.541	0.448	0.080	0.017	0.040	0.024	0.015	0.003
78	165	0.005	0.001	0.106	0.039	0.004	0.002	0.008	0.002
79	149	0.012	0.007	0.183	0.093	0.006	0.003	0.050	0.067
80	159	0.003	0.001	0.136	0.086	0.029	0.021	0.025	0.009
81	214	0.006	0.002	0.021	0.005	0.169	0.237	0.045	0.017
82	151	0.596	0.386	1.128	1.443	0.477	0.100	0.337	0.149
83	150	0.070	0.015	0.066	0.021	0.012	0.006	0.006	0.002
84	166	0.062	0.037	0.042	0.015	0.068	0.032	0.051	0.011
85	168	0.035	0.007	0.049	0.023	0.037	0.025	0.021	0.005
86	160	0.006	0.006	0.002	0.003	0.004	0.001	0.009	0.002
87	215	8.619	2.064	0.121	0.025	0.076	0.029	0.062	0.015
88	152	0.015	0.009	0.009	0.004	0.010	0.007	0.008	0.007
89	167	1.820	0.430	0.061	0.046	0.019	0.010	0.018	0.012
90	216	0.027	0.010	0.017	0.007	0.008	0.002	0.008	0.002
91	153	0.047	0.012	0.043	0.017	0.036	0.010	0.031	0.007
92	161	0.030	0.010	0.090	0.021	0.070	0.025	0.061	0.017
	Σ	34.345	2.726	35.993	2.594	39.871	1.903	27.435	1.336

¹ compounds name, carbon number, and species code for CMB according to table E.1

² CMB ID names:

GIRAR: Girardet Str., 19.09.01, 11:10-12:10; wind sector SE-E
UNI: University, 22.08.02, 15:06-16:06, wind sector N-NW
JOTAL1: Im Johannistal, 27.08.02, 15:55-17:05, wind sector W-NNW
JOTAL2: Im Johannistal, 27.08.02, 17:12-18:24, wind sector W-NNW

Table E.4.a: NMVOC concentrations measured at different receptor points, three concentration profiles obtained from measurements at dense traffic areas

	ID number ¹	BUNDA1 ²		BUNDA2 ²		MARKIS ²	
		concentr. µg/m ³	±	concentr. µg/m ³	±	concentr. µg/m ³	±
1	6	0.126	0.018	0.097	0.035	1.387	0.434
2	7	0.011	0.002	0.011	0.002	1.430	0.401
3	4	0.002	0.002	0.002	0.002	0.051	0.021
4	5	0.011	0.002	0.004	0.001	0.078	0.034
5	x13	0.011	0.003	0.006	0.002	0.058	0.054
6	13	0.225	0.032	0.162	0.046	0.984	0.297
7	10,11	1.371	0.195	0.854	0.211	2.310	0.692
8	8	0.074	0.011	0.050	0.009	0.096	0.087
9	14	0.309	0.044	0.229	0.116	2.293	0.692
10	9	0.089	0.013	0.064	0.011	0.454	0.138
11	203	0.018	0.003	0.009	0.002	0.013	0.005
12	12	0.070	0.010	0.054	0.014	0.416	0.132
13	x32	0.071	0.015	0.048	0.011	0.388	0.106
14	18	0.156	0.022	0.106	0.042	0.295	0.086
15	x34	0.119	0.017	0.133	0.090	0.157	0.054
16	x35	0.200	0.029	0.158	0.081	0.169	0.048
17	x37	5.014	0.715	3.234	2.648	1.920	0.523
18	25	2.854	0.407	2.119	0.783	5.476	1.580
19	x41	0.394	0.056	0.272	0.161	0.245	0.068
20	19	0.769	0.110	0.517	0.336	0.647	0.191
21	26, 20	5.053	0.720	3.489	1.883	3.082	1.356
22	16	2.264	0.323	1.534	0.810	0.340	0.167
23	21	0.813	0.116	0.574	0.444	0.474	0.179
24	22	0.403	0.057	0.270	0.166	0.242	0.072
25	x52	1.230	0.242	0.878	0.490	0.778	0.266
26	43	0.761	0.108	0.512	0.223	0.417	0.150
27	x60	0.028	0.006	0.040	0.043	0.006	0.002
28	17	0.063	0.009	0.054	0.026	0.372	0.106
29	x66	0.250	0.049	0.147	0.046	0.003	0.003
30	123	1.770	0.252	0.480	0.371	1.561	0.518
31	44,24	1.743	0.248	1.827	0.533	1.439	0.495
32	45	3.179	0.453	2.433	0.747	3.214	0.961
33	x71	0.415	0.059	0.280	0.125	0.152	0.047
34	46	1.788	0.255	1.383	0.448	1.736	0.523
35	37	0.271	0.039	0.206	0.061	0.160	0.047
36	47, 204	0.438	0.062	0.292	0.131	0.130	0.048
37	x77	1.724	0.246	1.455	0.454	1.830	0.513
38	205	0.038	0.005	0.030	0.009	0.035	0.021
39	41, 206	2.312	0.330	1.687	0.633	1.805	0.658
40	207	0.167	0.024	0.129	0.037	0.126	0.036
41	28	3.360	0.479	2.467	0.648	2.822	0.841
42	42, 58, 208	2.831	0.403	1.929	0.566	1.935	0.552
43	62	0.542	0.077	0.383	0.098	0.380	0.103
44	30	0.066	0.009	0.045	0.021	0.028	0.009
45	209	0.539	0.077	0.373	0.106	0.397	0.145
46	69	1.861	0.265	1.221	0.425	1.106	0.301
47	61	1.030	0.147	0.812	0.161	1.077	0.296
48	210	0.048	0.007	0.028	0.013	0.017	0.006
49	x122	0.847	0.121	0.602	0.206	0.764	0.234
50	x123	0.315	0.045	0.211	0.084	0.244	0.083
51	x124	0.255	0.036	0.160	0.037	0.210	0.060

Table E.4.b: NMVOC concentrations measured at different receptor points, three concentration profiles obtained from measurements at dense traffic areas

	ID number ¹	BUNDA1 ²		BUNDA2 ²		MARKIS ²	
		concentr. µg/m ³	±	concentr. µg/m ³	±	concentr. µg/m ³	±
52	70	0.602	0.086	0.410	0.093	0.402	0.111
53	48	10.281	1.465	8.300	1.926	18.353	6.098
54	78	0.573	0.082	0.506	0.081	1.049	0.499
55	79	0.263	0.037	0.167	0.032	0.243	0.111
56	80, 211	0.499	0.071	0.400	0.095	0.719	0.231
57	<i>x137</i>	0.007	0.001	0.007	0.003	0.055	0.066
58	212	0.431	0.061	0.250	0.148	0.975	0.289
59	<i>x140</i>	0.005	0.005	0.005	0.005	0.163	0.047
60	81	0.472	0.067	0.375	0.054	1.769	0.513
61	64	2.580	0.368	1.662	0.366	1.324	0.383
62	66,67	4.901	0.699	2.843	0.649	1.473	0.644
63	145	0.234	0.033	0.197	0.028	0.004	0.004
64	65	1.754	0.250	1.233	0.179	0.050	0.030
65	124	0.060	0.008	0.050	0.009	0.427	0.408
66	85	0.258	0.037	0.184	0.074	0.106	0.047
67	91	0.345	0.049	0.254	0.044	0.026	0.016
68	<i>x163</i>	0.202	0.029	0.171	0.070	0.025	0.011
69	<i>x166</i>	0.161	0.023	0.144	0.089	0.038	0.015
70	88	0.205	0.029	0.139	0.021	0.005	0.005
71	120	0.058	0.008	0.041	0.011	0.027	0.014
72	87, 213	0.529	0.075	0.291	0.087	0.163	0.057
73	193	0.023	0.003	0.021	0.003	0.005	0.005
74	86	0.064	0.009	0.039	0.007	0.012	0.003
75	115	0.005	0.005	0.005	0.005	0.006	0.006
76	139	0.384	0.079	0.357	0.172	8.309	4.763
77	164	0.108	0.022	0.060	0.052	0.533	0.329
78	165	0.003	0.001	0.013	0.012	0.137	0.059
79	149	0.030	0.006	0.065	0.016	0.359	0.124
80	159	0.010	0.002	0.028	0.006	0.161	0.151
81	214	0.006	0.001	0.037	0.017	0.054	0.024
82	151	0.076	0.016	0.057	0.013	0.106	0.043
83	150	0.041	0.008	0.040	0.019	0.971	0.476
84	166	0.017	0.003	0.059	0.036	0.169	0.080
85	168	0.046	0.010	0.030	0.010	0.038	0.014
86	160	0.020	0.004	0.008	0.006	0.003	0.001
87	215	0.013	0.003	0.117	0.081	0.089	0.020
88	152	0.014	0.003	0.013	0.005	0.003	0.002
89	167	0.035	0.007	0.038	0.017	0.045	0.038
90	216	0.005	0.001	0.009	0.009	0.020	0.009
91	153	0.018	0.004	0.047	0.011	0.073	0.036
92	161	0.036	0.007	0.075	0.037	0.045	0.021
	Σ	73.672	2.328	52.809	4.453	84.287	8.466

¹ compounds name, carbon number, and species code for CMB according to table E.1

² CMB ID names:

BUNDA1: Bundesallee, 26.08.02, 15:35-16:35; wind sector N-NE

BUNDA2: Bundesallee, 26.08.02, 16:40-17:40; wind sector N-NE

MARKIS: Märkisch Str., 15.10.03, 13:08-14:08, wind sector S-SE

Table E.5.a: NMVOC concentrations measured at different receptor points, three concentration profiles obtained from measurements close to the DuPont solvents factory

	ID number ¹	WILKHA ²		HATZEN ²		HATZEM ²	
		concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm
1	6	0.253	0.057	0.715	0.285	1.260	0.343
2	7	0.236	0.329	2.522	0.759	0.946	0.257
3	4	0.003	0.004	0.002	0.002	0.002	0.001
4	5	0.005	0.007	0.006	0.009	0.002	0.001
5	x13	0.002	0.003	0.025	0.031	0.006	0.002
6	13	0.131	0.113	0.553	0.385	0.397	0.108
7	10,11	0.640	0.133	1.903	0.277	3.211	0.873
8	8	0.046	0.015	0.083	0.039	0.079	0.022
9	14	0.303	0.366	1.646	0.448	0.644	0.175
10	9	0.050	0.013	0.223	0.103	0.086	0.023
11	203	0.004	0.005	0.035	0.029	0.015	0.004
12	12	0.037	0.006	0.187	0.089	0.072	0.020
13	x32	0.038	0.017	0.277	0.151	0.152	0.041
14	18	0.073	0.014	0.148	0.046	0.066	0.018
15	x34	0.074	0.016	0.268	0.065	0.071	0.019
16	x35	0.175	0.046	0.253	0.039	0.162	0.044
17	x37	1.379	0.902	1.945	1.216	4.939	1.343
18	25	1.187	0.758	3.844	1.631	1.654	0.450
19	x41	0.129	0.058	0.216	0.138	0.543	0.148
20	19	0.130	0.107	0.372	0.253	0.219	0.059
21	26, 20	1.236	1.649	1.815	1.365	0.525	0.143
22	16	0.543	0.704	0.993	0.796	0.094	0.026
23	21	0.079	0.096	0.322	0.324	0.038	0.010
24	22	0.038	0.037	0.275	0.130	0.336	0.091
25	x52	0.105	0.101	0.577	0.472	0.133	0.036
26	43	0.121	0.172	0.224	0.120	0.060	0.016
27	x60	0.017	0.006	0.049	0.011	0.003	0.003
28	17	0.027	0.005	0.160	0.117	0.029	0.008
29	x66	0.130	0.142	0.239	0.214	0.121	0.033
30	123	0.216	0.032	2.253	0.829	0.614	0.167
31	44,24	0.448	0.442	1.162	0.291	0.580	0.158
32	45	0.691	0.840	1.721	0.477	0.760	0.207
33	x71	0.107	0.062	0.344	0.172	0.257	0.070
34	46	0.423	0.523	0.995	0.275	0.105	0.028
35	37	0.070	0.016	0.183	0.039	0.216	0.059
36	47, 204	0.067	0.079	0.121	0.047	0.699	0.190
37	x77	0.598	0.691	1.140	0.206	0.394	0.107
38	205	0.005	0.001	0.020	0.010	0.030	0.008
39	41, 206	0.491	0.604	1.108	0.432	0.237	0.064
40	207	0.023	0.010	0.096	0.020	0.033	0.009
41	28	1.588	1.700	2.629	0.661	0.735	0.200
42	42, 58, 208	0.869	0.928	1.708	0.507	0.528	0.144
43	62	0.115	0.101	0.316	0.062	0.074	0.020
44	30	0.013	0.002	0.039	0.006	0.071	0.019
45	209	0.157	0.080	0.377	0.115	0.174	0.047
46	69	0.320	0.218	1.151	0.199	0.343	0.093
47	61	0.267	0.198	0.692	0.108	0.290	0.079
48	210	0.035	0.020	0.033	0.005	0.072	0.020
49	x122	0.216	0.206	0.568	0.142	0.220	0.060
50	x123	0.063	0.029	0.189	0.043	0.174	0.047
51	x124	0.043	0.038	0.169	0.033	0.346	0.094

Table E.5.b: NMVOC concentrations measured at different receptor points, three concentration profiles obtained from measurements close to the DuPont solvents factory

	ID number ¹	WILKHA ²		HATZEN ²		HATZEM ²	
		concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm
52	70	0.088	0.057	0.387	0.060	0.092	0.025
53	48	1.859	1.171	7.540	1.217	3.230	1.013
54	78	0.133	0.056	0.425	0.110	0.332	0.156
55	79	0.042	0.028	0.149	0.023	0.061	0.019
56	80, 211	0.096	0.061	0.384	0.065	0.154	0.048
57	<i>x137</i>	0.001	0.002	0.006	0.004	0.104	0.030
58	212	0.155	0.039	0.373	0.100	0.594	0.170
59	<i>x140</i>	0.005	0.005	0.005	0.005	14.948	4.280
60	81	0.156	0.035	0.307	0.046	1.733	0.496
61	64	0.823	0.436	1.704	0.314	2.729	0.781
62	66,67	1.740	0.825	2.876	0.817	4.192	1.200
63	145	0.079	0.012	0.155	0.087	0.119	0.034
64	65	0.675	0.269	1.098	0.515	0.065	0.019
65	124	0.050	0.028	0.044	0.016	1.009	0.289
66	85	0.082	0.025	0.180	0.154	0.143	0.041
67	91	0.188	0.087	0.276	0.055	0.023	0.006
68	<i>x163</i>	0.032	0.024	0.125	0.134	0.077	0.022
69	<i>x166</i>	0.029	0.004	0.112	0.111	0.032	0.009
70	88	0.058	0.021	0.166	0.154	0.011	0.003
71	120	0.062	0.017	0.065	0.048	0.024	0.007
72	87, 213	0.110	0.023	0.353	0.243	0.049	0.014
73	193	0.022	0.003	0.018	0.017	0.005	0.005
74	86	0.011	0.002	0.051	0.045	0.005	0.005
75	115	0.005	0.005	0.002	0.002	0.004	0.001
76	139	0.446	0.565	0.821	0.896	5.443	2.179
77	164	0.042	0.041	0.260	0.314	0.491	0.333
78	165	0.018	0.010	0.015	0.008	0.364	0.097
79	149	0.020	0.018	0.031	0.012	0.716	0.758
80	159	0.051	0.058	0.024	0.012	0.230	0.048
81	214	0.046	0.047	0.026	0.013	0.045	0.021
82	151	0.026	0.013	0.057	0.026	0.192	0.140
83	150	0.009	0.005	0.027	0.033	1.695	0.898
84	166	0.151	0.196	0.105	0.033	0.674	0.646
85	168	0.009	0.002	0.001	0.002	0.053	0.011
86	160	0.007	0.005	0.004	0.004	0.078	0.016
87	215	0.009	0.002	0.008	0.006	0.111	0.088
88	152	0.004	0.004	0.010	0.002	0.033	0.012
89	167	0.146	0.203	0.012	0.003	4.772	3.914
90	216	0.011	0.007	0.007	0.003	0.156	0.049
91	153	0.039	0.037	0.008	0.009	0.523	0.172
92	161	0.007	0.002	0.011	0.005	0.064	0.061
	Σ	21.561	3.688	55.124	3.742	68.189	5.642

¹ compounds name, carbon number, and species code for CMB according to table E.1

² CMB ID names:

WILKHA: Wilkhaus Str., 29.08.02, 13:06-14:10; wind sector NW
HATZEN: Hatzfelder Str., 29.08.02, 14:55-15:55; wind sector W-NW
HATZEM: Hatzfelder Str., 15.10.03, 12:55-14:00; wind sector S-SE

Table E.6.a: NMVOC concentrations measured at different receptor points, four concentration profiles obtained from measurements close to the PPG solvent factory

	ID number ¹	BISSIN ²		LUTZOW ²		BISSIM ²		YOREK ²	
		concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm
1	6	0.494	0.070	0.240	0.055	0.827	0.571	0.427	0.116
2	7	0.773	0.122	0.513	0.086	1.668	0.776	0.825	0.224
3	4	0.002	0.002	0.002	0.002	0.013	0.009	0.002	0.002
4	5	0.011	0.002	0.011	0.002	0.014	0.008	0.002	0.002
5	x13	0.006	0.002	0.002	0.002	0.006	0.003	0.002	0.002
6	13	0.331	0.051	0.439	0.071	0.563	0.323	0.420	0.114
7	10,11	1.730	0.966	0.928	0.201	2.623	0.954	2.338	0.636
8	8	0.058	0.012	0.043	0.006	0.081	0.023	0.066	0.018
9	14	0.869	0.126	0.561	0.126	0.884	0.406	1.285	0.349
10	9	0.128	0.035	0.078	0.017	0.133	0.043	0.096	0.026
11	203	0.020	0.007	0.004	0.005	0.016	0.009	0.022	0.006
12	12	0.102	0.027	0.060	0.014	0.097	0.037	0.085	0.023
13	x32	0.182	0.082	0.125	0.026	0.284	0.077	0.125	0.034
14	18	0.045	0.016	0.045	0.012	0.115	0.032	0.086	0.023
15	x34	0.505	0.414	0.572	0.198	0.203	0.113	0.092	0.025
16	x35	0.251	0.125	0.394	0.110	0.207	0.068	0.190	0.052
17	x37	2.540	0.698	0.822	0.135	3.197	1.057	0.003	0.003
18	25	2.691	0.467	2.269	0.677	1.543	0.454	1.736	0.472
19	x41	0.538	0.765	0.149	0.022	0.135	0.044	0.085	0.023
20	19	0.185	0.027	0.145	0.053	0.165	0.066	0.090	0.025
21	26, 20	0.878	0.126	1.343	0.265	0.465	0.264	0.273	0.074
22	16	0.387	0.074	0.727	0.140	0.132	0.053	0.122	0.033
23	21	0.192	0.028	0.169	0.040	0.104	0.055	0.036	0.010
24	22	0.286	0.102	0.175	0.030	0.067	0.031	0.022	0.006
25	x52	0.341	0.067	0.252	0.062	0.206	0.090	0.107	0.029
26	43	0.128	0.032	0.144	0.022	0.032	0.015	0.031	0.008
27	x60	0.187	0.205	0.229	0.085	0.006	0.002	0.003	0.003
28	17	0.065	0.010	0.041	0.006	0.078	0.031	0.040	0.011
29	x66	0.176	0.039	0.311	0.095	0.014	0.017	0.156	0.042
30	123	0.674	0.224	0.712	0.114	0.398	0.325	0.202	0.055
31	44,24	0.399	0.084	0.289	0.047	0.353	0.097	0.211	0.057
32	45	0.557	0.084	0.706	0.109	0.533	0.145	0.443	0.120
33	x71	0.704	0.359	0.709	0.203	0.204	0.067	0.127	0.034
34	46	0.307	0.055	0.406	0.061	0.365	0.106	0.291	0.079
35	37	0.091	0.018	0.084	0.013	0.118	0.035	0.067	0.018
36	47, 204	1.015	0.145	0.151	0.027	0.462	0.207	0.803	0.218
37	x77	0.408	0.066	0.558	0.085	0.429	0.124	0.392	0.107
38	205	0.003	0.003	0.002	0.003	0.146	0.076	0.013	0.003
39	41, 206	0.414	0.085	0.505	0.074	0.222	0.083	0.186	0.050
40	207	0.041	0.006	0.052	0.010	0.028	0.008	0.025	0.007
41	28	0.672	0.099	0.923	0.132	0.612	0.184	0.510	0.139
42	42, 58, 208	0.615	0.089	0.744	0.108	0.341	0.100	0.289	0.078
43	62	0.123	0.022	0.121	0.022	0.075	0.022	0.063	0.017
44	30	0.021	0.017	0.061	0.012	0.033	0.010	0.025	0.007
45	209	0.151	0.033	0.127	0.027	0.175	0.054	0.076	0.021
46	69	0.442	0.106	0.394	0.060	0.225	0.061	0.185	0.050
47	61	0.454	0.129	0.514	0.092	0.198	0.054	0.200	0.054
48	210	0.140	0.084	0.030	0.006	0.018	0.015	0.015	0.004
49	x122	0.316	0.060	0.209	0.030	0.148	0.040	0.103	0.028
50	x123	0.106	0.026	0.058	0.009	0.113	0.107	0.041	0.011
51	x124	0.088	0.042	0.039	0.007	0.054	0.030	0.083	0.022

Table E.6.b: NMVOC concentrations measured at different receptor points, four concentration profiles obtained from measurements close to the PPG solvent factory

	ID number ¹	BISSIN ²		LUTZOW ²		BISSIM ²		YOREK ²	
		concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm
52	70	0.112	0.021	0.108	0.023	0.049	0.013	0.033	0.009
53	48	2.070	0.344	2.747	0.480	2.296	0.759	2.328	0.730
54	78	0.199	0.036	0.201	0.031	0.222	0.106	0.190	0.089
55	79	0.050	0.007	0.048	0.007	0.044	0.015	0.041	0.013
56	80, 211	0.198	0.029	0.139	0.021	0.140	0.044	0.072	0.023
57	<i>x137</i>	0.004	0.001	0.026	0.029	0.004	0.001	0.036	0.010
58	212	0.185	0.042	0.159	0.053	1.039	0.366	0.358	0.103
59	<i>x140</i>	0.005	0.005	0.005	0.005	0.068	0.019	0.029	0.008
60	81	0.444	0.068	0.444	0.072	1.000	0.304	0.398	0.114
61	64	1.477	0.451	0.808	0.292	0.420	0.167	0.465	0.133
62	66,67	4.019	1.651	1.719	0.524	0.494	0.202	0.544	0.156
63	145	0.038	0.026	0.094	0.067	0.002	0.003	0.012	0.004
64	65	0.929	0.456	0.968	0.341	0.108	0.077	0.050	0.014
65	124	0.026	0.004	0.066	0.014	0.458	0.210	0.234	0.067
66	85	0.048	0.033	0.105	0.054	0.017	0.009	0.052	0.015
67	91	0.111	0.064	0.123	0.059	0.006	0.008	0.005	0.002
68	<i>x163</i>	0.041	0.023	0.069	0.059	0.017	0.009	0.012	0.003
69	<i>x166</i>	0.041	0.022	0.067	0.038	0.001	0.002	0.005	0.005
70	88	0.054	0.024	0.161	0.119	0.006	0.009	0.021	0.006
71	120	0.042	0.029	0.094	0.062	0.020	0.011	0.023	0.007
72	87, 213	0.171	0.091	0.198	0.122	0.026	0.009	0.017	0.005
73	193	0.009	0.003	0.039	0.019	0.003	0.004	0.002	0.005
74	86	0.023	0.008	0.018	0.009	0.005	0.003	0.003	0.005
75	115	0.001	0.002	0.005	0.005	0.006	0.009	0.003	0.005
76	139	2.969	1.895	0.848	0.794	3.834	0.792	3.396	1.405
77	164	0.424	0.229	0.153	0.032	0.514	0.155	0.171	0.045
78	165	0.015	0.004	0.007	0.004	0.470	0.570	1.388	0.290
79	149	0.073	0.029	0.044	0.010	1.096	0.253	0.520	0.425
80	159	0.209	0.126	0.025	0.012	0.156	0.034	0.266	0.085
81	214	0.126	0.144	0.083	0.017	0.070	0.023	0.050	0.029
82	151	0.209	0.181	0.050	0.011	0.048	0.064	0.098	0.033
83	150	0.363	0.089	0.285	0.180	0.867	0.522	0.286	0.064
84	166	0.265	0.326	0.033	0.008	0.041	0.018	0.105	0.041
85	168	0.018	0.011	0.013	0.003	0.012	0.010	0.021	0.005
86	160	0.021	0.017	0.012	0.004	0.016	0.019	0.005	0.003
87	215	0.046	0.029	0.009	0.006	0.020	0.013	0.065	0.018
88	152	0.023	0.006	0.011	0.008	0.013	0.010	0.014	0.009
89	167	0.175	0.233	0.019	0.007	0.026	0.022	0.033	0.018
90	216	0.005	0.002	0.006	0.006	0.009	0.003	0.026	0.013
91	153	0.511	0.192	0.083	0.018	0.053	0.024	0.041	0.030
92	161	0.004	0.004	0.004	0.001	0.052	0.018	0.077	0.023
	Σ	37.593	3.159	28.281	1.511	32.872	2.470	24.609	1.959

¹ compounds name, carbon number, and species code for CMB according to table E.1

² CMB ID names:

BISSIN: Bissing Str., 03.09.02, 12:52-13:52; wind sector E

LUTZOW: Lützw Str., 04.09.02, 14:29-15:30, wind sector SW

BISSIM: Bissing Str., 13.10.03, 13:06-14:06, wind sector E-SE

YOREK: Yorck Str., 13.10.03, 13:06-14:06, wind sector E-SE

Table E.7.a: NMVOC concentrations measured at different receptor points, four concentration profiles obtained from measurements close to the Gorn workshop and the Conrads solvent factory

	ID number ¹	SIMONS ²		SIMONB ²		SIMONM ²		VIEHOF ²	
		concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm	concentr. $\mu\text{g}/\text{m}^3$	\pm
1	6	0.281	0.073	0.839	0.236	0.914	0.439	0.280	0.041
2	7	0.781	0.136	0.496	0.179	1.271	0.599	0.283	0.069
3	4	0.002	0.003	0.019	0.010	0.011	0.003	0.002	0.002
4	5	0.009	0.001	0.001	0.002	0.004	0.003	0.002	0.003
5	x13	0.002	0.002	0.002	0.003	0.004	0.003	0.010	0.004
6	13	0.327	0.058	0.957	0.266	1.246	0.640	0.535	0.079
7	10,11	0.863	0.259	1.392	0.569	1.538	0.518	0.900	0.150
8	8	0.032	0.011	0.071	0.021	0.075	0.033	0.038	0.007
9	14	0.701	0.108	1.299	0.375	2.759	2.293	0.318	0.053
10	9	0.077	0.022	0.100	0.027	0.190	0.133	0.094	0.014
11	203	0.011	0.003	0.012	0.004	0.024	0.013	0.012	0.002
12	12	0.065	0.016	0.117	0.033	0.178	0.132	0.078	0.011
13	x32	0.031	0.044	0.210	0.065	0.621	0.660	0.052	0.025
14	18	0.059	0.009	0.169	0.046	0.145	0.070	0.052	0.028
15	x34	0.142	0.133	0.092	0.052	0.097	0.084	1.100	0.183
16	x35	0.215	0.098	0.173	0.051	0.173	0.061	0.324	0.046
17	x37	1.777	0.256	1.471	0.404	3.823	3.635	0.487	0.175
18	25	1.128	0.353	3.259	0.893	2.649	0.751	5.286	2.118
19	x41	0.159	0.024	0.087	0.126	1.903	2.599	0.278	0.073
20	19	0.121	0.022	0.377	0.105	0.362	0.127	0.502	0.247
21	26, 20	0.801	0.142	1.625	0.642	1.864	0.636	3.144	0.916
22	16	1.363	0.255	0.166	0.079	0.156	0.047	1.738	0.525
23	21	0.129	0.026	0.086	0.120	0.189	0.109	0.567	0.199
24	22	0.077	0.014	0.874	0.268	0.583	0.172	0.328	0.083
25	x52	0.182	0.037	0.352	0.103	0.415	0.139	0.832	0.309
26	43	0.112	0.016	0.353	0.184	0.317	0.092	0.442	0.111
27	x60	0.093	0.044	0.035	0.026	0.016	0.005	0.537	0.148
28	17	0.050	0.007	0.063	0.019	0.107	0.059	0.110	0.115
29	x66	0.018	0.015	0.166	0.046	0.124	0.096	0.245	0.049
30	123	0.239	0.180	0.760	0.491	1.702	0.738	0.970	0.185
31	44,24	0.282	0.132	1.603	0.566	1.635	0.492	1.044	0.306
32	45	0.441	0.065	2.791	0.933	2.269	0.672	1.977	0.334
33	x71	0.238	0.059	0.290	0.112	0.508	0.301	0.922	0.158
34	46	0.248	0.035	1.533	0.548	1.271	0.377	1.132	0.192
35	37	0.080	0.013	0.263	0.097	0.208	0.058	0.149	0.021
36	47, 204	0.264	0.040	0.748	0.238	0.777	0.254	0.242	0.039
37	x77	0.277	0.040	1.789	0.529	1.296	0.384	1.384	0.215
38	205	0.004	0.005	0.017	0.007	0.021	0.024	0.029	0.006
39	41, 206	0.341	0.053	1.659	0.663	1.307	0.390	1.511	0.336
40	207	0.032	0.006	0.107	0.042	0.077	0.021	0.151	0.028
41	28	0.563	0.089	3.038	0.865	2.318	0.655	2.096	0.322
42	42, 58, 208	0.636	0.117	3.217	0.912	2.296	0.688	1.826	0.309
43	62	0.123	0.018	0.671	0.183	0.453	0.133	0.351	0.053
44	30	0.014	0.010	0.046	0.023	0.079	0.025	0.025	0.006
45	209	0.160	0.023	0.624	0.176	0.434	0.119	0.269	0.039
46	69	0.263	0.054	1.603	0.447	1.068	0.329	1.181	0.173
47	61	0.543	0.116	2.191	0.601	1.366	0.413	1.033	0.154
48	210	0.009	0.002	0.062	0.020	0.049	0.026	0.009	0.001
49	x122	0.284	0.056	1.448	0.426	0.960	0.300	0.580	0.085
50	x123	0.045	0.016	0.648	0.260	0.392	0.135	0.215	0.031
51	x124	0.048	0.010	0.393	0.110	0.265	0.134	0.125	0.020

Table E.7.b: NMVOC concentrations measured at different receptor points, four concentration profiles obtained from measurements close to the Gorn workshop and the Conrads solvent factory

	ID number ¹	SIMONS ²		SIMONB ²		SIMONM ²		VIEHOF ²	
		concentr. µg/m ³	±	concentr. µg/m ³	±	concentr. µg/m ³	±	concentr. µg/m ³	±
52	70	0.051	0.010	0.437	0.119	0.248	0.101	0.430	0.062
53	48	1.609	0.250	25.356	8.003	9.641	2.702	7.844	1.132
54	78	0.130	0.027	1.636	0.782	0.644	0.265	0.516	0.082
55	79	0.043	0.006	0.392	0.148	0.135	0.043	0.154	0.022
56	80, 211	0.105	0.015	1.090	0.388	0.501	0.153	0.392	0.056
57	x137	0.002	0.002	0.047	0.025	0.006	0.009	0.006	0.004
58	212	0.210	0.045	1.694	0.488	1.078	1.169	0.157	0.092
59	x140	0.005	0.005	4.716	1.675	0.789	0.783	0.005	0.005
60	81	0.191	0.036	4.953	1.429	1.823	1.509	0.357	0.055
61	64	1.097	0.175	7.536	2.441	2.865	1.136	2.138	0.326
62	66,67	2.730	0.437	13.233	5.080	5.975	3.711	4.558	0.830
63	145	0.158	0.054	0.285	0.114	0.182	0.055	0.158	0.044
64	65	0.897	0.162	0.118	0.091	0.327	0.471	1.387	0.309
65	124	0.069	0.028	3.799	1.821	2.614	2.153	0.130	0.019
66	85	0.191	0.056	0.255	0.087	0.160	0.070	0.161	0.058
67	91	0.254	0.046	0.143	0.072	0.366	0.458	0.128	0.031
68	x163	0.153	0.052	0.091	0.035	0.446	0.602	0.114	0.050
69	x166	0.148	0.068	0.081	0.030	0.485	0.650	0.101	0.021
70	88	0.238	0.113	0.078	0.088	0.335	0.483	0.167	0.076
71	120	0.129	0.071	0.077	0.024	0.248	0.272	0.041	0.017
72	87, 213	0.553	0.323	0.351	0.140	1.256	1.576	0.352	0.138
73	193	0.069	0.018	0.022	0.009	0.069	0.083	0.027	0.005
74	86	0.054	0.041	0.030	0.010	0.116	0.145	0.037	0.010
75	115	0.005	0.005	0.006	0.002	0.003	0.001	0.005	0.005
76	139	3.172	2.797	4.777	1.117	10.165	7.219	0.718	0.311
77	164	0.152	0.047	1.125	0.232	0.536	0.264	0.077	0.085
78	165	0.016	0.006	0.397	0.096	0.583	0.520	0.011	0.002
79	149	0.055	0.072	0.839	0.210	1.315	0.371	0.012	0.005
80	159	0.061	0.026	0.141	0.062	0.107	0.090	0.072	0.042
81	214	0.029	0.018	0.070	0.019	0.110	0.076	0.081	0.018
82	151	0.120	0.026	0.136	0.070	0.120	0.049	0.045	0.019
83	150	0.575	0.119	7.198	2.392	1.501	0.542	0.493	0.106
84	166	0.050	0.038	0.711	0.405	0.927	0.858	0.039	0.022
85	168	0.009	0.002	0.135	0.032	0.091	0.019	0.018	0.005
86	160	0.003	0.001	0.150	0.206	0.005	0.001	0.012	0.003
87	215	0.013	0.005	0.153	0.118	0.109	0.024	0.028	0.007
88	152	0.017	0.004	0.014	0.004	0.016	0.008	0.007	0.010
89	167	0.034	0.018	1.047	0.423	0.184	0.212	0.131	0.139
90	216	0.009	0.009	0.235	0.264	0.015	0.007	0.004	0.002
91	153	0.095	0.068	0.132	0.060	0.047	0.020	0.075	0.016
92	161	0.009	0.007	0.076	0.016	0.056	0.024	0.007	0.002
	Σ	28.252	2.973	124.128	10.938	88.706	10.966	56.989	3.008

¹ compounds name, carbon number, and species code for CMB according to table E.1

² CMB ID names:

SIMONS: Simon Str., 03.09.02, 10:35-11:40; wind sector N
SIMONB: Simon Str., 17.10.03, 09:45-10:45; wind sector NE
SIMONM: Simon Str., 17.10.03, 09:45-10:55; wind sector NE
VIEHOF: Viehhof Str., 04.09.02, 16:17-17:17; wind sector SW

Annex F: CMB results

Table F.1.a: Results of CMB analysis for receptor point GIRAR (Girardet Str., 19.09.01, down-wind from the city centre)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS8	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.354	0.055	0.162	0.121	0.030	0.009
2	<i>propane</i>	0.093	0.017	0.022	0.015	0.100	0.017
3	<i>propadiene</i>	0.003	0.001	0.002	0.002	0.000	0.000
4	<i>propyne</i>	0.007	0.002	0.003	0.002	0.001	0.001
5	<i>X5/13a</i>	0.106	0.065	0.109	0.117	0.004	0.001
6	<i>2-methylpropane</i>	0.155	0.031	0.041	0.014	0.017	0.003
7	<i>1-butene, 2-methylpropene</i>	2.892	1.070	0.910	0.933	0.150	0.035
8	<i>1,3-butadiene</i>	0.103	0.018	0.039	0.037	0.005	0.001
9	<i>n-butane</i>	0.087	0.014	0.044	0.020	0.037	0.007
10	<i>trans-2-butene</i>	0.079	0.038	0.029	0.022	0.008	0.002
11	<i>1-butyne</i>	0.003	0.005	0.002	0.000	0.000	0.000
12	<i>cis-2-butene</i>	0.042	0.008	0.015	0.014	0.005	0.001
13	<i>X12/18d</i>	0.023	0.032	0.000	0.000	0.010	0.003
14	<i>3-methyl-1-butene</i>	0.049	0.015	0.017	0.007	0.003	0.001
15	<i>X18/25a</i>	0.123	0.076	0.102	0.112	0.007	0.002
16	<i>X18/25b</i>	0.230	0.064	0.148	0.140	0.012	0.004
17	<i>X18/25d</i>	1.984	0.355	0.664	0.240	0.227	0.037
18	<i>2-methylbutane</i>	2.561	0.400	0.330	0.075	0.132	0.021
19	<i>X25/19c</i>	0.121	0.019	0.056	0.029	0.003	0.001
20	<i>1-pentene</i>	0.110	0.033	0.092	0.027	0.001	0.001
21	<i>n-pentane, 2-methyl-1-butene</i>	0.324	0.185	0.279	0.272	0.000	0.000
22	<i>2-methyl-1,3-butadiene</i>	0.214	0.088	0.158	0.100	0.003	0.002
23	<i>trans-2-pentene</i>	0.037	0.017	0.065	0.056	0.000	0.000
24	<i>cis-2-pentene</i>	0.054	0.011	0.039	0.027	0.001	0.000
25	<i>X22/43b</i>	0.131	0.051	0.133	0.097	0.003	0.001
26	<i>2,2-dimethylbutane</i>	0.047	0.011	0.053	0.027	0.000	0.000
27	<i>X43/17c</i>	0.036	0.013	0.031	0.037	0.001	0.001
28	<i>cyclopentene</i>	0.054	0.011	0.022	0.005	0.003	0.001
29	<i>X17/123c</i>	0.003	0.003	0.012	0.017	0.011	0.003
30	<i>methyl tert-butyl ether</i>	0.645	0.112	0.157	0.075	0.012	0.003
31	<i>2,3-dimethylbutane, cyclopentane</i>	1.062	0.372	0.112	0.065	0.017	0.003
32	<i>2-methylpentane</i>	0.325	0.052	0.402	0.090	0.000	0.000
33	<i>X45/46b</i>	0.173	0.055	0.061	0.024	0.011	0.003
34	<i>3-methylpentane</i>	0.241	0.053	0.243	0.068	0.000	0.000
35	<i>1-hexene</i>	0.113	0.018	0.083	0.015	0.003	0.001
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.044	0.063	0.007	0.010	0.004	0.001
37	<i>X37/47b</i>	0.323	0.052	0.233	0.044	0.000	0.000
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.019	0.007	0.010	0.002	0.001	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.208	0.050	0.262	0.073	0.000	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.050	0.029	0.056	0.019	0.002	0.001
41	<i>benzene</i>	0.580	0.090	0.630	0.126	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	1.269	0.197	0.155	0.032	0.023	0.004
43	<i>2-methylhexane</i>	0.083	0.014	0.048	0.010	0.000	0.000
44	<i>cyclohexene</i>	0.011	0.004	0.020	0.012	0.000	0.000
45	<i>1-heptene</i>	0.105	0.029	0.083	0.019	0.002	0.000
46	<i>2,2,4-trimethylpentane</i>	0.319	0.093	0.172	0.034	0.004	0.001

Table F.1.b: Results of CMB analysis for receptor point GIRAR (Girardet Str., 19.09.01, down-wind from the city centre)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS8	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	0.268	0.041	0.145	0.051	0.000	0.000
48	1,4-cyclohexadiene	0.014	0.002	0.005	0.002	0.002	0.001
49	X210/70h	0.161	0.029	0.111	0.022	0.000	0.000
50	X210/70i	0.054	0.016	0.041	0.010	0.001	0.000
51	X210/70j	0.079	0.068	0.087	0.017	0.005	0.003
52	2,3,4-trimethylpentane	0.063	0.012	0.053	0.012	0.000	0.000
53	toluene	1.448	0.224	1.768	0.334	0.021	0.003
54	2-methylheptane	0.125	0.019	0.133	0.031	0.005	0.001
55	3-methylheptane	0.031	0.006	0.024	0.005	0.000	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.070	0.011	0.068	0.014	0.000	0.000
57	X211/212c	0.118	0.024	0.095	0.017	0.013	0.002
58	1-octene	0.149	0.037	0.085	0.043	0.003	0.001
59	X212/81a	0.099	0.028	0.116	0.024	0.054	0.009
60	<i>n</i> -octane	0.129	0.025	0.080	0.019	0.005	0.001
61	ethylbenzene	0.215	0.051	0.422	0.080	0.033	0.006
62	meta- and para-xylene	0.291	0.095	0.754	0.141	0.093	0.015
63	styrene	0.016	0.004	0.022	0.012	0.001	0.001
64	ortho-xylene	0.008	0.005	0.085	0.032	0.027	0.004
65	alpha-pinene	0.080	0.028	0.257	0.048	0.000	0.000
66	<i>n</i> -propylbenzene	0.010	0.005	0.029	0.009	0.000	0.000
67	4-ethyltoluene	0.005	0.005	0.019	0.009	0.003	0.002
68	X67/145c	0.001	0.002	0.010	0.003	0.000	0.000
69	X88/120c	0.005	0.005	0.005	0.003	0.000	0.000
70	1,3,5-trimethylbenzene	0.005	0.005	0.014	0.005	0.000	0.000
71	<i>n</i> -decane	0.004	0.006	0.002	0.002	0.000	0.000
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.005	0.003	0.027	0.010	0.000	0.000
73	X213/86b	0.005	0.005	0.000	0.000	0.000	0.000
74	1,2,3-trimethylbenzene	0.005	0.005	0.003	0.002	0.000	0.000
75	1,2,3,4-tetramethylbenzene	0.003	0.001	0.002	0.002	0.000	0.000
76	acetone	3.398	1.011	0.313	0.265	0.035	0.010
77	methyl acetate	0.541	0.448	0.078	0.044	0.009	0.002
78	ethyl acetate	0.005	0.001	0.000	0.000	0.000	0.000
79	methanol	0.012	0.007	0.003	0.002	0.001	0.001
80	2-butanone	0.003	0.001	0.005	0.003	0.000	0.000
81	isopropyl acetate	0.006	0.002	0.002	0.000	0.000	0.000
82	2-propanol	0.596	0.386	0.094	0.094	0.008	0.004
83	ethanol	0.070	0.015	0.048	0.026	0.002	0.001
84	propyl acetate	0.062	0.037	0.015	0.003	0.000	0.000
85	isobutyl acetate	0.035	0.007	0.043	0.010	0.008	0.002
86	4-methyl-2-pentanone	0.006	0.006	0.019	0.007	0.000	0.000
87	2-butanol	8.619	2.064	4.889	1.453	0.311	0.080
88	1-propanol	0.015	0.010	0.005	0.003	0.000	0.000
89	butyl acetate	1.820	0.430	0.706	0.167	0.215	0.082
90	2-hexanone	0.027	0.011	0.005	0.003	0.000	0.000
91	1-butanol	0.047	0.012	0.015	0.003	0.008	0.009
92	cyclohexanone	0.030	0.010	0.007	0.002	0.003	0.001
	Σ NMVOC	34.349	2.726	17.016	0.913	1.717	0.393

names of unknown compounds are explained in table E.1 in Annex E

Table F.2.a: Results of CMB analysis for receptor point UNI (University, 22.08.02, down-wind from the city centre)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS3	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.225	0.101	0.143	0.047	0.043	0.012
2	<i>propane</i>	0.225	0.046	0.149	0.096	0.137	0.028
3	<i>propadiene</i>	0.012	0.009	0.006	0.006	0.000	0.000
4	<i>propyne</i>	0.004	0.005	0.003	0.006	0.002	0.000
5	<i>X5/13a</i>	0.002	0.003	0.009	0.006	0.000	0.000
6	<i>2-methylpropane</i>	0.158	0.042	0.204	0.064	0.047	0.010
7	<i>1-butene, 2-methylpropene</i>	1.334	1.091	0.551	0.149	0.123	0.039
8	<i>1,3-butadiene</i>	0.054	0.031	0.035	0.009	0.004	0.001
9	<i>n-butane</i>	0.302	0.124	0.312	0.102	0.110	0.021
10	<i>trans-2-butene</i>	0.068	0.041	0.044	0.012	0.012	0.004
11	<i>1-butyne</i>	0.016	0.003	0.006	0.003	0.002	0.000
12	<i>cis-2-butene</i>	0.039	0.020	0.041	0.012	0.010	0.003
13	<i>X12/18d</i>	0.007	0.010	0.041	0.015	0.003	0.004
14	<i>3-methyl-1-butene</i>	0.049	0.010	0.061	0.012	0.007	0.001
15	<i>X18/25a</i>	0.027	0.021	0.055	0.020	0.023	0.022
16	<i>X18/25b</i>	0.096	0.036	0.073	0.020	0.035	0.016
17	<i>X18/25d</i>	1.253	0.666	1.398	0.333	0.235	0.042
18	<i>2-methylbutane</i>	0.661	0.350	1.438	0.426	0.109	0.036
19	<i>X25/19c</i>	0.093	0.133	0.131	0.026	0.021	0.004
20	<i>1-pentene</i>	0.202	0.077	0.257	0.055	0.005	0.001
21	<i>n-pentane, 2-methyl-1-butene</i>	1.632	0.542	1.535	0.327	0.041	0.009
22	<i>2-methyl-1,3-butadiene</i>	1.094	0.250	0.476	0.120	0.223	0.048
23	<i>trans-2-pentene</i>	0.258	0.158	0.271	0.064	0.005	0.001
24	<i>cis-2-pentene</i>	0.119	0.056	0.131	0.029	0.005	0.001
25	<i>X22/43b</i>	0.366	0.102	0.411	0.055	0.005	0.001
26	<i>2,2-dimethylbutane</i>	0.209	0.044	0.231	0.047	0.005	0.001
27	<i>X43/17c</i>	0.075	0.010	0.012	0.003	0.017	0.008
28	<i>cyclopentene</i>	0.034	0.008	0.044	0.012	0.006	0.001
29	<i>X17/123c</i>	0.071	0.039	0.079	0.029	0.000	0.000
30	<i>methyl tert-butyl ether</i>	0.221	0.118	0.455	0.114	0.012	0.009
31	<i>2,3-dimethylbutane, cyclopentane</i>	0.367	0.100	0.694	0.149	0.003	0.002
32	<i>2-methylpentane</i>	1.273	0.248	1.158	0.228	0.000	0.000
33	<i>X45/46b</i>	0.068	0.042	0.114	0.041	0.037	0.010
34	<i>3-methylpentane</i>	0.765	0.147	0.651	0.128	0.000	0.000
35	<i>1-hexene</i>	0.144	0.030	0.108	0.020	0.007	0.001
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.034	0.010	0.117	0.032	0.042	0.008
37	<i>X37/47b</i>	0.966	0.225	0.762	0.149	0.000	0.000
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.016	0.006	0.020	0.009	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.896	0.174	0.887	0.172	0.000	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.082	0.020	0.070	0.015	0.001	0.000
41	<i>benzene</i>	1.428	0.276	1.473	0.283	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	1.302	0.250	0.995	0.198	0.049	0.010
43	<i>2-methylhexane</i>	0.258	0.050	0.213	0.044	0.008	0.001
44	<i>cyclohexene</i>	0.023	0.006	0.026	0.006	0.001	0.001
45	<i>1-heptene</i>	0.235	0.048	0.190	0.038	0.016	0.003
46	<i>2,2,4-trimethylpentane</i>	0.746	0.148	0.636	0.126	0.004	0.001

Table F.2.b: Results of CMB analysis for receptor point UNI (University, 22.08.02, down-wind from the city centre)

	compounds	measured concentration		CMB calculated concentrations			
		µg/m ³	±	TRAFFIC1		SOLVENTS3	
				µg/m ³	±	µg/m ³	±
47	<i>n</i> -heptane	0.643	0.129	0.438	0.090	0.071	0.017
48	1,4-cyclohexadiene	0.016	0.004	0.012	0.003	0.001	0.000
49	X210/70h	0.462	0.091	0.327	0.067	0.030	0.007
50	X210/70i	0.138	0.029	0.111	0.023	0.001	0.000
51	X210/70j	0.178	0.086	0.090	0.018	0.003	0.001
52	2,3,4-trimethylpentane	0.237	0.046	0.219	0.047	0.000	0.000
53	toluene	5.410	1.046	4.540	0.919	0.000	0.000
54	2-methylheptane	0.366	0.114	0.266	0.053	0.006	0.001
55	3-methylheptane	0.071	0.017	0.099	0.020	0.001	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.232	0.080	0.251	0.055	0.002	0.000
57	X211/212c	0.012	0.011	0.006	0.003	0.000	0.000
58	1-octene	0.143	0.043	0.108	0.023	0.032	0.008
59	X212/81a	0.005	0.005	0.003	0.000	0.001	0.001
60	<i>n</i> -octane	0.253	0.054	0.204	0.041	0.021	0.005
61	ethylbenzene	1.133	0.219	0.896	0.193	0.143	0.027
62	meta- and para-xylene	2.460	0.522	1.555	0.341	0.404	0.078
63	styrene	0.188	0.056	0.149	0.047	0.019	0.007
64	ortho-xylene	1.058	0.214	0.624	0.146	0.124	0.026
65	alpha-pinene	0.137	0.030	0.114	0.047	0.005	0.002
66	<i>n</i> -propylbenzene	0.256	0.061	0.128	0.038	0.027	0.008
67	4-ethyltoluene	0.063	0.016	0.064	0.020	0.044	0.009
68	X67/145c	0.228	0.049	0.099	0.032	0.022	0.008
69	X88/120c	0.216	0.044	0.111	0.038	0.020	0.010
70	1,3,5-trimethylbenzene	0.266	0.061	0.128	0.047	0.036	0.017
71	<i>n</i> -decane	0.141	0.048	0.053	0.023	0.021	0.012
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.837	0.212	0.365	0.140	0.078	0.047
73	X213/86b	0.044	0.012	0.012	0.003	0.012	0.003
74	1,2,3-trimethylbenzene	0.083	0.026	0.041	0.018	0.007	0.006
75	1,2,3,4-tetramethylbenzene	0.051	0.053	0.003	0.000	0.001	0.001
76	acetone	1.006	0.436	0.776	0.476	0.544	0.483
77	methyl acetate	0.080	0.017	0.076	0.026	0.023	0.008
78	ethyl acetate	0.106	0.039	0.047	0.020	0.000	0.000
79	methanol	0.183	0.093	0.020	0.006	0.009	0.012
80	2-butanone	0.136	0.086	0.038	0.015	0.009	0.004
81	isopropyl acetate	0.021	0.005	0.020	0.015	0.004	0.002
82	2-propanol	1.128	1.000	0.085	0.032	0.016	0.004
83	ethanol	0.066	0.021	0.184	0.146	0.096	0.022
84	propyl acetate	0.042	0.016	0.035	0.032	0.007	0.005
85	isobutyl acetate	0.049	0.023	0.015	0.003	0.001	0.000
86	4-methyl-2-pentanone	0.002	0.003	0.015	0.023	0.000	0.000
87	2-butanol	0.121	0.025	0.044	0.023	0.000	0.000
88	1-propanol	0.009	0.004	0.009	0.003	0.003	0.001
89	butyl acetate	0.062	0.046	0.026	0.015	0.005	0.002
90	2-hexanone	0.017	0.007	0.015	0.015	0.001	0.001
91	1-butanol	0.043	0.017	0.023	0.009	0.016	0.012
92	cyclohexanone	0.090	0.021	0.020	0.006	0.000	0.000
	Σ NMVOC	35.993	2.594	29.176	1.648	3.274	0.949

names of unknown compounds are explained in table E.1 in Annex E

Table F.3.a: Results of CMB analysis for receptor point JOTAL1 (Im Johannistal, 27.08.02, residential area, down-wind from the city centre)

	compounds	measured concentration		CMB calculated concentrations					
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS2		SOLVENTS4	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.338	0.122	0.135	0.044	0.025	0.004	0.008	0.001
2	<i>propane</i>	0.634	0.322	0.141	0.091	0.041	0.007	0.007	0.002
3	<i>propadiene</i>	0.007	0.002	0.006	0.006	0.000	0.000	0.000	0.000
4	<i>propyne</i>	0.011	0.008	0.003	0.006	0.001	0.000	0.000	0.000
5	<i>X5/13a</i>	0.011	0.007	0.008	0.006	0.000	0.000	0.000	0.000
6	<i>2-methylpropane</i>	0.264	0.087	0.193	0.061	0.014	0.002	0.025	0.004
7	<i>1-butene, 2-methylpropene</i>	0.798	0.298	0.521	0.141	0.086	0.048	0.012	0.002
8	<i>1,3-butadiene</i>	0.052	0.010	0.033	0.008	0.003	0.001	0.000	0.000
9	<i>n-butane</i>	0.883	0.365	0.295	0.097	0.042	0.007	0.000	0.000
10	<i>trans-2-butene</i>	0.128	0.051	0.041	0.011	0.006	0.002	0.004	0.001
11	<i>1-butyne</i>	0.006	0.001	0.006	0.003	0.001	0.000	0.000	0.000
12	<i>cis-2-butene</i>	0.097	0.035	0.039	0.011	0.005	0.001	0.002	0.000
13	<i>X12/18d</i>	0.166	0.035	0.039	0.014	0.010	0.004	0.000	0.000
14	<i>3-methyl-1-butene</i>	0.111	0.021	0.058	0.011	0.001	0.000	0.000	0.000
15	<i>X18/25a</i>	0.207	0.035	0.052	0.019	0.028	0.023	0.102	0.018
16	<i>X18/25b</i>	0.202	0.047	0.069	0.019	0.013	0.006	0.022	0.003
17	<i>X18/25d</i>	1.577	0.260	1.321	0.314	0.110	0.032	0.000	0.000
18	<i>2-methylbutane</i>	3.792	1.016	1.359	0.403	0.118	0.023	0.323	0.131
19	<i>X25/19c</i>	0.229	0.062	0.124	0.025	0.028	0.039	0.009	0.002
20	<i>1-pentene</i>	0.423	0.118	0.243	0.052	0.004	0.001	0.014	0.007
21	<i>n-pentane, 2-methyl-1-butene</i>	3.110	0.719	1.450	0.309	0.010	0.002	0.096	0.028
22	<i>2-methyl-1,3-butadiene</i>	1.178	0.222	0.449	0.113	0.010	0.002	0.106	0.033
23	<i>trans-2-pentene</i>	0.445	0.118	0.256	0.061	0.004	0.001	0.018	0.006
24	<i>cis-2-pentene</i>	0.200	0.047	0.124	0.028	0.013	0.005	0.014	0.004
25	<i>X22/43b</i>	0.631	0.168	0.389	0.052	0.009	0.002	0.025	0.009
26	<i>2,2-dimethylbutane</i>	0.386	0.082	0.218	0.044	0.001	0.000	0.012	0.003
27	<i>X43/17c</i>	0.041	0.011	0.011	0.003	0.011	0.012	0.052	0.015
28	<i>cyclopentene</i>	0.067	0.027	0.041	0.011	0.003	0.000	0.005	0.005
29	<i>X17/123c</i>	0.067	0.027	0.074	0.028	0.008	0.002	0.014	0.003
30	<i>methyl tert-butyl ether</i>	0.592	0.206	0.430	0.108	0.027	0.009	0.032	0.006
31	<i>2,3-dimethylbutane, cyclopentane</i>	0.895	0.141	0.656	0.141	0.005	0.001	0.006	0.002
32	<i>2-methylpentane</i>	1.428	0.300	1.094	0.215	0.002	0.000	0.033	0.006
33	<i>X45/46b</i>	0.330	0.058	0.108	0.039	0.038	0.020	0.076	0.014
34	<i>3-methylpentane</i>	0.785	0.169	0.615	0.121	0.001	0.000	0.021	0.004
35	<i>1-hexene</i>	0.115	0.032	0.102	0.019	0.002	0.001	0.000	0.000
36	<i>n-hexane, 2-ethyl-1-butene</i>	2.479	0.483	0.110	0.030	0.056	0.009	0.008	0.001
37	<i>X37/47b</i>	1.070	0.188	0.720	0.141	0.004	0.001	0.030	0.005
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.006	0.001	0.019	0.008	0.000	0.000	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.961	0.190	0.838	0.163	0.001	0.000	0.025	0.006
40	<i>2,3-dimethyl-2-butene</i>	0.046	0.008	0.066	0.014	0.001	0.000	0.005	0.001
41	<i>benzene</i>	1.921	0.442	1.392	0.267	0.000	0.000	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	1.372	0.271	0.940	0.188	0.009	0.002	0.041	0.007
43	<i>2-methylhexane</i>	0.205	0.042	0.201	0.041	0.002	0.000	0.005	0.001
44	<i>cyclohexene</i>	0.019	0.010	0.025	0.006	0.001	0.000	0.000	0.000
45	<i>1-heptene</i>	0.172	0.029	0.179	0.036	0.004	0.001	0.000	0.000
46	<i>2,2,4-trimethylpentane</i>	0.534	0.127	0.601	0.119	0.009	0.002	0.027	0.004

Table F.3.a: Results of CMB analysis for receptor point JOTAL1 (Im Johannistal, 27.08.02, residential area, down-wind from the city centre)

	compounds	measured concentration		CMB calculated concentrations					
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS2		SOLVENTS4	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	0.451	0.079	0.414	0.086	0.015	0.004	0.041	0.006
48	1,4-cyclohexadiene	0.039	0.007	0.011	0.003	0.008	0.005	0.000	0.000
49	X210/70h	0.377	0.073	0.309	0.063	0.010	0.002	0.012	0.002
50	X210/70i	0.092	0.019	0.105	0.022	0.003	0.001	0.006	0.001
51	X210/70j	0.099	0.045	0.086	0.017	0.003	0.001	0.000	0.000
52	2,3,4-trimethylpentane	0.127	0.021	0.207	0.044	0.001	0.000	0.012	0.002
53	toluene	3.717	0.744	4.290	0.868	0.000	0.000	0.138	0.021
54	2-methylheptane	0.257	0.041	0.251	0.050	0.005	0.001	0.014	0.002
55	3-methylheptane	0.090	0.022	0.094	0.019	0.000	0.000	0.001	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.174	0.030	0.237	0.052	0.005	0.001	0.004	0.001
57	X211/212c	0.003	0.000	0.006	0.003	0.000	0.000	0.000	0.000
58	1-octene	0.104	0.017	0.102	0.022	0.008	0.002	0.000	0.000
59	X212/81a	0.005	0.005	0.003	0.000	0.000	0.000	0.000	0.000
60	<i>n</i> -octane	0.206	0.035	0.193	0.039	0.020	0.004	0.007	0.001
61	ethylbenzene	0.844	0.126	0.846	0.182	0.062	0.020	0.086	0.014
62	meta- and para-xylene	1.468	0.221	1.469	0.323	0.192	0.080	0.234	0.044
63	styrene	0.081	0.052	0.141	0.044	0.000	0.000	0.000	0.000
64	ortho-xylene	0.607	0.127	0.590	0.138	0.037	0.019	0.050	0.011
65	alpha-pinene	0.137	0.020	0.108	0.044	0.000	0.000	0.000	0.000
66	<i>n</i> -propylbenzene	0.079	0.050	0.121	0.036	0.000	0.000	0.000	0.000
67	4-ethyltoluene	0.047	0.007	0.061	0.019	0.005	0.003	0.004	0.001
68	X67/145c	0.058	0.050	0.094	0.030	0.000	0.000	0.000	0.000
69	X88/120c	0.048	0.041	0.105	0.036	0.000	0.000	0.000	0.000
70	1,3,5-trimethylbenzene	0.105	0.056	0.121	0.044	0.000	0.000	0.000	0.000
71	<i>n</i> -decane	0.075	0.043	0.050	0.022	0.001	0.001	0.000	0.000
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.156	0.067	0.345	0.132	0.000	0.000	0.000	0.000
73	X213/86b	0.037	0.020	0.011	0.003	0.000	0.000	0.001	0.000
74	1,2,3-trimethylbenzene	0.013	0.004	0.039	0.017	0.000	0.000	0.000	0.000
75	1,2,3,4-tetramethylbenzene	0.006	0.006	0.003	0.000	0.000	0.000	0.000	0.000
76	acetone	0.318	0.078	0.733	0.449	0.151	0.097	0.000	0.000
77	methyl acetate	0.040	0.024	0.072	0.025	0.023	0.012	0.000	0.000
78	ethyl acetate	0.004	0.002	0.044	0.019	0.000	0.000	0.000	0.000
79	methanol	0.006	0.003	0.019	0.006	0.004	0.001	0.000	0.000
80	2-butanone	0.029	0.021	0.036	0.014	0.011	0.007	0.002	0.001
81	isopropyl acetate	0.169	0.237	0.019	0.014	0.007	0.008	0.005	0.001
82	2-propanol	0.477	0.100	0.080	0.030	0.010	0.009	0.000	0.000
83	ethanol	0.012	0.006	0.174	0.138	0.016	0.004	0.023	0.005
84	propyl acetate	0.069	0.032	0.033	0.030	0.014	0.018	0.000	0.000
85	isobutyl acetate	0.037	0.025	0.014	0.003	0.001	0.000	0.000	0.000
86	4-methyl-2-pentanone	0.004	0.001	0.014	0.022	0.001	0.001	0.000	0.000
87	2-butanol	0.076	0.029	0.041	0.022	0.002	0.001	0.000	0.000
88	1-propanol	0.010	0.007	0.008	0.003	0.001	0.000	0.000	0.000
89	butyl acetate	0.019	0.010	0.025	0.014	0.010	0.013	0.009	0.010
90	2-hexanone	0.008	0.002	0.014	0.014	0.000	0.000	0.000	0.000
91	1-butanol	0.036	0.010	0.022	0.008	0.029	0.011	0.004	0.001
92	cyclohexanone	0.070	0.025	0.019	0.006	0.000	0.000	0.000	0.000
	Σ NMVOC	39.871	1.903	27.567	1.416	1.412	0.638	1.827	0.574

names of unknown compounds are explained in table E.1 in Annex E

Table F.4.a: Results of CMB analysis for receptor point JOTAL2 (Im Johannistal, 27.08.02, residential area, down-wind from the city centre)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS4	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.219	0.036	0.114	0.037	0.004	0.001
2	<i>propane</i>	0.024	0.005	0.119	0.077	0.004	0.001
3	<i>propadiene</i>	0.002	0.002	0.005	0.005	0.000	0.000
4	<i>propyne</i>	0.012	0.002	0.002	0.005	0.000	0.000
5	<i>X5/13a</i>	0.002	0.002	0.007	0.005	0.000	0.000
6	<i>2-methylpropane</i>	0.042	0.012	0.163	0.051	0.014	0.002
7	<i>1-butene, 2-methylpropene</i>	0.648	0.125	0.441	0.119	0.007	0.001
8	<i>1,3-butadiene</i>	0.040	0.007	0.028	0.007	0.000	0.000
9	<i>n-butane</i>	0.062	0.013	0.250	0.082	0.000	0.000
10	<i>trans-2-butene</i>	0.052	0.020	0.035	0.009	0.002	0.000
11	<i>1-butyne</i>	0.009	0.001	0.005	0.002	0.000	0.000
12	<i>cis-2-butene</i>	0.040	0.006	0.033	0.009	0.001	0.000
13	<i>X12/18d</i>	0.050	0.010	0.033	0.012	0.000	0.000
14	<i>3-methyl-1-butene</i>	0.067	0.011	0.049	0.009	0.000	0.000
15	<i>X18/25a</i>	0.134	0.024	0.044	0.016	0.058	0.010
16	<i>X18/25b</i>	0.155	0.025	0.058	0.016	0.013	0.002
17	<i>X18/25d</i>	0.916	0.131	1.117	0.266	0.000	0.000
18	<i>2-methylbutane</i>	0.891	0.172	1.150	0.341	0.184	0.075
19	<i>X25/19c</i>	0.082	0.019	0.105	0.021	0.005	0.001
20	<i>1-pentene</i>	0.084	0.013	0.205	0.044	0.008	0.004
21	<i>n-pentane, 2-methyl-1-butene</i>	1.109	0.432	1.227	0.261	0.055	0.016
22	<i>2-methyl-1,3-butadiene</i>	0.386	0.110	0.380	0.096	0.060	0.019
23	<i>trans-2-pentene</i>	0.061	0.012	0.217	0.051	0.010	0.004
24	<i>cis-2-pentene</i>	0.068	0.017	0.105	0.023	0.008	0.002
25	<i>X22/43b</i>	0.195	0.058	0.329	0.044	0.014	0.005
26	<i>2,2-dimethylbutane</i>	0.200	0.091	0.184	0.037	0.007	0.002
27	<i>X43/17c</i>	0.032	0.010	0.009	0.002	0.030	0.008
28	<i>cyclopentene</i>	0.015	0.002	0.035	0.009	0.003	0.003
29	<i>X17/123c</i>	0.189	0.037	0.063	0.023	0.008	0.002
30	<i>methyl tert-butyl ether</i>	0.268	0.267	0.364	0.091	0.018	0.004
31	<i>2,3-dimethylbutane, cyclopentane</i>	0.471	0.403	0.555	0.119	0.003	0.001
32	<i>2-methylpentane</i>	1.161	0.305	0.926	0.182	0.019	0.003
33	<i>X45/46b</i>	0.134	0.019	0.091	0.033	0.043	0.008
34	<i>3-methylpentane</i>	0.636	0.173	0.520	0.103	0.012	0.002
35	<i>1-hexene</i>	0.094	0.017	0.086	0.016	0.000	0.000
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.003	0.003	0.093	0.026	0.004	0.001
37	<i>X37/47b</i>	1.664	0.357	0.609	0.119	0.017	0.003
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.004	0.006	0.016	0.007	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.640	0.206	0.709	0.138	0.014	0.003
40	<i>2,3-dimethyl-2-butene</i>	0.040	0.013	0.056	0.012	0.003	0.001
41	<i>benzene</i>	1.505	0.352	1.178	0.226	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	1.133	0.265	0.795	0.159	0.023	0.004
43	<i>2-methylhexane</i>	0.210	0.038	0.170	0.035	0.003	0.000
44	<i>cyclohexene</i>	0.014	0.003	0.021	0.005	0.000	0.000
45	<i>1-heptene</i>	0.188	0.034	0.152	0.030	0.000	0.000
46	<i>2,2,4-trimethylpentane</i>	0.575	0.107	0.508	0.100	0.016	0.002

Table F.4.b: Results of CMB analysis for receptor point JOTAL2 (Im Johannistal, 27.08.02, residential area, down-wind from the city centre)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS4	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	0.508	0.083	0.350	0.072	0.023	0.004
48	1,4-cyclohexadiene	0.054	0.009	0.009	0.002	0.000	0.000
49	X210/70h	0.324	0.065	0.261	0.054	0.007	0.001
50	X210/70i	0.084	0.012	0.089	0.019	0.003	0.001
51	X210/70j	0.086	0.013	0.072	0.014	0.000	0.000
52	2,3,4-trimethylpentane	0.178	0.027	0.175	0.037	0.007	0.001
53	toluene	4.260	0.724	3.629	0.735	0.079	0.012
54	2-methylheptane	0.288	0.046	0.212	0.042	0.008	0.001
55	3-methylheptane	0.092	0.017	0.079	0.016	0.001	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.190	0.034	0.201	0.044	0.002	0.000
57	X211/212c	0.004	0.004	0.005	0.002	0.000	0.000
58	1-octene	0.107	0.015	0.086	0.019	0.000	0.000
59	X212/81a	0.005	0.005	0.002	0.000	0.000	0.000
60	<i>n</i> -octane	0.218	0.038	0.163	0.033	0.004	0.001
61	ethylbenzene	1.081	0.186	0.716	0.154	0.049	0.008
62	meta- and para-xylene	1.987	0.342	1.243	0.273	0.134	0.025
63	styrene	0.103	0.024	0.119	0.037	0.000	0.000
64	ortho-xylene	0.959	0.165	0.499	0.117	0.028	0.007
65	alpha-pinene	0.110	0.031	0.091	0.037	0.000	0.000
66	<i>n</i> -propylbenzene	0.186	0.041	0.103	0.030	0.000	0.000
67	4-ethyltoluene	0.093	0.016	0.051	0.016	0.002	0.001
68	X67/145c	0.126	0.030	0.079	0.026	0.000	0.000
69	X88/120c	0.069	0.016	0.089	0.030	0.000	0.000
70	1,3,5-trimethylbenzene	0.180	0.047	0.103	0.037	0.000	0.000
71	<i>n</i> -decane	0.219	0.052	0.042	0.019	0.000	0.000
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.369	0.101	0.292	0.112	0.000	0.000
73	X213/86b	0.078	0.017	0.009	0.002	0.001	0.000
74	1,2,3-trimethylbenzene	0.026	0.009	0.033	0.014	0.000	0.000
75	1,2,3,4-tetramethylbenzene	0.003	0.006	0.002	0.000	0.000	0.000
76	acetone	0.171	0.035	0.620	0.380	0.000	0.000
77	methyl acetate	0.015	0.003	0.061	0.021	0.000	0.000
78	ethyl acetate	0.008	0.002	0.037	0.016	0.000	0.000
79	methanol	0.051	0.067	0.016	0.005	0.000	0.000
80	2-butanone	0.025	0.009	0.030	0.012	0.001	0.001
81	isopropyl acetate	0.045	0.017	0.016	0.012	0.003	0.001
82	2-propanol	0.337	0.149	0.068	0.026	0.000	0.000
83	ethanol	0.006	0.002	0.147	0.117	0.013	0.003
84	propyl acetate	0.051	0.011	0.028	0.026	0.000	0.000
85	isobutyl acetate	0.021	0.005	0.012	0.002	0.000	0.000
86	4-methyl-2-pentanone	0.009	0.002	0.012	0.019	0.000	0.000
87	2-butanol	0.062	0.015	0.035	0.019	0.000	0.000
88	1-propanol	0.008	0.007	0.007	0.002	0.000	0.000
89	butyl acetate	0.019	0.012	0.021	0.012	0.005	0.006
90	2-hexanone	0.008	0.002	0.012	0.012	0.000	0.000
91	1-butanol	0.032	0.007	0.019	0.007	0.002	0.001
92	cyclohexanone	0.061	0.017	0.016	0.005	0.000	0.000
	Σ NMVOC	27.435	1.336	23.323	1.008	1.041	0.329

names of unknown compounds are explained in table E.1 in Annex E

Table F.5.a: Results of CMB analysis for receptor point BUNDA1 (Bundesallee, 26.08.02, city centre of Wuppertal, dense traffic intersection)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.126	0.018	0.340	0.111	0.000	0.000
2	<i>propane</i>	0.011	0.002	0.354	0.229	0.000	0.000
3	<i>propadiene</i>	0.002	0.002	0.014	0.014	0.000	0.000
4	<i>propyne</i>	0.012	0.002	0.007	0.014	0.000	0.000
5	<i>X5/13a</i>	0.011	0.003	0.021	0.014	0.000	0.000
6	<i>2-methylpropane</i>	0.225	0.032	0.486	0.153	0.000	0.000
7	<i>1-butene, 2-methylpropene</i>	1.371	0.195	1.312	0.354	0.000	0.000
8	<i>1,3-butadiene</i>	0.074	0.011	0.083	0.021	0.000	0.000
9	<i>n-butane</i>	0.309	0.044	0.743	0.243	0.000	0.000
10	<i>trans-2-butene</i>	0.089	0.013	0.104	0.028	0.000	0.000
11	<i>1-butyne</i>	0.018	0.003	0.014	0.007	0.000	0.000
12	<i>cis-2-butene</i>	0.070	0.010	0.097	0.028	0.000	0.000
13	<i>X12/18d</i>	0.071	0.015	0.097	0.035	0.000	0.000
14	<i>3-methyl-1-butene</i>	0.156	0.022	0.146	0.028	0.000	0.000
15	<i>X18/25a</i>	0.119	0.017	0.132	0.049	0.000	0.000
16	<i>X18/25b</i>	0.200	0.029	0.174	0.049	0.000	0.000
17	<i>X18/25d</i>	5.014	0.715	3.325	0.791	0.000	0.000
18	<i>2-methylbutane</i>	2.854	0.407	3.422	1.014	0.000	0.000
19	<i>X25/19c</i>	0.394	0.056	0.312	0.063	0.000	0.000
20	<i>1-pentene</i>	0.769	0.110	0.611	0.132	0.000	0.000
21	<i>n-pentane, 2-methyl-1-butene</i>	5.053	0.720	3.651	0.778	0.000	0.000
22	<i>2-methyl-1,3-butadiene</i>	2.264	0.323	1.132	0.285	0.000	0.000
23	<i>trans-2-pentene</i>	0.813	0.116	0.646	0.153	0.000	0.000
24	<i>cis-2-pentene</i>	0.403	0.058	0.312	0.069	0.000	0.000
25	<i>X22/43b</i>	1.231	0.242	0.979	0.132	0.000	0.000
26	<i>2,2-dimethylbutane</i>	0.761	0.108	0.548	0.111	0.000	0.000
27	<i>X43/17c</i>	0.028	0.006	0.028	0.007	0.000	0.000
28	<i>cyclopentene</i>	0.064	0.009	0.104	0.028	0.000	0.000
29	<i>X17/123c</i>	0.250	0.049	0.187	0.069	0.000	0.000
30	<i>methyl tert-butyl ether</i>	1.770	0.252	1.083	0.271	0.000	0.000
31	<i>2,3-dimethylbutane, cyclopentane</i>	1.743	0.248	1.652	0.354	0.000	0.000
32	<i>2-methylpentane</i>	3.179	0.453	2.756	0.542	0.000	0.000
33	<i>X45/46b</i>	0.415	0.059	0.271	0.097	0.000	0.000
34	<i>3-methylpentane</i>	1.788	0.255	1.548	0.305	0.000	0.000
35	<i>1-hexene</i>	0.272	0.039	0.257	0.049	0.000	0.000
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.438	0.062	0.278	0.076	0.000	0.000
37	<i>X37/47b</i>	1.724	0.246	1.812	0.354	0.000	0.000
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.038	0.005	0.049	0.021	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	2.312	0.330	2.110	0.410	0.000	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.167	0.024	0.167	0.035	0.000	0.000
41	<i>benzene</i>	3.360	0.479	3.506	0.673	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	2.831	0.404	2.367	0.472	0.000	0.000
43	<i>2-methylhexane</i>	0.542	0.077	0.507	0.104	0.000	0.000
44	<i>cyclohexene</i>	0.066	0.009	0.063	0.014	0.000	0.000
45	<i>1-heptene</i>	0.539	0.077	0.451	0.090	0.000	0.000
46	<i>2,2,4-trimethylpentane</i>	1.861	0.265	1.513	0.299	0.000	0.000

Table F.5.b: Results of CMB analysis for receptor point BUNDA1 (Bundesallee, 26.08.02, city centre of Wuppertal, dense traffic intersection)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n-heptane</i>	1.030	0.147	1.041	0.215	0.000	0.000
48	<i>1,4-cyclohexadiene</i>	0.048	0.007	0.028	0.007	0.000	0.000
49	<i>X210/70h</i>	0.847	0.121	0.778	0.160	0.000	0.000
50	<i>X210/70i</i>	0.315	0.045	0.264	0.056	0.000	0.000
51	<i>X210/70j</i>	0.255	0.036	0.215	0.042	0.000	0.000
52	<i>2,3,4-trimethylpentane</i>	0.602	0.086	0.521	0.111	0.000	0.000
53	<i>toluene</i>	10.281	1.465	10.801	2.187	0.000	0.000
54	<i>2-methylheptane</i>	0.573	0.082	0.632	0.125	0.000	0.000
55	<i>3-methylheptane</i>	0.263	0.038	0.236	0.049	0.000	0.000
56	<i>4-methylheptane, 1-methyl-1-cyclohexene</i>	0.499	0.071	0.597	0.132	0.000	0.000
57	<i>X211/212c</i>	0.008	0.001	0.014	0.007	0.000	0.000
58	<i>1-octene</i>	0.431	0.062	0.257	0.056	0.000	0.000
59	<i>X212/81a</i>	0.005	0.005	0.007	0.000	0.000	0.000
60	<i>n-octane</i>	0.472	0.067	0.486	0.097	0.000	0.000
61	<i>ethylbenzene</i>	2.580	0.368	2.131	0.458	0.000	0.000
62	<i>meta- and para-xylene</i>	4.902	0.699	3.700	0.812	0.000	0.000
63	<i>styrene</i>	0.234	0.033	0.354	0.111	0.000	0.000
64	<i>ortho-xylene</i>	1.754	0.250	1.486	0.347	0.000	0.000
65	<i>alpha-pinene</i>	0.060	0.009	0.271	0.111	0.000	0.000
66	<i>n-propylbenzene</i>	0.258	0.037	0.305	0.090	0.000	0.000
67	<i>4-ethyltoluene</i>	0.345	0.049	0.153	0.049	0.000	0.000
68	<i>X67/145c</i>	0.202	0.029	0.236	0.076	0.000	0.000
69	<i>X88/120c</i>	0.161	0.023	0.264	0.090	0.000	0.000
70	<i>1,3,5-trimethylbenzene</i>	0.205	0.029	0.305	0.111	0.000	0.000
71	<i>n-decane</i>	0.058	0.008	0.125	0.056	0.000	0.000
72	<i>1,2,4-trimethylbenzene, tetrabutylbenzene</i>	0.529	0.075	0.868	0.333	0.000	0.000
73	<i>X213/86b</i>	0.023	0.003	0.028	0.007	0.000	0.000
74	<i>1,2,3-trimethylbenzene</i>	0.064	0.009	0.097	0.042	0.000	0.000
75	<i>1,2,3,4-tetramethylbenzene</i>	0.006	0.006	0.007	0.000	0.000	0.000
76	<i>acetone</i>	0.384	0.079	1.847	1.132	0.000	0.000
77	<i>methyl acetate</i>	0.109	0.022	0.181	0.063	0.000	0.000
78	<i>ethyl acetate</i>	0.003	0.001	0.111	0.049	0.000	0.000
79	<i>methanol</i>	0.030	0.006	0.049	0.014	0.000	0.000
80	<i>2-butanone</i>	0.010	0.002	0.090	0.035	0.000	0.000
81	<i>isopropyl acetate</i>	0.006	0.001	0.049	0.035	0.000	0.000
82	<i>2-propanol</i>	0.076	0.016	0.201	0.076	0.000	0.000
83	<i>ethanol</i>	0.041	0.009	0.437	0.347	0.000	0.000
84	<i>propyl acetate</i>	0.017	0.003	0.083	0.076	0.000	0.000
85	<i>isobutyl acetate</i>	0.047	0.010	0.035	0.007	0.000	0.000
86	<i>4-methyl-2-pentanone</i>	0.020	0.004	0.035	0.056	0.000	0.000
87	<i>2-butanol</i>	0.013	0.003	0.104	0.056	0.000	0.000
88	<i>1-propanol</i>	0.014	0.003	0.021	0.007	0.000	0.000
89	<i>butyl acetate</i>	0.035	0.007	0.063	0.035	0.000	0.000
90	<i>2-hexanone</i>	0.005	0.001	0.035	0.035	0.000	0.000
91	<i>1-butanol</i>	0.018	0.004	0.056	0.021	0.000	0.000
92	<i>cyclohexanone</i>	0.036	0.007	0.049	0.014	0.000	0.000
	Σ NMVOC	73.672	2.328	69.417	2.328	0.000	0.000

names of unknown compounds are explained in table E.1 in Annex E

Table F.6.a: Results of CMB analysis for receptor point BUNDA2 (Bundesallee, 26.08.02, city centre of Wuppertal, dense traffic intersection)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.097	0.035	0.227	0.074	0.000	0.000
2	<i>propane</i>	0.011	0.002	0.236	0.153	0.000	0.000
3	<i>propadiene</i>	0.002	0.002	0.009	0.009	0.000	0.000
4	<i>propyne</i>	0.004	0.001	0.005	0.009	0.000	0.000
5	<i>X5/13a</i>	0.007	0.002	0.014	0.009	0.000	0.000
6	<i>2-methylpropane</i>	0.162	0.046	0.324	0.102	0.000	0.000
7	<i>1-butene, 2-methylpropene</i>	0.854	0.211	0.875	0.236	0.000	0.000
8	<i>1,3-butadiene</i>	0.050	0.009	0.056	0.014	0.000	0.000
9	<i>n-butane</i>	0.229	0.116	0.496	0.162	0.000	0.000
10	<i>trans-2-butene</i>	0.064	0.011	0.070	0.019	0.000	0.000
11	<i>1-butyne</i>	0.009	0.002	0.009	0.005	0.000	0.000
12	<i>cis-2-butene</i>	0.054	0.014	0.065	0.019	0.000	0.000
13	<i>X12/18d</i>	0.049	0.011	0.065	0.023	0.000	0.000
14	<i>3-methyl-1-butene</i>	0.106	0.042	0.097	0.019	0.000	0.000
15	<i>X18/25a</i>	0.133	0.090	0.088	0.032	0.000	0.000
16	<i>X18/25b</i>	0.158	0.081	0.116	0.032	0.000	0.000
17	<i>X18/25d</i>	3.234	2.648	2.218	0.528	0.000	0.000
18	<i>2-methylbutane</i>	2.119	0.783	2.283	0.676	0.000	0.000
19	<i>X25/19c</i>	0.272	0.161	0.208	0.042	0.000	0.000
20	<i>1-pentene</i>	0.517	0.336	0.408	0.088	0.000	0.000
21	<i>n-pentane, 2-methyl-1-butene</i>	3.490	1.883	2.436	0.519	0.000	0.000
22	<i>2-methyl-1,3-butadiene</i>	1.534	0.810	0.755	0.190	0.000	0.000
23	<i>trans-2-pentene</i>	0.575	0.444	0.431	0.102	0.000	0.000
24	<i>cis-2-pentene</i>	0.270	0.166	0.208	0.046	0.000	0.000
25	<i>X22/43b</i>	0.878	0.490	0.653	0.088	0.000	0.000
26	<i>2,2-dimethylbutane</i>	0.512	0.223	0.366	0.074	0.000	0.000
27	<i>X43/17c</i>	0.040	0.043	0.019	0.005	0.000	0.000
28	<i>cyclopentene</i>	0.054	0.026	0.070	0.019	0.000	0.000
29	<i>X17/123c</i>	0.147	0.046	0.125	0.046	0.000	0.000
30	<i>methyl tert-butyl ether</i>	0.480	0.371	0.723	0.181	0.000	0.000
31	<i>2,3-dimethylbutane, cyclopentane</i>	1.827	0.533	1.102	0.236	0.000	0.000
32	<i>2-methylpentane</i>	2.433	0.747	1.839	0.361	0.000	0.000
33	<i>X45/46b</i>	0.280	0.125	0.181	0.065	0.000	0.000
34	<i>3-methylpentane</i>	1.383	0.448	1.033	0.204	0.000	0.000
35	<i>1-hexene</i>	0.207	0.061	0.171	0.032	0.000	0.000
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.292	0.131	0.185	0.051	0.000	0.000
37	<i>X37/47b</i>	1.455	0.454	1.209	0.236	0.000	0.000
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.030	0.009	0.032	0.014	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	1.688	0.633	1.408	0.273	0.000	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.129	0.037	0.111	0.023	0.000	0.000
41	<i>benzene</i>	2.467	0.648	2.339	0.449	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	1.929	0.566	1.579	0.315	0.000	0.000
43	<i>2-methylhexane</i>	0.383	0.099	0.338	0.070	0.000	0.000
44	<i>cyclohexene</i>	0.045	0.021	0.042	0.009	0.000	0.000
45	<i>1-heptene</i>	0.373	0.106	0.301	0.060	0.000	0.000
46	<i>2,2,4-trimethylpentane</i>	1.221	0.425	1.010	0.199	0.000	0.000

Table F.6.b: Results of CMB analysis for receptor point BUNDA2 (Bundesallee, 26.08.02, city centre of Wuppertal, dense traffic intersection)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	0.812	0.161	0.695	0.144	0.000	0.000
48	1,4-cyclohexadiene	0.029	0.013	0.019	0.005	0.000	0.000
49	X210/70h	0.602	0.206	0.519	0.107	0.000	0.000
50	X210/70i	0.211	0.084	0.176	0.037	0.000	0.000
51	X210/70j	0.160	0.037	0.144	0.028	0.000	0.000
52	2,3,4-trimethylpentane	0.410	0.093	0.347	0.074	0.000	0.000
53	toluene	8.300	1.926	7.206	1.459	0.000	0.000
54	2-methylheptane	0.506	0.081	0.422	0.083	0.000	0.000
55	3-methylheptane	0.167	0.032	0.158	0.032	0.000	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.400	0.095	0.398	0.088	0.000	0.000
57	X211/212c	0.007	0.003	0.009	0.005	0.000	0.000
58	1-octene	0.250	0.148	0.171	0.037	0.000	0.000
59	X212/81a	0.005	0.005	0.005	0.000	0.000	0.000
60	<i>n</i> -octane	0.375	0.054	0.324	0.065	0.000	0.000
61	ethylbenzene	1.662	0.366	1.422	0.306	0.000	0.000
62	meta- and para-xylene	2.844	0.649	2.469	0.542	0.000	0.000
63	styrene	0.197	0.028	0.236	0.074	0.000	0.000
64	ortho-xylene	1.234	0.179	0.991	0.232	0.000	0.000
65	alpha-pinene	0.050	0.009	0.181	0.074	0.000	0.000
66	<i>n</i> -propylbenzene	0.184	0.074	0.204	0.060	0.000	0.000
67	4-ethyltoluene	0.254	0.044	0.102	0.032	0.000	0.000
68	X67/145c	0.171	0.070	0.158	0.051	0.000	0.000
69	X88/120c	0.144	0.089	0.176	0.060	0.000	0.000
70	1,3,5-trimethylbenzene	0.139	0.021	0.204	0.074	0.000	0.000
71	<i>n</i> -decane	0.042	0.011	0.083	0.037	0.000	0.000
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.291	0.087	0.579	0.222	0.000	0.000
73	X213/86b	0.021	0.003	0.019	0.005	0.000	0.000
74	1,2,3-trimethylbenzene	0.039	0.007	0.065	0.028	0.000	0.000
75	1,2,3,4-tetramethylbenzene	0.006	0.006	0.005	0.000	0.000	0.000
76	acetone	0.357	0.173	1.232	0.755	0.000	0.000
77	methyl acetate	0.060	0.052	0.120	0.042	0.000	0.000
78	ethyl acetate	0.013	0.012	0.074	0.032	0.000	0.000
79	methanol	0.065	0.016	0.032	0.009	0.000	0.000
80	2-butanone	0.028	0.006	0.060	0.023	0.000	0.000
81	isopropyl acetate	0.037	0.017	0.032	0.023	0.000	0.000
82	2-propanol	0.057	0.013	0.134	0.051	0.000	0.000
83	ethanol	0.040	0.019	0.292	0.232	0.000	0.000
84	propyl acetate	0.059	0.036	0.056	0.051	0.000	0.000
85	isobutyl acetate	0.030	0.010	0.023	0.005	0.000	0.000
86	4-methyl-2-pentanone	0.008	0.006	0.023	0.037	0.000	0.000
87	2-butanol	0.117	0.081	0.070	0.037	0.000	0.000
88	1-propanol	0.013	0.005	0.014	0.005	0.000	0.000
89	butyl acetate	0.038	0.017	0.042	0.023	0.000	0.000
90	2-hexanone	0.009	0.009	0.023	0.023	0.000	0.000
91	1-butanol	0.047	0.011	0.037	0.014	0.000	0.000
92	cyclohexanone	0.075	0.037	0.032	0.009	0.000	0.000
	Σ NMVOC	52.809	4.453	46.314	2.215	0.000	0.000

names of unknown compounds are explained in table E.1 in Annex E

Table F.7.a: Results of CMB analysis for receptor point MARKIS (Märkisch Str., 15.10.03, close to free-way A46)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS8	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	1.387	0.434	0.181	0.059	0.014	0.004
2	<i>propane</i>	1.430	0.401	0.189	0.122	0.011	0.003
3	<i>propadiene</i>	0.051	0.021	0.007	0.007	0.000	0.000
4	<i>propyne</i>	0.078	0.034	0.004	0.007	0.000	0.000
5	<i>X5/13a</i>	0.058	0.054	0.011	0.007	0.000	0.000
6	<i>2-methylpropane</i>	0.984	0.297	0.259	0.081	0.004	0.001
7	<i>1-butene, 2-methylpropene</i>	2.310	0.692	0.699	0.189	0.035	0.010
8	<i>1,3-butadiene</i>	0.096	0.087	0.044	0.011	0.001	0.000
9	<i>n-butane</i>	2.293	0.692	0.396	0.129	0.006	0.002
10	<i>trans-2-butene</i>	0.454	0.138	0.056	0.015	0.001	0.000
11	<i>1-butyne</i>	0.013	0.005	0.007	0.004	0.000	0.000
12	<i>cis-2-butene</i>	0.416	0.132	0.052	0.015	0.001	0.000
13	<i>X12/18d</i>	0.388	0.106	0.052	0.019	0.002	0.001
14	<i>3-methyl-1-butene</i>	0.295	0.086	0.078	0.015	0.000	0.000
15	<i>X18/25a</i>	0.157	0.054	0.070	0.026	0.001	0.000
16	<i>X18/25b</i>	0.170	0.048	0.092	0.026	0.002	0.000
17	<i>X18/25d</i>	1.920	0.523	1.771	0.421	0.051	0.014
18	<i>2-methylbutane</i>	5.476	1.580	1.823	0.540	0.011	0.003
19	<i>X25/19c</i>	0.245	0.068	0.166	0.033	0.006	0.002
20	<i>1-pentene</i>	0.647	0.191	0.325	0.070	0.001	0.000
21	<i>n-pentane, 2-methyl-1-butene</i>	3.082	1.356	1.945	0.414	0.000	0.000
22	<i>2-methyl-1,3-butadiene</i>	0.340	0.167	0.603	0.152	0.000	0.000
23	<i>trans-2-pentene</i>	0.474	0.179	0.344	0.081	0.000	0.000
24	<i>cis-2-pentene</i>	0.242	0.072	0.166	0.037	0.003	0.001
25	<i>X22/43b</i>	0.778	0.266	0.521	0.070	0.000	0.000
26	<i>2,2-dimethylbutane</i>	0.417	0.150	0.292	0.059	0.000	0.000
27	<i>X43/17c</i>	0.006	0.003	0.015	0.004	0.000	0.000
28	<i>cyclopentene</i>	0.372	0.106	0.056	0.015	0.000	0.000
29	<i>X17/123c</i>	0.003	0.003	0.100	0.037	0.001	0.000
30	<i>methyl tert-butyl ether</i>	1.561	0.518	0.577	0.144	0.005	0.001
31	<i>2,3-dimethylbutane, cyclopentane</i>	1.439	0.495	0.880	0.189	0.003	0.001
32	<i>2-methylpentane</i>	3.214	0.961	1.468	0.288	0.002	0.001
33	<i>X45/46b</i>	0.152	0.047	0.144	0.052	0.002	0.001
34	<i>3-methylpentane</i>	1.736	0.523	0.824	0.163	0.000	0.000
35	<i>1-hexene</i>	0.160	0.047	0.137	0.026	0.002	0.001
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.131	0.048	0.148	0.041	0.008	0.002
37	<i>X37/47b</i>	1.831	0.513	0.965	0.189	0.000	0.000
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.035	0.021	0.026	0.011	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	1.805	0.658	1.124	0.218	0.000	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.126	0.036	0.089	0.019	0.000	0.000
41	<i>benzene</i>	2.822	0.841	1.867	0.359	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	1.935	0.552	1.261	0.251	0.000	0.000
43	<i>2-methylhexane</i>	0.380	0.103	0.270	0.056	0.000	0.000
44	<i>cyclohexene</i>	0.028	0.009	0.033	0.007	0.001	0.000
45	<i>1-heptene</i>	0.397	0.145	0.240	0.048	0.001	0.000
46	<i>2,2,4-trimethylpentane</i>	1.106	0.301	0.806	0.159	0.000	0.000

Table F.7.b: Results of CMB analysis for receptor point MARKIS (Märkisch Str., 15.10.03, close to free-way A46)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS8	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	1.077	0.296	0.555	0.115	0.001	0.000
48	1,4-cyclohexadiene	0.017	0.006	0.015	0.004	0.001	0.000
49	X210/70h	0.764	0.234	0.414	0.085	0.001	0.000
50	X210/70i	0.244	0.083	0.141	0.030	0.002	0.000
51	X210/70j	0.210	0.060	0.115	0.022	0.004	0.001
52	2,3,4-trimethylpentane	0.402	0.111	0.277	0.059	0.000	0.000
53	toluene	18.353	6.098	5.752	1.165	0.012	0.004
54	2-methylheptane	1.049	0.499	0.336	0.067	0.002	0.001
55	3-methylheptane	0.243	0.111	0.126	0.026	0.000	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.719	0.231	0.318	0.070	0.000	0.000
57	X211/212c	0.055	0.066	0.007	0.004	0.001	0.000
58	1-octene	0.975	0.289	0.137	0.030	0.007	0.002
59	X212/81a	0.163	0.047	0.004	0.000	0.179	0.053
60	<i>n</i> -octane	1.769	0.513	0.259	0.052	0.020	0.006
61	ethylbenzene	1.324	0.383	1.135	0.244	0.027	0.008
62	meta- and para-xylene	1.473	0.644	1.970	0.433	0.041	0.012
63	styrene	0.004	0.004	0.189	0.059	0.001	0.000
64	ortho-xylene	0.050	0.030	0.791	0.185	0.000	0.000
65	alpha-pinene	0.427	0.408	0.144	0.059	0.011	0.003
66	<i>n</i> -propylbenzene	0.106	0.047	0.163	0.048	0.001	0.000
67	4-ethyltoluene	0.026	0.016	0.081	0.026	0.000	0.000
68	X67/145c	0.025	0.011	0.126	0.041	0.000	0.000
69	X88/120c	0.038	0.015	0.141	0.048	0.000	0.000
70	1,3,5-trimethylbenzene	0.005	0.005	0.163	0.059	0.000	0.000
71	<i>n</i> -decane	0.027	0.014	0.067	0.030	0.000	0.000
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.163	0.057	0.462	0.177	0.000	0.000
73	X213/86b	0.005	0.005	0.015	0.004	0.000	0.000
74	1,2,3-trimethylbenzene	0.012	0.004	0.052	0.022	0.000	0.000
75	1,2,3,4-tetramethylbenzene	0.006	0.006	0.004	0.000	0.000	0.000
76	acetone	8.309	4.763	0.983	0.603	0.061	0.025
77	methyl acetate	0.533	0.329	0.096	0.033	0.005	0.004
78	ethyl acetate	0.137	0.059	0.059	0.026	0.004	0.001
79	methanol	0.359	0.124	0.026	0.007	0.009	0.009
80	2-butanone	0.161	0.151	0.048	0.019	0.003	0.001
81	isopropyl acetate	0.054	0.024	0.026	0.019	0.000	0.000
82	2-propanol	0.106	0.043	0.107	0.041	0.002	0.001
83	ethanol	0.971	0.476	0.233	0.185	0.019	0.010
84	propyl acetate	0.169	0.080	0.044	0.041	0.008	0.008
85	isobutyl acetate	0.038	0.014	0.019	0.004	0.001	0.000
86	4-methyl-2-pentanone	0.003	0.001	0.019	0.030	0.001	0.000
87	2-butanol	0.089	0.020	0.056	0.030	0.001	0.001
88	1-propanol	0.003	0.002	0.011	0.004	0.000	0.000
89	butyl acetate	0.045	0.038	0.033	0.019	0.057	0.047
90	2-hexanone	0.020	0.009	0.019	0.019	0.002	0.001
91	1-butanol	0.073	0.036	0.030	0.011	0.006	0.002
92	cyclohexanone	0.045	0.021	0.026	0.007	0.001	0.001
	Σ NMVOC	84.287	8.466	36.968	2.209	0.662	0.247

names of unknown compounds are explained in table E.1 in Annex E

Table F.8.a: Results of CMB analysis for receptor point WILKHA (Wilkhau Str., 29.08.02, industrial area, close to DuPont solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS3	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.253	0.058	0.062	0.020	0.052	0.015
2	<i>propane</i>	0.236	0.329	0.065	0.042	0.167	0.034
3	<i>propadiene</i>	0.003	0.004	0.003	0.003	0.000	0.000
4	<i>propyne</i>	0.005	0.007	0.001	0.003	0.002	0.000
5	<i>X5/13a</i>	0.002	0.003	0.004	0.003	0.000	0.000
6	<i>2-methylpropane</i>	0.131	0.113	0.089	0.028	0.058	0.012
7	<i>1-butene, 2-methylpropene</i>	0.640	0.133	0.240	0.065	0.151	0.048
8	<i>1,3-butadiene</i>	0.046	0.015	0.015	0.004	0.004	0.002
9	<i>n-butane</i>	0.303	0.366	0.136	0.044	0.134	0.025
10	<i>trans-2-butene</i>	0.051	0.013	0.019	0.005	0.014	0.004
11	<i>1-butyne</i>	0.004	0.005	0.003	0.001	0.002	0.000
12	<i>cis-2-butene</i>	0.037	0.006	0.018	0.005	0.012	0.003
13	<i>X12/18d</i>	0.038	0.017	0.018	0.006	0.004	0.005
14	<i>3-methyl-1-butene</i>	0.073	0.014	0.027	0.005	0.008	0.002
15	<i>X18/25a</i>	0.074	0.016	0.024	0.009	0.028	0.026
16	<i>X18/25b</i>	0.175	0.046	0.032	0.009	0.043	0.020
17	<i>X18/25d</i>	1.379	0.902	0.608	0.145	0.287	0.051
18	<i>2-methylbutane</i>	1.187	0.758	0.626	0.185	0.134	0.044
19	<i>X25/19c</i>	0.130	0.058	0.057	0.011	0.025	0.004
20	<i>1-pentene</i>	0.130	0.107	0.112	0.024	0.006	0.001
21	<i>n-pentane, 2-methyl-1-butene</i>	1.236	1.649	0.668	0.142	0.050	0.010
22	<i>2-methyl-1,3-butadiene</i>	0.543	0.704	0.207	0.052	0.273	0.058
23	<i>trans-2-pentene</i>	0.079	0.096	0.118	0.028	0.006	0.001
24	<i>cis-2-pentene</i>	0.038	0.037	0.057	0.013	0.006	0.001
25	<i>X22/43b</i>	0.105	0.101	0.179	0.024	0.006	0.001
26	<i>2,2-dimethylbutane</i>	0.121	0.172	0.100	0.020	0.006	0.001
27	<i>X43/17c</i>	0.017	0.007	0.005	0.001	0.021	0.010
28	<i>cyclopentene</i>	0.027	0.005	0.019	0.005	0.008	0.001
29	<i>X17/123c</i>	0.130	0.142	0.034	0.013	0.000	0.000
30	<i>methyl tert-butyl ether</i>	0.216	0.032	0.198	0.050	0.015	0.011
31	<i>2,3-dimethylbutane, cyclopentane</i>	0.448	0.442	0.302	0.065	0.004	0.002
32	<i>2-methylpentane</i>	0.691	0.840	0.504	0.099	0.000	0.000
33	<i>X45/46b</i>	0.107	0.062	0.050	0.018	0.045	0.012
34	<i>3-methylpentane</i>	0.423	0.523	0.283	0.056	0.000	0.000
35	<i>1-hexene</i>	0.070	0.016	0.047	0.009	0.009	0.002
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.067	0.079	0.051	0.014	0.051	0.009
37	<i>X37/47b</i>	0.598	0.691	0.331	0.065	0.000	0.000
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.005	0.001	0.009	0.004	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.491	0.604	0.386	0.075	0.000	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.023	0.010	0.031	0.006	0.001	0.000
41	<i>benzene</i>	1.589	1.700	0.641	0.123	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	0.869	0.928	0.433	0.086	0.059	0.012
43	<i>2-methylhexane</i>	0.115	0.102	0.093	0.019	0.010	0.002
44	<i>cyclohexene</i>	0.014	0.002	0.011	0.003	0.001	0.001
45	<i>1-heptene</i>	0.157	0.080	0.083	0.017	0.020	0.004
46	<i>2,2,4-trimethylpentane</i>	0.320	0.218	0.277	0.055	0.005	0.001

Table F.8.b: Results of CMB analysis for receptor point WILKHA (Wilkhau Str., 29.08.02, industrial area, close to DuPont solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		µg/m ³	±	TRAFFIC1		SOLVENTS3	
				µg/m ³	±	µg/m ³	±
47	<i>n</i> -heptane	0.267	0.198	0.190	0.039	0.087	0.021
48	1,4-cyclohexadiene	0.035	0.020	0.005	0.001	0.001	0.000
49	X210/70h	0.216	0.206	0.142	0.029	0.037	0.008
50	X210/70i	0.063	0.029	0.048	0.010	0.001	0.000
51	X210/70j	0.043	0.038	0.039	0.008	0.003	0.001
52	2,3,4-trimethylpentane	0.088	0.057	0.095	0.020	0.000	0.000
53	toluene	1.859	1.171	1.975	0.400	0.000	0.000
54	2-methylheptane	0.133	0.056	0.116	0.023	0.007	0.002
55	3-methylheptane	0.042	0.028	0.043	0.009	0.001	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.096	0.061	0.109	0.024	0.002	0.000
57	X211/212c	0.001	0.002	0.003	0.001	0.000	0.000
58	1-octene	0.155	0.039	0.047	0.010	0.039	0.009
59	X212/81a	0.005	0.005	0.001	0.000	0.001	0.001
60	<i>n</i> -octane	0.156	0.035	0.089	0.018	0.026	0.006
61	ethylbenzene	0.823	0.436	0.390	0.084	0.174	0.033
62	meta- and para-xylene	1.740	0.825	0.677	0.149	0.493	0.095
63	styrene	0.079	0.012	0.065	0.020	0.023	0.008
64	ortho-xylene	0.675	0.269	0.272	0.064	0.152	0.032
65	alpha-pinene	0.050	0.028	0.050	0.020	0.006	0.002
66	<i>n</i> -propylbenzene	0.082	0.025	0.056	0.017	0.033	0.010
67	4-ethyltoluene	0.188	0.087	0.028	0.009	0.053	0.011
68	X67/145c	0.032	0.024	0.043	0.014	0.026	0.010
69	X88/120c	0.029	0.004	0.048	0.017	0.025	0.012
70	1,3,5-trimethylbenzene	0.058	0.021	0.056	0.020	0.044	0.021
71	<i>n</i> -decane	0.062	0.017	0.023	0.010	0.025	0.014
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.110	0.023	0.159	0.061	0.096	0.057
73	X213/86b	0.022	0.003	0.005	0.001	0.015	0.004
74	1,2,3-trimethylbenzene	0.011	0.002	0.018	0.008	0.009	0.007
75	1,2,3,4-tetramethylbenzene	0.006	0.006	0.001	0.000	0.001	0.001
76	acetone	0.446	0.565	0.338	0.207	0.664	0.590
77	methyl acetate	0.042	0.041	0.033	0.011	0.028	0.009
78	ethyl acetate	0.018	0.010	0.020	0.009	0.000	0.000
79	methanol	0.020	0.018	0.009	0.003	0.011	0.014
80	2-butanone	0.051	0.058	0.017	0.006	0.011	0.005
81	isopropyl acetate	0.046	0.047	0.009	0.006	0.005	0.003
82	2-propanol	0.026	0.013	0.037	0.014	0.020	0.005
83	ethanol	0.009	0.005	0.080	0.064	0.117	0.027
84	propyl acetate	0.151	0.196	0.015	0.014	0.008	0.006
85	isobutyl acetate	0.009	0.002	0.006	0.001	0.001	0.000
86	4-methyl-2-pentanone	0.007	0.005	0.006	0.010	0.000	0.000
87	2-butanol	0.009	0.002	0.019	0.010	0.000	0.000
88	1-propanol	0.004	0.004	0.004	0.001	0.003	0.001
89	butyl acetate	0.146	0.204	0.011	0.006	0.006	0.003
90	2-hexanone	0.011	0.008	0.006	0.006	0.001	0.001
91	1-butanol	0.039	0.037	0.010	0.004	0.020	0.014
92	cyclohexanone	0.007	0.003	0.009	0.003	0.000	0.000
	Σ NMVOC	21.561	3.688	12.695	1.242	3.998	0.816

names of unknown compounds are explained in table E.1 in Annex E

Table F.9.a: Results of CMB analysis for receptor point HATZEN (Hatzfelder Str., 29.08.02, industrial area, close to DuPont solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS3	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.715	0.285	0.195	0.064	0.061	0.017
2	<i>propane</i>	2.522	0.759	0.203	0.131	0.195	0.040
3	<i>propadiene</i>	0.002	0.002	0.008	0.008	0.000	0.000
4	<i>propyne</i>	0.006	0.009	0.004	0.008	0.002	0.001
5	<i>X5/13a</i>	0.025	0.031	0.012	0.008	0.000	0.000
6	<i>2-methylpropane</i>	0.553	0.385	0.278	0.087	0.067	0.014
7	<i>1-butene, 2-methylpropene</i>	1.903	0.277	0.751	0.203	0.175	0.056
8	<i>1,3-butadiene</i>	0.083	0.039	0.048	0.012	0.005	0.002
9	<i>n-butane</i>	1.646	0.448	0.425	0.139	0.156	0.029
10	<i>trans-2-butene</i>	0.223	0.103	0.060	0.016	0.016	0.005
11	<i>1-butyne</i>	0.035	0.029	0.008	0.004	0.002	0.001
12	<i>cis-2-butene</i>	0.188	0.089	0.056	0.016	0.014	0.004
13	<i>X12/18d</i>	0.277	0.151	0.056	0.020	0.004	0.006
14	<i>3-methyl-1-butene</i>	0.148	0.046	0.083	0.016	0.010	0.002
15	<i>X18/25a</i>	0.268	0.065	0.076	0.028	0.032	0.031
16	<i>X18/25b</i>	0.253	0.039	0.099	0.028	0.050	0.023
17	<i>X18/25d</i>	1.945	1.216	1.903	0.453	0.334	0.060
18	<i>2-methylbutane</i>	3.844	1.631	1.958	0.580	0.155	0.051
19	<i>X25/19c</i>	0.216	0.138	0.179	0.036	0.029	0.005
20	<i>1-pentene</i>	0.372	0.253	0.350	0.076	0.007	0.001
21	<i>n-pentane, 2-methyl-1-butene</i>	1.815	1.365	2.089	0.445	0.058	0.012
22	<i>2-methyl-1,3-butadiene</i>	0.993	0.796	0.648	0.163	0.317	0.068
23	<i>trans-2-pentene</i>	0.322	0.324	0.369	0.087	0.007	0.001
24	<i>cis-2-pentene</i>	0.275	0.130	0.179	0.040	0.007	0.001
25	<i>X22/43b</i>	0.578	0.472	0.560	0.076	0.007	0.001
26	<i>2,2-dimethylbutane</i>	0.224	0.120	0.314	0.064	0.007	0.001
27	<i>X43/17c</i>	0.049	0.011	0.016	0.004	0.024	0.012
28	<i>cyclopentene</i>	0.160	0.117	0.060	0.016	0.009	0.001
29	<i>X17/123c</i>	0.239	0.214	0.107	0.040	0.000	0.000
30	<i>methyl tert-butyl ether</i>	2.253	0.829	0.620	0.155	0.017	0.013
31	<i>2,3-dimethylbutane, cyclopentane</i>	1.162	0.292	0.945	0.203	0.005	0.002
32	<i>2-methylpentane</i>	1.722	0.477	1.577	0.310	0.000	0.000
33	<i>X45/46b</i>	0.344	0.172	0.155	0.056	0.052	0.014
34	<i>3-methylpentane</i>	0.995	0.275	0.886	0.175	0.000	0.000
35	<i>1-hexene</i>	0.183	0.039	0.147	0.028	0.010	0.002
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.121	0.047	0.159	0.044	0.059	0.011
37	<i>X37/47b</i>	1.140	0.206	1.037	0.203	0.000	0.000
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.020	0.010	0.028	0.012	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	1.108	0.432	1.208	0.234	0.001	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.096	0.020	0.095	0.020	0.001	0.001
41	<i>benzene</i>	2.629	0.661	2.006	0.385	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	1.708	0.507	1.355	0.270	0.069	0.014
43	<i>2-methylhexane</i>	0.316	0.062	0.290	0.060	0.011	0.002
44	<i>cyclohexene</i>	0.039	0.006	0.036	0.008	0.001	0.001
45	<i>1-heptene</i>	0.377	0.115	0.258	0.052	0.023	0.004
46	<i>2,2,4-trimethylpentane</i>	1.151	0.199	0.866	0.171	0.006	0.001

Table F.8.b: Results of CMB analysis for receptor point WILKHA (Wilkhau Str., 29.08.02, industrial area, close to DuPont solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS3	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	0.692	0.108	0.596	0.123	0.101	0.024
48	1,4-cyclohexadiene	0.033	0.005	0.016	0.004	0.001	0.000
49	X210/70h	0.568	0.142	0.445	0.091	0.043	0.009
50	X210/70i	0.189	0.043	0.151	0.032	0.001	0.001
51	X210/70j	0.169	0.033	0.123	0.024	0.004	0.001
52	2,3,4-trimethylpentane	0.387	0.060	0.298	0.064	0.000	0.000
53	toluene	7.540	1.217	6.181	1.251	0.000	0.000
54	2-methylheptane	0.425	0.110	0.362	0.072	0.008	0.002
55	3-methylheptane	0.150	0.023	0.135	0.028	0.001	0.001
56	4-methylheptane, 1-methyl-1-cyclohexene	0.384	0.065	0.342	0.076	0.002	0.001
57	X211/212c	0.006	0.004	0.008	0.004	0.000	0.000
58	1-octene	0.373	0.100	0.147	0.032	0.045	0.011
59	X212/81a	0.005	0.005	0.004	0.000	0.001	0.001
60	<i>n</i> -octane	0.307	0.046	0.278	0.056	0.030	0.007
61	ethylbenzene	1.704	0.314	1.219	0.262	0.203	0.039
62	meta- and para-xylene	2.876	0.817	2.117	0.465	0.574	0.110
63	styrene	0.155	0.087	0.203	0.064	0.027	0.010
64	ortho-xylene	1.098	0.515	0.850	0.199	0.177	0.037
65	alpha-pinene	0.044	0.016	0.155	0.064	0.007	0.003
66	<i>n</i> -propylbenzene	0.181	0.154	0.175	0.052	0.038	0.012
67	4-ethyltoluene	0.276	0.055	0.087	0.028	0.062	0.013
68	X67/145c	0.125	0.134	0.135	0.044	0.031	0.011
69	X88/120c	0.112	0.111	0.151	0.052	0.029	0.014
70	1,3,5-trimethylbenzene	0.167	0.154	0.175	0.064	0.051	0.025
71	<i>n</i> -decane	0.065	0.048	0.072	0.032	0.029	0.016
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.353	0.243	0.497	0.191	0.111	0.066
73	X213/86b	0.018	0.017	0.016	0.004	0.017	0.005
74	1,2,3-trimethylbenzene	0.051	0.045	0.056	0.024	0.010	0.008
75	1,2,3,4-tetramethylbenzene	0.002	0.002	0.004	0.000	0.001	0.001
76	acetone	0.821	0.896	1.057	0.648	0.773	0.687
77	methyl acetate	0.260	0.314	0.103	0.036	0.033	0.011
78	ethyl acetate	0.015	0.008	0.064	0.028	0.000	0.000
79	methanol	0.031	0.012	0.028	0.008	0.013	0.017
80	2-butanone	0.024	0.012	0.052	0.020	0.013	0.006
81	isopropyl acetate	0.026	0.013	0.028	0.020	0.006	0.003
82	2-propanol	0.058	0.026	0.115	0.044	0.023	0.006
83	ethanol	0.027	0.033	0.250	0.199	0.136	0.032
84	propyl acetate	0.105	0.033	0.048	0.044	0.010	0.007
85	isobutyl acetate	0.001	0.002	0.020	0.004	0.001	0.001
86	4-methyl-2-pentanone	0.004	0.004	0.020	0.032	0.000	0.000
87	2-butanol	0.008	0.006	0.060	0.032	0.000	0.000
88	1-propanol	0.010	0.002	0.012	0.004	0.004	0.001
89	butyl acetate	0.012	0.003	0.036	0.020	0.007	0.003
90	2-hexanone	0.007	0.003	0.020	0.020	0.001	0.001
91	1-butanol	0.008	0.009	0.032	0.012	0.023	0.017
92	cyclohexanone	0.011	0.005	0.028	0.008	0.001	0.000
	Σ NMVOC	55.124	3.742	39.721	2.379	4.654	1.507

names of unknown compounds are explained in table E.1 in Annex E

Table F.10.a: Results of CMB analysis for receptor point HATZEM (Hatzfelder Str., 15.10.03, industrial area, close to DuPont solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS8	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	1.260	0.343	0.041	0.014	1.355	0.384
2	<i>propane</i>	0.946	0.257	0.043	0.028	0.996	0.284
3	<i>propadiene</i>	0.002	0.001	0.002	0.002	0.000	0.000
4	<i>propyne</i>	0.002	0.001	0.001	0.002	0.000	0.000
5	<i>X5/13a</i>	0.006	0.002	0.003	0.002	0.000	0.000
6	<i>2-methylpropane</i>	0.397	0.108	0.059	0.019	0.340	0.095
7	<i>1-butene, 2-methylpropene</i>	3.211	0.873	0.159	0.043	3.352	0.952
8	<i>1,3-butadiene</i>	0.079	0.022	0.010	0.003	0.069	0.019
9	<i>n-butane</i>	0.644	0.175	0.090	0.029	0.555	0.158
10	<i>trans-2-butene</i>	0.086	0.023	0.013	0.003	0.076	0.019
11	<i>1-butyne</i>	0.015	0.004	0.002	0.001	0.013	0.006
12	<i>cis-2-butene</i>	0.072	0.020	0.012	0.003	0.057	0.019
13	<i>X12/18d</i>	0.152	0.041	0.012	0.004	0.151	0.044
14	<i>3-methyl-1-butene</i>	0.066	0.018	0.018	0.003	0.038	0.013
15	<i>X18/25a</i>	0.071	0.019	0.016	0.006	0.050	0.013
16	<i>X18/25b</i>	0.162	0.044	0.021	0.006	0.145	0.038
17	<i>X18/25d</i>	4.939	1.343	0.403	0.096	4.839	1.374
18	<i>2-methylbutane</i>	1.654	0.450	0.414	0.123	1.071	0.303
19	<i>X25/19c</i>	0.543	0.148	0.038	0.008	0.542	0.158
20	<i>1-pentene</i>	0.219	0.060	0.074	0.016	0.101	0.032
21	<i>n-pentane, 2-methyl-1-butene</i>	0.525	0.143	0.442	0.094	0.000	0.000
22	<i>2-methyl-1,3-butadiene</i>	0.094	0.026	0.137	0.035	0.000	0.000
23	<i>trans-2-pentene</i>	0.038	0.010	0.078	0.019	0.000	0.000
24	<i>cis-2-pentene</i>	0.336	0.091	0.038	0.008	0.309	0.088
25	<i>X22/43b</i>	0.133	0.036	0.119	0.016	0.000	0.000
26	<i>2,2-dimethylbutane</i>	0.060	0.016	0.066	0.014	0.000	0.000
27	<i>X43/17c</i>	0.003	0.003	0.003	0.001	0.000	0.000
28	<i>cyclopentene</i>	0.029	0.008	0.013	0.003	0.006	0.000
29	<i>X17/123c</i>	0.121	0.033	0.023	0.008	0.095	0.025
30	<i>methyl tert-butyl ether</i>	0.614	0.167	0.131	0.033	0.441	0.126
31	<i>2,3-dimethylbutane, cyclopentane</i>	0.580	0.158	0.200	0.043	0.265	0.076
32	<i>2-methylpentane</i>	0.760	0.207	0.334	0.066	0.208	0.057
33	<i>X45/46b</i>	0.257	0.070	0.033	0.012	0.227	0.063
34	<i>3-methylpentane</i>	0.105	0.029	0.188	0.037	0.000	0.000
35	<i>1-hexene</i>	0.216	0.059	0.031	0.006	0.183	0.050
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.699	0.190	0.034	0.009	0.731	0.208
37	<i>X37/47b</i>	0.394	0.107	0.219	0.043	0.019	0.006
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.030	0.008	0.006	0.003	0.025	0.006
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.237	0.064	0.256	0.050	0.000	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.033	0.009	0.020	0.004	0.000	0.000
41	<i>benzene</i>	0.735	0.200	0.425	0.082	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	0.529	0.144	0.287	0.057	0.038	0.013
43	<i>2-methylhexane</i>	0.074	0.020	0.061	0.013	0.000	0.000
44	<i>cyclohexene</i>	0.071	0.019	0.008	0.002	0.063	0.019
45	<i>1-heptene</i>	0.174	0.047	0.055	0.011	0.088	0.025
46	<i>2,2,4-trimethylpentane</i>	0.343	0.093	0.183	0.036	0.032	0.006

Table F.10.b: Results of CMB analysis for receptor point HATZEM (Hatzfelder Str., 15.10.03, industrial area, close to DuPont solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		µg/m ³	±	TRAFFIC1		SOLVENTS8	
				µg/m ³	±	µg/m ³	±
47	<i>n</i> -heptane	0.290	0.079	0.126	0.026	0.082	0.025
48	1,4-cyclohexadiene	0.072	0.020	0.003	0.001	0.076	0.019
49	X210/70h	0.220	0.060	0.094	0.019	0.063	0.019
50	X210/70i	0.174	0.047	0.032	0.007	0.139	0.038
51	X210/70j	0.346	0.094	0.026	0.005	0.347	0.101
52	2,3,4-trimethylpentane	0.092	0.025	0.063	0.014	0.000	0.000
53	toluene	3.230	1.013	1.308	0.265	1.103	0.359
54	2-methylheptane	0.332	0.156	0.077	0.015	0.227	0.107
55	3-methylheptane	0.061	0.019	0.029	0.006	0.013	0.006
56	4-methylheptane, 1-methyl-1-cyclohexene	0.154	0.048	0.072	0.016	0.032	0.013
57	X211/212c	0.104	0.030	0.002	0.001	0.113	0.032
58	1-octene	0.594	0.170	0.031	0.007	0.618	0.183
59	X212/81a	14.948	4.280	0.001	0.000	17.058	5.085
60	<i>n</i> -octane	1.733	0.496	0.059	0.012	1.859	0.555
61	ethylbenzene	2.729	0.781	0.258	0.056	2.603	0.775
62	meta- and para-xylene	4.192	1.200	0.448	0.098	3.901	1.160
63	styrene	0.119	0.034	0.043	0.014	0.050	0.013
64	ortho-xylene	0.065	0.019	0.180	0.042	0.000	0.000
65	alpha-pinene	1.009	0.289	0.033	0.014	1.084	0.321
66	<i>n</i> -propylbenzene	0.143	0.041	0.037	0.011	0.088	0.025
67	4-ethyltoluene	0.023	0.007	0.019	0.006	0.000	0.000
68	X67/145c	0.077	0.022	0.029	0.009	0.032	0.006
69	X88/120c	0.032	0.009	0.032	0.011	0.000	0.000
70	1,3,5-trimethylbenzene	0.011	0.003	0.037	0.014	0.000	0.000
71	<i>n</i> -decane	0.024	0.007	0.015	0.007	0.000	0.000
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.049	0.014	0.105	0.040	0.000	0.000
73	X213/86b	0.005	0.005	0.003	0.001	0.000	0.000
74	1,2,3-trimethylbenzene	0.005	0.005	0.012	0.005	0.000	0.000
75	1,2,3,4-tetramethylbenzene	0.004	0.001	0.001	0.000	0.000	0.000
76	acetone	5.443	2.179	0.224	0.137	5.772	2.357
77	methyl acetate	0.491	0.333	0.022	0.008	0.517	0.353
78	ethyl acetate	0.364	0.097	0.014	0.006	0.391	0.107
79	methanol	0.716	0.758	0.006	0.002	0.807	0.857
80	2-butanone	0.230	0.048	0.011	0.004	0.240	0.057
81	isopropyl acetate	0.045	0.021	0.006	0.004	0.038	0.019
82	2-propanol	0.192	0.140	0.024	0.009	0.170	0.126
83	ethanol	1.695	0.899	0.053	0.042	1.827	0.983
84	propyl acetate	0.674	0.646	0.010	0.009	0.750	0.718
85	isobutyl acetate	0.053	0.011	0.004	0.001	0.050	0.013
86	4-methyl-2-pentanone	0.078	0.016	0.004	0.007	0.082	0.019
87	2-butanol	0.111	0.088	0.013	0.007	0.101	0.082
88	1-propanol	0.033	0.012	0.003	0.001	0.032	0.013
89	butyl acetate	4.772	3.914	0.008	0.004	5.432	4.474
90	2-hexanone	0.157	0.049	0.004	0.004	0.170	0.057
91	1-butanol	0.523	0.172	0.007	0.003	0.586	0.195
92	cyclohexanone	0.064	0.061	0.006	0.002	0.063	0.057
	Σ NMVOC	68.189	5.642	8.407	0.642	63.014	3.882

names of unknown compounds are explained in table E.1 in Annex E

Table F.11.a: Results of CMB analysis for receptor point BISSIN (Bissing Str., 03.09.02, industrial areas, close to PPG solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS2	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.494	0.070	0.062	0.020	0.438	0.072
2	<i>propane</i>	0.773	0.122	0.065	0.042	0.719	0.129
3	<i>propadiene</i>	0.002	0.002	0.003	0.003	0.000	0.000
4	<i>propyne</i>	0.011	0.002	0.001	0.003	0.010	0.003
5	<i>X5/13a</i>	0.006	0.002	0.004	0.003	0.003	0.000
6	<i>2-methylpropane</i>	0.331	0.051	0.089	0.028	0.244	0.042
7	<i>1-butene, 2-methylpropene</i>	1.730	0.966	0.239	0.065	1.509	0.851
8	<i>1,3-butadiene</i>	0.059	0.012	0.015	0.004	0.045	0.010
9	<i>n-butane</i>	0.869	0.126	0.135	0.044	0.742	0.125
10	<i>trans-2-butene</i>	0.128	0.035	0.019	0.005	0.110	0.032
11	<i>1-butyne</i>	0.020	0.007	0.003	0.001	0.017	0.005
12	<i>cis-2-butene</i>	0.102	0.028	0.018	0.005	0.085	0.025
13	<i>X12/18d</i>	0.182	0.082	0.018	0.006	0.167	0.077
14	<i>3-methyl-1-butene</i>	0.045	0.016	0.027	0.005	0.017	0.008
15	<i>X18/25a</i>	0.505	0.414	0.024	0.009	0.488	0.403
16	<i>X18/25b</i>	0.251	0.125	0.032	0.009	0.222	0.112
17	<i>X18/25d</i>	2.540	0.699	0.606	0.144	1.942	0.558
18	<i>2-methylbutane</i>	2.691	0.467	0.623	0.185	2.076	0.401
19	<i>X25/19c</i>	0.538	0.765	0.057	0.011	0.488	0.695
20	<i>1-pentene</i>	0.185	0.027	0.111	0.024	0.070	0.012
21	<i>n-pentane, 2-methyl-1-butene</i>	0.878	0.126	0.665	0.142	0.182	0.030
22	<i>2-methyl-1,3-butadiene</i>	0.387	0.074	0.206	0.052	0.174	0.037
23	<i>trans-2-pentene</i>	0.192	0.028	0.118	0.028	0.070	0.012
24	<i>cis-2-pentene</i>	0.286	0.102	0.057	0.013	0.232	0.085
25	<i>X22/43b</i>	0.341	0.067	0.178	0.024	0.157	0.035
26	<i>2,2-dimethylbutane</i>	0.128	0.032	0.100	0.020	0.025	0.008
27	<i>X43/17c</i>	0.187	0.205	0.005	0.001	0.187	0.204
28	<i>cyclopentene</i>	0.065	0.010	0.019	0.005	0.045	0.008
29	<i>X17/123c</i>	0.176	0.039	0.034	0.013	0.144	0.035
30	<i>methyl tert-butyl ether</i>	0.674	0.224	0.197	0.049	0.475	0.164
31	<i>2,3-dimethylbutane, cyclopentane</i>	0.399	0.084	0.301	0.065	0.085	0.020
32	<i>2-methylpentane</i>	0.557	0.084	0.502	0.099	0.030	0.005
33	<i>X45/46b</i>	0.704	0.360	0.049	0.018	0.665	0.344
34	<i>3-methylpentane</i>	0.307	0.055	0.282	0.056	0.010	0.003
35	<i>1-hexene</i>	0.091	0.018	0.047	0.009	0.042	0.010
36	<i>n-hexane, 2-ethyl-1-butene</i>	1.015	0.145	0.051	0.014	0.983	0.162
37	<i>X37/47b</i>	0.408	0.066	0.330	0.065	0.062	0.012
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.003	0.003	0.009	0.004	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.414	0.085	0.384	0.075	0.010	0.003
40	<i>2,3-dimethyl-2-butene</i>	0.041	0.006	0.030	0.006	0.010	0.003
41	<i>benzene</i>	0.672	0.099	0.639	0.123	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	0.615	0.089	0.431	0.086	0.164	0.027
43	<i>2-methylhexane</i>	0.123	0.022	0.092	0.019	0.027	0.005
44	<i>cyclohexene</i>	0.021	0.017	0.011	0.003	0.010	0.008
45	<i>1-heptene</i>	0.151	0.033	0.082	0.016	0.065	0.015
46	<i>2,2,4-trimethylpentane</i>	0.442	0.106	0.276	0.054	0.154	0.040

Table F.11.b: Results of CMB analysis for receptor point BISSIN (Bissing Str., 03.09.02, industrial areas, close to PPG solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		µg/m ³	±	TRAFFIC1		SOLVENTS2	
				µg/m ³	±	µg/m ³	±
47	<i>n</i> -heptane	0.454	0.130	0.190	0.039	0.259	0.077
48	1,4-cyclohexadiene	0.140	0.084	0.005	0.001	0.137	0.085
49	X210/70h	0.316	0.060	0.142	0.029	0.172	0.035
50	X210/70i	0.106	0.026	0.048	0.010	0.057	0.015
51	X210/70j	0.088	0.042	0.039	0.008	0.047	0.022
52	2,3,4-trimethylpentane	0.112	0.021	0.095	0.020	0.012	0.003
53	toluene	2.070	0.344	1.967	0.398	0.000	0.000
54	2-methylheptane	0.199	0.036	0.115	0.023	0.080	0.015
55	3-methylheptane	0.051	0.008	0.043	0.009	0.005	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.198	0.029	0.109	0.024	0.085	0.015
57	X211/212c	0.004	0.001	0.003	0.001	0.000	0.000
58	1-octene	0.185	0.042	0.047	0.010	0.139	0.032
59	X212/81a	0.005	0.005	0.001	0.000	0.005	0.005
60	<i>n</i> -octane	0.444	0.068	0.089	0.018	0.359	0.062
61	ethylbenzene	1.477	0.451	0.388	0.084	1.090	0.346
62	meta- and para-xylene	4.019	1.651	0.674	0.148	3.378	1.416
63	styrene	0.038	0.027	0.065	0.020	0.000	0.000
64	ortho-xylene	0.929	0.456	0.271	0.063	0.657	0.326
65	alpha-pinene	0.026	0.004	0.049	0.020	0.000	0.000
66	<i>n</i> -propylbenzene	0.048	0.033	0.056	0.016	0.000	0.000
67	4-ethyltoluene	0.111	0.064	0.028	0.009	0.082	0.050
68	X67/145c	0.041	0.023	0.043	0.014	0.000	0.000
69	X88/120c	0.041	0.023	0.048	0.016	0.000	0.000
70	1,3,5-trimethylbenzene	0.054	0.024	0.056	0.020	0.000	0.000
71	<i>n</i> -decane	0.042	0.029	0.023	0.010	0.020	0.012
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.171	0.091	0.158	0.061	0.005	0.003
73	X213/86b	0.009	0.003	0.005	0.001	0.005	0.003
74	1,2,3-trimethylbenzene	0.023	0.008	0.018	0.008	0.005	0.003
75	1,2,3,4-tetramethylbenzene	0.001	0.002	0.001	0.000	0.000	0.000
76	acetone	2.969	1.895	0.336	0.206	2.669	1.718
77	methyl acetate	0.424	0.230	0.033	0.011	0.398	0.217
78	ethyl acetate	0.015	0.004	0.020	0.009	0.000	0.000
79	methanol	0.073	0.029	0.009	0.003	0.065	0.025
80	2-butanone	0.209	0.126	0.016	0.006	0.197	0.120
81	isopropyl acetate	0.126	0.144	0.009	0.006	0.120	0.137
82	2-propanol	0.209	0.181	0.037	0.014	0.174	0.152
83	ethanol	0.363	0.089	0.080	0.063	0.284	0.075
84	propyl acetate	0.265	0.327	0.015	0.014	0.254	0.314
85	isobutyl acetate	0.018	0.011	0.006	0.001	0.012	0.008
86	4-methyl-2-pentanone	0.021	0.017	0.006	0.010	0.015	0.012
87	2-butanol	0.046	0.029	0.019	0.010	0.027	0.017
88	1-propanol	0.023	0.006	0.004	0.001	0.020	0.005
89	butyl acetate	0.175	0.233	0.011	0.006	0.167	0.222
90	2-hexanone	0.005	0.002	0.006	0.006	0.000	0.000
91	1-butanol	0.511	0.192	0.010	0.004	0.510	0.197
92	cyclohexanone	0.004	0.004	0.009	0.003	0.000	0.000
	Σ NMVOC	37.593	3.159	12.644	0.837	24.893	1.714

names of unknown compounds are explained in table E.1 in Annex E

Table F.12.a: Results of CMB analysis for receptor point LUTZOW (Lützow Str., 04.09.02, industrial areas, close to PPG solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS8	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.240	0.055	0.083	0.027	0.132	0.022
2	<i>propane</i>	0.513	0.086	0.086	0.056	0.217	0.039
3	<i>propadiene</i>	0.002	0.002	0.003	0.003	0.000	0.000
4	<i>propyne</i>	0.012	0.002	0.002	0.003	0.003	0.001
5	<i>X5/13a</i>	0.002	0.002	0.005	0.003	0.001	0.000
6	<i>2-methylpropane</i>	0.439	0.071	0.118	0.037	0.073	0.013
7	<i>1-butene, 2-methylpropene</i>	0.928	0.201	0.319	0.086	0.454	0.256
8	<i>1,3-butadiene</i>	0.043	0.006	0.020	0.005	0.014	0.003
9	<i>n-butane</i>	0.561	0.126	0.181	0.059	0.223	0.038
10	<i>trans-2-butene</i>	0.078	0.017	0.025	0.007	0.033	0.010
11	<i>1-butyne</i>	0.004	0.005	0.003	0.002	0.005	0.002
12	<i>cis-2-butene</i>	0.060	0.014	0.024	0.007	0.026	0.008
13	<i>X12/18d</i>	0.125	0.026	0.024	0.008	0.050	0.023
14	<i>3-methyl-1-butene</i>	0.045	0.012	0.035	0.007	0.005	0.002
15	<i>X18/25a</i>	0.572	0.198	0.032	0.012	0.147	0.121
16	<i>X18/25b</i>	0.394	0.110	0.042	0.012	0.067	0.034
17	<i>X18/25d</i>	0.822	0.135	0.808	0.192	0.585	0.168
18	<i>2-methylbutane</i>	2.269	0.677	0.832	0.246	0.625	0.121
19	<i>X25/19c</i>	0.149	0.023	0.076	0.015	0.147	0.209
20	<i>1-pentene</i>	0.145	0.053	0.148	0.032	0.021	0.004
21	<i>n-pentane, 2-methyl-1-butene</i>	1.343	0.265	0.887	0.189	0.055	0.009
22	<i>2-methyl-1,3-butadiene</i>	0.727	0.140	0.275	0.069	0.053	0.011
23	<i>trans-2-pentene</i>	0.169	0.040	0.157	0.037	0.021	0.004
24	<i>cis-2-pentene</i>	0.175	0.030	0.076	0.017	0.070	0.026
25	<i>X22/43b</i>	0.252	0.062	0.238	0.032	0.047	0.011
26	<i>2,2-dimethylbutane</i>	0.144	0.022	0.133	0.027	0.008	0.002
27	<i>X43/17c</i>	0.229	0.085	0.007	0.002	0.056	0.061
28	<i>cyclopentene</i>	0.041	0.007	0.025	0.007	0.014	0.002
29	<i>X17/123c</i>	0.311	0.095	0.046	0.017	0.044	0.011
30	<i>methyl tert-butyl ether</i>	0.712	0.114	0.263	0.066	0.143	0.050
31	<i>2,3-dimethylbutane, cyclopentane</i>	0.289	0.047	0.401	0.086	0.026	0.006
32	<i>2-methylpentane</i>	0.706	0.109	0.670	0.132	0.009	0.002
33	<i>X45/46b</i>	0.709	0.203	0.066	0.024	0.200	0.103
34	<i>3-methylpentane</i>	0.407	0.061	0.376	0.074	0.003	0.001
35	<i>1-hexene</i>	0.084	0.013	0.062	0.012	0.013	0.003
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.151	0.027	0.068	0.019	0.296	0.049
37	<i>X37/47b</i>	0.558	0.085	0.440	0.086	0.019	0.004
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.002	0.003	0.012	0.005	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.505	0.074	0.513	0.100	0.003	0.001
40	<i>2,3-dimethyl-2-butene</i>	0.052	0.010	0.041	0.008	0.003	0.001
41	<i>benzene</i>	0.923	0.132	0.852	0.164	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	0.744	0.108	0.575	0.115	0.050	0.008
43	<i>2-methylhexane</i>	0.121	0.022	0.123	0.025	0.008	0.002
44	<i>cyclohexene</i>	0.061	0.012	0.015	0.003	0.003	0.002
45	<i>1-heptene</i>	0.127	0.027	0.110	0.022	0.020	0.005
46	<i>2,2,4-trimethylpentane</i>	0.394	0.060	0.368	0.073	0.047	0.012

Table F.12.b: Results of CMB analysis for receptor point LUTZOW (Lützow Str., 04.09.02, industrial areas, close to PPG solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		µg/m ³	±	TRAFFIC1		SOLVENTS8	
				µg/m ³	±	µg/m ³	±
47	<i>n</i> -heptane	0.514	0.092	0.253	0.052	0.078	0.023
48	1,4-cyclohexadiene	0.030	0.006	0.007	0.002	0.041	0.026
49	X210/70h	0.209	0.030	0.189	0.039	0.052	0.011
50	X210/70i	0.058	0.009	0.064	0.014	0.017	0.005
51	X210/70j	0.039	0.007	0.052	0.010	0.014	0.007
52	2,3,4-trimethylpentane	0.108	0.023	0.127	0.027	0.004	0.001
53	toluene	2.747	0.480	2.625	0.531	0.000	0.000
54	2-methylheptane	0.201	0.031	0.154	0.030	0.024	0.005
55	3-methylheptane	0.048	0.007	0.057	0.012	0.002	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.139	0.021	0.145	0.032	0.026	0.005
57	X211/212c	0.026	0.029	0.003	0.002	0.000	0.000
58	1-octene	0.160	0.053	0.062	0.014	0.042	0.010
59	X212/81a	0.005	0.005	0.002	0.000	0.002	0.002
60	<i>n</i> -octane	0.444	0.072	0.118	0.024	0.108	0.019
61	ethylbenzene	0.808	0.292	0.518	0.111	0.328	0.104
62	meta- and para-xylene	1.719	0.524	0.899	0.197	1.017	0.426
63	styrene	0.094	0.068	0.086	0.027	0.000	0.000
64	ortho-xylene	0.968	0.341	0.361	0.084	0.198	0.098
65	alpha-pinene	0.066	0.014	0.066	0.027	0.000	0.000
66	<i>n</i> -propylbenzene	0.105	0.054	0.074	0.022	0.000	0.000
67	4-ethyltoluene	0.123	0.059	0.037	0.012	0.025	0.015
68	X67/145c	0.069	0.059	0.057	0.019	0.000	0.000
69	X88/120c	0.067	0.039	0.064	0.022	0.000	0.000
70	1,3,5-trimethylbenzene	0.161	0.119	0.074	0.027	0.000	0.000
71	<i>n</i> -decane	0.094	0.062	0.030	0.014	0.006	0.004
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.198	0.122	0.211	0.081	0.002	0.001
73	X213/86b	0.039	0.019	0.007	0.002	0.002	0.001
74	1,2,3-trimethylbenzene	0.018	0.009	0.024	0.010	0.002	0.001
75	1,2,3,4-tetramethylbenzene	0.006	0.006	0.002	0.000	0.000	0.000
76	acetone	0.848	0.794	0.449	0.275	0.803	0.517
77	methyl acetate	0.153	0.032	0.044	0.015	0.120	0.065
78	ethyl acetate	0.007	0.004	0.027	0.012	0.000	0.000
79	methanol	0.044	0.010	0.012	0.003	0.020	0.008
80	2-butanone	0.025	0.012	0.022	0.008	0.059	0.036
81	isopropyl acetate	0.083	0.017	0.012	0.008	0.036	0.041
82	2-propanol	0.050	0.011	0.049	0.019	0.053	0.046
83	ethanol	0.285	0.180	0.106	0.084	0.085	0.023
84	propyl acetate	0.033	0.008	0.020	0.019	0.076	0.094
85	isobutyl acetate	0.013	0.003	0.008	0.002	0.004	0.002
86	4-methyl-2-pentanone	0.012	0.004	0.008	0.014	0.005	0.004
87	2-butanol	0.009	0.006	0.025	0.014	0.008	0.005
88	1-propanol	0.011	0.008	0.005	0.002	0.006	0.002
89	butyl acetate	0.019	0.007	0.015	0.008	0.050	0.067
90	2-hexanone	0.006	0.006	0.008	0.008	0.000	0.000
91	1-butanol	0.083	0.018	0.014	0.005	0.154	0.059
92	cyclohexanone	0.004	0.001	0.012	0.003	0.000	0.000
	Σ NMVOC	28.281	1.511	16.867	0.897	7.493	0.854

names of unknown compounds are explained in table E.1 in Annex E

Table F.13.a: Results of CMB analysis for receptor point BISSIM (Bissing Str., 13.10.03, industrial areas, close to PPG solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS2	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.827	0.571	0.030	0.010	0.193	0.032
2	<i>propane</i>	1.668	0.776	0.031	0.020	0.316	0.057
3	<i>propadiene</i>	0.013	0.009	0.001	0.001	0.000	0.000
4	<i>propyne</i>	0.014	0.008	0.001	0.001	0.004	0.001
5	<i>X5/13a</i>	0.006	0.003	0.002	0.001	0.001	0.000
6	<i>2-methylpropane</i>	0.563	0.323	0.043	0.014	0.107	0.019
7	<i>1-butene, 2-methylpropene</i>	2.623	0.954	0.116	0.031	0.664	0.375
8	<i>1,3-butadiene</i>	0.081	0.023	0.007	0.002	0.020	0.004
9	<i>n-butane</i>	0.884	0.406	0.066	0.022	0.326	0.055
10	<i>trans-2-butene</i>	0.133	0.043	0.009	0.003	0.048	0.014
11	<i>1-butyne</i>	0.016	0.009	0.001	0.001	0.008	0.002
12	<i>cis-2-butene</i>	0.097	0.037	0.009	0.003	0.037	0.011
13	<i>X12/18d</i>	0.284	0.077	0.009	0.003	0.073	0.034
14	<i>3-methyl-1-butene</i>	0.115	0.032	0.013	0.003	0.008	0.003
15	<i>X18/25a</i>	0.203	0.113	0.012	0.004	0.215	0.177
16	<i>X18/25b</i>	0.207	0.068	0.015	0.004	0.097	0.049
17	<i>X18/25d</i>	3.197	1.057	0.294	0.070	0.854	0.245
18	<i>2-methylbutane</i>	1.543	0.454	0.302	0.090	0.913	0.176
19	<i>X25/19c</i>	0.135	0.045	0.028	0.006	0.215	0.306
20	<i>1-pentene</i>	0.166	0.066	0.054	0.012	0.031	0.006
21	<i>n-pentane, 2-methyl-1-butene</i>	0.465	0.264	0.323	0.069	0.080	0.013
22	<i>2-methyl-1,3-butadiene</i>	0.132	0.053	0.100	0.025	0.077	0.016
23	<i>trans-2-pentene</i>	0.104	0.055	0.057	0.014	0.031	0.006
24	<i>cis-2-pentene</i>	0.067	0.031	0.028	0.006	0.102	0.037
25	<i>X22/43b</i>	0.206	0.090	0.087	0.012	0.069	0.015
26	<i>2,2-dimethylbutane</i>	0.032	0.015	0.049	0.010	0.011	0.003
27	<i>X43/17c</i>	0.006	0.002	0.003	0.001	0.082	0.090
28	<i>cyclopentene</i>	0.078	0.031	0.009	0.003	0.020	0.003
29	<i>X17/123c</i>	0.014	0.017	0.017	0.006	0.064	0.015
30	<i>methyl tert-butyl ether</i>	0.398	0.325	0.096	0.024	0.209	0.072
31	<i>2,3-dimethylbutane, cyclopentane</i>	0.353	0.097	0.146	0.031	0.037	0.009
32	<i>2-methylpentane</i>	0.533	0.146	0.244	0.048	0.013	0.002
33	<i>X45/46b</i>	0.204	0.067	0.024	0.009	0.292	0.151
34	<i>3-methylpentane</i>	0.365	0.106	0.137	0.027	0.004	0.001
35	<i>1-hexene</i>	0.118	0.035	0.023	0.004	0.019	0.004
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.463	0.207	0.025	0.007	0.433	0.071
37	<i>X37/47b</i>	0.429	0.124	0.160	0.031	0.027	0.006
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.146	0.076	0.004	0.002	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.222	0.083	0.187	0.036	0.004	0.001
40	<i>2,3-dimethyl-2-butene</i>	0.028	0.008	0.015	0.003	0.004	0.001
41	<i>benzene</i>	0.612	0.184	0.310	0.060	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	0.341	0.100	0.209	0.042	0.072	0.012
43	<i>2-methylhexane</i>	0.076	0.022	0.045	0.009	0.012	0.002
44	<i>cyclohexene</i>	0.033	0.010	0.006	0.001	0.004	0.003
45	<i>1-heptene</i>	0.175	0.054	0.040	0.008	0.029	0.007
46	<i>2,2,4-trimethylpentane</i>	0.225	0.061	0.134	0.026	0.068	0.018

Table F.13.b: Results of CMB analysis for receptor point BISSIM (Bissing Str., 13.10.03, industrial areas, close to PPG solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS2	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	0.198	0.054	0.092	0.019	0.114	0.034
48	1,4-cyclohexadiene	0.018	0.015	0.003	0.001	0.060	0.037
49	X210/70h	0.148	0.040	0.069	0.014	0.076	0.015
50	X210/70i	0.113	0.107	0.023	0.005	0.025	0.007
51	X210/70j	0.054	0.030	0.019	0.004	0.021	0.010
52	2,3,4-trimethylpentane	0.049	0.013	0.046	0.010	0.006	0.001
53	toluene	2.296	0.759	0.955	0.193	0.000	0.000
54	2-methylheptane	0.222	0.106	0.056	0.011	0.035	0.007
55	3-methylheptane	0.044	0.015	0.021	0.004	0.002	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.140	0.044	0.053	0.012	0.037	0.007
57	X211/212c	0.004	0.001	0.001	0.001	0.000	0.000
58	1-octene	1.039	0.366	0.023	0.005	0.061	0.014
59	X212/81a	0.068	0.019	0.001	0.000	0.002	0.002
60	<i>n</i> -octane	1.000	0.304	0.043	0.009	0.158	0.027
61	ethylbenzene	0.421	0.168	0.188	0.041	0.480	0.152
62	meta- and para-xylene	0.494	0.202	0.327	0.072	1.486	0.623
63	styrene	0.002	0.003	0.031	0.010	0.000	0.000
64	ortho-xylene	0.108	0.077	0.131	0.031	0.289	0.143
65	alpha-pinene	0.458	0.210	0.024	0.010	0.000	0.000
66	<i>n</i> -propylbenzene	0.017	0.009	0.027	0.008	0.000	0.000
67	4-ethyltoluene	0.006	0.002	0.014	0.004	0.036	0.022
68	X67/145c	0.017	0.009	0.021	0.007	0.000	0.000
69	X88/120c	0.001	0.002	0.023	0.008	0.000	0.000
70	1,3,5-trimethylbenzene	0.006	0.009	0.027	0.010	0.000	0.000
71	<i>n</i> -decane	0.020	0.011	0.011	0.005	0.009	0.006
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.026	0.009	0.077	0.029	0.002	0.001
73	X213/86b	0.003	0.004	0.003	0.001	0.002	0.001
74	1,2,3-trimethylbenzene	0.005	0.003	0.009	0.004	0.002	0.001
75	1,2,3,4-tetramethylbenzene	0.007	0.009	0.001	0.000	0.000	0.000
76	acetone	3.834	0.792	0.163	0.100	1.174	0.756
77	methyl acetate	0.514	0.155	0.016	0.006	0.175	0.095
78	ethyl acetate	0.470	0.570	0.010	0.004	0.000	0.000
79	methanol	1.096	0.253	0.004	0.001	0.029	0.011
80	2-butanone	0.156	0.034	0.008	0.003	0.087	0.053
81	isopropyl acetate	0.070	0.023	0.004	0.003	0.053	0.060
82	2-propanol	0.048	0.064	0.018	0.007	0.077	0.067
83	ethanol	0.867	0.522	0.039	0.031	0.125	0.033
84	propyl acetate	0.041	0.018	0.007	0.007	0.112	0.138
85	isobutyl acetate	0.012	0.010	0.003	0.001	0.006	0.003
86	4-methyl-2-pentanone	0.017	0.019	0.003	0.005	0.007	0.006
87	2-butanol	0.020	0.013	0.009	0.005	0.012	0.008
88	1-propanol	0.013	0.010	0.002	0.001	0.009	0.002
89	butyl acetate	0.026	0.022	0.006	0.003	0.073	0.097
90	2-hexanone	0.009	0.003	0.003	0.003	0.000	0.000
91	1-butanol	0.053	0.024	0.005	0.002	0.225	0.087
92	cyclohexanone	0.052	0.018	0.004	0.001	0.000	0.000
	Σ NMVOC	32.873	2.470	6.134	0.646	10.949	1.333

names of unknown compounds are explained in table E.1 in Annex E

Table F.14.a: Results of CMB analysis for receptor point YOREK (Yorck Str., 13.10.03, industrial areas, close to PPG solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS2	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.427	0.116	0.027	0.009	0.143	0.024
2	<i>propane</i>	0.825	0.224	0.028	0.018	0.235	0.042
3	<i>propadiene</i>	0.002	0.002	0.001	0.001	0.000	0.000
4	<i>propyne</i>	0.002	0.002	0.001	0.001	0.003	0.001
5	<i>X5/13a</i>	0.002	0.002	0.002	0.001	0.001	0.000
6	<i>2-methylpropane</i>	0.420	0.114	0.038	0.012	0.080	0.014
7	<i>1-butene, 2-methylpropene</i>	2.338	0.636	0.102	0.028	0.492	0.278
8	<i>1,3-butadiene</i>	0.066	0.018	0.007	0.002	0.015	0.003
9	<i>n-butane</i>	1.285	0.349	0.058	0.019	0.242	0.041
10	<i>trans-2-butene</i>	0.096	0.026	0.008	0.002	0.036	0.011
11	<i>1-butyne</i>	0.022	0.006	0.001	0.001	0.006	0.002
12	<i>cis-2-butene</i>	0.085	0.023	0.008	0.002	0.028	0.008
13	<i>X12/18d</i>	0.125	0.034	0.008	0.003	0.054	0.025
14	<i>3-methyl-1-butene</i>	0.086	0.023	0.011	0.002	0.006	0.002
15	<i>X18/25a</i>	0.093	0.025	0.010	0.004	0.159	0.132
16	<i>X18/25b</i>	0.190	0.052	0.014	0.004	0.072	0.037
17	<i>X18/25d</i>	0.003	0.003	0.259	0.062	0.634	0.182
18	<i>2-methylbutane</i>	1.736	0.472	0.267	0.079	0.678	0.131
19	<i>X25/19c</i>	0.085	0.023	0.024	0.005	0.159	0.227
20	<i>1-pentene</i>	0.090	0.025	0.048	0.010	0.023	0.004
21	<i>n-pentane, 2-methyl-1-butene</i>	0.273	0.074	0.285	0.061	0.059	0.010
22	<i>2-methyl-1,3-butadiene</i>	0.122	0.033	0.088	0.022	0.057	0.012
23	<i>trans-2-pentene</i>	0.036	0.010	0.050	0.012	0.023	0.004
24	<i>cis-2-pentene</i>	0.022	0.006	0.024	0.005	0.076	0.028
25	<i>X22/43b</i>	0.107	0.029	0.076	0.010	0.051	0.011
26	<i>2,2-dimethylbutane</i>	0.031	0.008	0.043	0.009	0.008	0.002
27	<i>X43/17c</i>	0.003	0.003	0.002	0.001	0.061	0.067
28	<i>cyclopentene</i>	0.040	0.011	0.008	0.002	0.015	0.002
29	<i>X17/123c</i>	0.156	0.042	0.015	0.005	0.047	0.011
30	<i>methyl tert-butyl ether</i>	0.203	0.055	0.085	0.021	0.155	0.054
31	<i>2,3-dimethylbutane, cyclopentane</i>	0.211	0.058	0.129	0.028	0.028	0.007
32	<i>2-methylpentane</i>	0.443	0.120	0.215	0.042	0.010	0.002
33	<i>X45/46b</i>	0.127	0.034	0.021	0.008	0.217	0.112
34	<i>3-methylpentane</i>	0.292	0.079	0.121	0.024	0.003	0.001
35	<i>1-hexene</i>	0.067	0.018	0.020	0.004	0.014	0.003
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.803	0.218	0.022	0.006	0.321	0.053
37	<i>X37/47b</i>	0.392	0.107	0.141	0.028	0.020	0.004
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.013	0.004	0.004	0.002	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.186	0.051	0.165	0.032	0.003	0.001
40	<i>2,3-dimethyl-2-butene</i>	0.025	0.007	0.013	0.003	0.003	0.001
41	<i>benzene</i>	0.510	0.139	0.274	0.053	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	0.289	0.079	0.185	0.037	0.054	0.009
43	<i>2-methylhexane</i>	0.063	0.017	0.040	0.008	0.009	0.002
44	<i>cyclohexene</i>	0.025	0.007	0.005	0.001	0.003	0.002
45	<i>1-heptene</i>	0.076	0.021	0.035	0.007	0.021	0.005
46	<i>2,2,4-trimethylpentane</i>	0.185	0.050	0.118	0.023	0.050	0.013

Table F.14.b: Results of CMB analysis for receptor point YOREK (Yorck Str., 13.10.03, industrial areas, close to PPG solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS2	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	0.200	0.054	0.081	0.017	0.085	0.025
48	1,4-cyclohexadiene	0.015	0.004	0.002	0.001	0.045	0.028
49	X210/70h	0.103	0.028	0.061	0.013	0.056	0.011
50	X210/70i	0.041	0.011	0.021	0.004	0.019	0.005
51	X210/70j	0.083	0.022	0.017	0.003	0.015	0.007
52	2,3,4-trimethylpentane	0.033	0.009	0.041	0.009	0.004	0.001
53	toluene	2.328	0.730	0.843	0.171	0.000	0.000
54	2-methylheptane	0.190	0.089	0.049	0.010	0.026	0.005
55	3-methylheptane	0.041	0.013	0.018	0.004	0.002	0.000
56	4-methylheptane, 1-methyl-1-cyclohexene	0.072	0.023	0.047	0.010	0.028	0.005
57	X211/212c	0.036	0.010	0.001	0.001	0.000	0.000
58	1-octene	0.358	0.103	0.020	0.004	0.046	0.011
59	X212/81a	0.029	0.008	0.001	0.000	0.002	0.002
60	<i>n</i> -octane	0.398	0.114	0.038	0.008	0.117	0.020
61	ethylbenzene	0.466	0.133	0.166	0.036	0.356	0.113
62	meta- and para-xylene	0.544	0.156	0.289	0.063	1.103	0.462
63	styrene	0.012	0.004	0.028	0.009	0.000	0.000
64	ortho-xylene	0.050	0.014	0.116	0.027	0.215	0.106
65	alpha-pinene	0.234	0.067	0.021	0.009	0.000	0.000
66	<i>n</i> -propylbenzene	0.052	0.015	0.024	0.007	0.000	0.000
67	4-ethyltoluene	0.005	0.002	0.012	0.004	0.027	0.016
68	X67/145c	0.012	0.003	0.018	0.006	0.000	0.000
69	X88/120c	0.005	0.005	0.021	0.007	0.000	0.000
70	1,3,5-trimethylbenzene	0.021	0.006	0.024	0.009	0.000	0.000
71	<i>n</i> -decane	0.023	0.007	0.010	0.004	0.007	0.004
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.017	0.005	0.068	0.026	0.002	0.001
73	X213/86b	0.002	0.005	0.002	0.001	0.002	0.001
74	1,2,3-trimethylbenzene	0.003	0.005	0.008	0.003	0.002	0.001
75	1,2,3,4-tetramethylbenzene	0.003	0.006	0.001	0.000	0.000	0.000
76	acetone	3.396	1.405	0.144	0.088	0.871	0.561
77	methyl acetate	0.171	0.045	0.014	0.005	0.130	0.071
78	ethyl acetate	1.388	0.290	0.009	0.004	0.000	0.000
79	methanol	0.520	0.425	0.004	0.001	0.021	0.008
80	2-butanone	0.266	0.085	0.007	0.003	0.064	0.039
81	isopropyl acetate	0.050	0.029	0.004	0.003	0.039	0.045
82	2-propanol	0.098	0.033	0.016	0.006	0.057	0.050
83	ethanol	0.286	0.064	0.034	0.027	0.093	0.024
84	propyl acetate	0.105	0.041	0.007	0.006	0.083	0.102
85	isobutyl acetate	0.021	0.005	0.003	0.001	0.004	0.002
86	4-methyl-2-pentanone	0.005	0.003	0.003	0.004	0.005	0.004
87	2-butanol	0.065	0.019	0.008	0.004	0.009	0.006
88	1-propanol	0.015	0.009	0.002	0.001	0.007	0.002
89	butyl acetate	0.033	0.018	0.005	0.003	0.054	0.072
90	2-hexanone	0.026	0.013	0.003	0.003	0.000	0.000
91	1-butanol	0.041	0.030	0.004	0.002	0.167	0.064
92	cyclohexanone	0.077	0.023	0.004	0.001	0.000	0.000
	Σ NMVOC	24.609	1.959	5.416	0.487	8.125	0.912

names of unknown compounds are explained in table E.1 in Annex E

Table F.15.a: Results of CMB analysis for receptor point SIMONS (Simon Str., 03.09.02, industrial area, close to Gorn workshop)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS3	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.282	0.073	0.052	0.017	0.232	0.066
2	<i>propane</i>	0.781	0.136	0.054	0.035	0.741	0.151
3	<i>propadiene</i>	0.002	0.003	0.002	0.002	0.000	0.000
4	<i>propyne</i>	0.009	0.001	0.001	0.002	0.009	0.002
5	<i>X5/13a</i>	0.002	0.002	0.003	0.002	0.000	0.000
6	<i>2-methylpropane</i>	0.327	0.058	0.075	0.024	0.255	0.053
7	<i>1-butene, 2-methylpropene</i>	0.863	0.259	0.202	0.054	0.668	0.213
8	<i>1,3-butadiene</i>	0.032	0.011	0.013	0.003	0.020	0.007
9	<i>n-butane</i>	0.701	0.108	0.114	0.037	0.595	0.112
10	<i>trans-2-butene</i>	0.077	0.022	0.016	0.004	0.062	0.020
11	<i>1-butyne</i>	0.011	0.003	0.002	0.001	0.009	0.002
12	<i>cis-2-butene</i>	0.065	0.016	0.015	0.004	0.051	0.014
13	<i>X12/18d</i>	0.031	0.044	0.015	0.005	0.016	0.023
14	<i>3-methyl-1-butene</i>	0.059	0.009	0.022	0.004	0.037	0.007
15	<i>X18/25a</i>	0.142	0.133	0.020	0.008	0.122	0.117
16	<i>X18/25b</i>	0.215	0.098	0.027	0.008	0.191	0.089
17	<i>X18/25d</i>	1.777	0.257	0.511	0.122	1.272	0.227
18	<i>2-methylbutane</i>	1.128	0.353	0.526	0.156	0.592	0.195
19	<i>X25/19c</i>	0.159	0.024	0.048	0.010	0.112	0.020
20	<i>1-pentene</i>	0.122	0.022	0.094	0.020	0.025	0.005
21	<i>n-pentane, 2-methyl-1-butene</i>	0.801	0.143	0.561	0.119	0.220	0.046
22	<i>2-methyl-1,3-butadiene</i>	1.363	0.255	0.174	0.044	1.208	0.259
23	<i>trans-2-pentene</i>	0.129	0.026	0.099	0.024	0.025	0.005
24	<i>cis-2-pentene</i>	0.077	0.014	0.048	0.011	0.027	0.005
25	<i>X22/43b</i>	0.182	0.037	0.150	0.020	0.027	0.005
26	<i>2,2-dimethylbutane</i>	0.112	0.016	0.084	0.017	0.025	0.005
27	<i>X43/17c</i>	0.093	0.044	0.004	0.001	0.092	0.044
28	<i>cyclopentene</i>	0.050	0.007	0.016	0.004	0.034	0.005
29	<i>X17/123c</i>	0.018	0.015	0.029	0.011	0.000	0.000
30	<i>methyl tert-butyl ether</i>	0.239	0.180	0.166	0.042	0.066	0.050
31	<i>2,3-dimethylbutane, cyclopentane</i>	0.283	0.132	0.254	0.054	0.018	0.009
32	<i>2-methylpentane</i>	0.441	0.065	0.423	0.083	0.000	0.000
33	<i>X45/46b</i>	0.238	0.060	0.042	0.015	0.198	0.053
34	<i>3-methylpentane</i>	0.249	0.036	0.238	0.047	0.000	0.000
35	<i>1-hexene</i>	0.080	0.013	0.040	0.008	0.039	0.007
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.264	0.040	0.043	0.012	0.225	0.041
37	<i>X37/47b</i>	0.277	0.040	0.278	0.054	0.000	0.000
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.004	0.005	0.008	0.003	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	0.341	0.053	0.324	0.063	0.002	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.033	0.006	0.026	0.005	0.005	0.002
41	<i>benzene</i>	0.563	0.089	0.538	0.103	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	0.636	0.117	0.364	0.073	0.262	0.055
43	<i>2-methylhexane</i>	0.123	0.018	0.078	0.016	0.043	0.007
44	<i>cyclohexene</i>	0.014	0.010	0.010	0.002	0.004	0.004
45	<i>1-heptene</i>	0.160	0.024	0.069	0.014	0.089	0.016
46	<i>2,2,4-trimethylpentane</i>	0.263	0.054	0.232	0.046	0.021	0.005

Table F.15.b: Results of CMB analysis for receptor point SIMONS (Simon Str., 03.09.02, industrial area, close to Gorn workshop)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS3	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	0.543	0.116	0.160	0.033	0.385	0.092
48	1,4-cyclohexadiene	0.009	0.002	0.004	0.001	0.004	0.000
49	X210/70h	0.284	0.056	0.119	0.025	0.163	0.035
50	X210/70i	0.045	0.016	0.041	0.009	0.004	0.002
51	X210/70j	0.048	0.010	0.033	0.006	0.014	0.004
52	2,3,4-trimethylpentane	0.051	0.010	0.080	0.017	0.000	0.000
53	toluene	1.609	0.250	1.659	0.336	0.000	0.000
54	2-methylheptane	0.130	0.028	0.097	0.019	0.030	0.007
55	3-methylheptane	0.043	0.006	0.036	0.008	0.005	0.002
56	4-methylheptane, 1-methyl-1-cyclohexene	0.105	0.015	0.092	0.020	0.009	0.002
57	X211/212c	0.002	0.002	0.002	0.001	0.000	0.000
58	1-octene	0.210	0.045	0.040	0.009	0.172	0.041
59	X212/81a	0.005	0.005	0.001	0.000	0.004	0.004
60	<i>n</i> -octane	0.191	0.036	0.075	0.015	0.115	0.025
61	ethylbenzene	1.097	0.175	0.327	0.070	0.773	0.147
62	meta- and para-xylene	2.730	0.437	0.568	0.125	2.186	0.420
63	styrene	0.158	0.054	0.054	0.017	0.103	0.037
64	ortho-xylene	0.897	0.162	0.228	0.053	0.673	0.140
65	alpha-pinene	0.069	0.028	0.042	0.017	0.025	0.011
66	<i>n</i> -propylbenzene	0.191	0.056	0.047	0.014	0.145	0.044
67	4-ethyltoluene	0.254	0.046	0.024	0.008	0.236	0.050
68	X67/145c	0.153	0.052	0.036	0.012	0.117	0.043
69	X88/120c	0.148	0.068	0.041	0.014	0.110	0.051
70	1,3,5-trimethylbenzene	0.238	0.113	0.047	0.017	0.193	0.094
71	<i>n</i> -decane	0.129	0.071	0.019	0.009	0.112	0.062
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.553	0.324	0.133	0.051	0.424	0.252
73	X213/86b	0.069	0.018	0.004	0.001	0.066	0.018
74	1,2,3-trimethylbenzene	0.054	0.041	0.015	0.006	0.039	0.030
75	1,2,3,4-tetramethylbenzene	0.006	0.006	0.001	0.000	0.005	0.005
76	acetone	3.172	2.797	0.284	0.174	2.945	2.615
77	methyl acetate	0.152	0.047	0.028	0.010	0.126	0.041
78	ethyl acetate	0.016	0.006	0.017	0.008	0.000	0.000
79	methanol	0.055	0.072	0.008	0.002	0.048	0.064
80	2-butanone	0.061	0.026	0.014	0.005	0.048	0.021
81	isopropyl acetate	0.029	0.018	0.008	0.005	0.021	0.012
82	2-propanol	0.120	0.026	0.031	0.012	0.089	0.021
83	ethanol	0.575	0.119	0.067	0.053	0.517	0.121
84	propyl acetate	0.050	0.038	0.013	0.012	0.037	0.028
85	isobutyl acetate	0.009	0.002	0.005	0.001	0.004	0.002
86	4-methyl-2-pentanone	0.004	0.001	0.005	0.009	0.000	0.000
87	2-butanol	0.013	0.006	0.016	0.009	0.000	0.000
88	1-propanol	0.017	0.004	0.003	0.001	0.014	0.004
89	butyl acetate	0.034	0.018	0.010	0.005	0.025	0.012
90	2-hexanone	0.010	0.009	0.005	0.005	0.004	0.004
91	1-butanol	0.095	0.069	0.009	0.003	0.087	0.064
92	cyclohexanone	0.009	0.007	0.008	0.002	0.002	0.000
	Σ NMVOC	28.252	2.973	10.662	0.662	17.718	1.112

names of unknown compounds are explained in table E.1 in Annex E

Table F.16.a: Results of CMB analysis for receptor point SIMONB (Simon Str., 17.10.03, industrial area, close to Gorn workshop)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS8	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.839	0.236	0.193	0.063	0.602	0.171
2	<i>propane</i>	0.496	0.179	0.201	0.130	0.443	0.126
3	<i>propadiene</i>	0.019	0.010	0.008	0.008	0.000	0.000
4	<i>propyne</i>	0.001	0.002	0.004	0.008	0.000	0.000
5	<i>X5/13a</i>	0.002	0.003	0.012	0.008	0.000	0.000
6	<i>2-methylpropane</i>	0.957	0.266	0.276	0.087	0.151	0.042
7	<i>1-butene, 2-methylpropene</i>	1.393	0.569	0.744	0.201	1.490	0.423
8	<i>1,3-butadiene</i>	0.071	0.021	0.047	0.012	0.031	0.008
9	<i>n-butane</i>	1.299	0.375	0.421	0.138	0.247	0.070
10	<i>trans-2-butene</i>	0.100	0.027	0.059	0.016	0.034	0.008
11	<i>1-butyne</i>	0.012	0.004	0.008	0.004	0.006	0.003
12	<i>cis-2-butene</i>	0.117	0.033	0.055	0.016	0.025	0.008
13	<i>X12/18d</i>	0.210	0.065	0.055	0.020	0.067	0.020
14	<i>3-methyl-1-butene</i>	0.169	0.046	0.083	0.016	0.017	0.006
15	<i>X18/25a</i>	0.092	0.052	0.075	0.028	0.022	0.006
16	<i>X18/25b</i>	0.173	0.051	0.098	0.028	0.064	0.017
17	<i>X18/25d</i>	1.471	0.404	1.886	0.449	2.151	0.611
18	<i>2-methylbutane</i>	3.259	0.893	1.941	0.575	0.476	0.134
19	<i>X25/19c</i>	0.087	0.126	0.177	0.035	0.241	0.070
20	<i>1-pentene</i>	0.377	0.105	0.346	0.075	0.045	0.014
21	<i>n-pentane, 2-methyl-1-butene</i>	1.625	0.643	2.071	0.441	0.000	0.000
22	<i>2-methyl-1,3-butadiene</i>	0.166	0.079	0.642	0.161	0.000	0.000
23	<i>trans-2-pentene</i>	0.086	0.120	0.366	0.087	0.000	0.000
24	<i>cis-2-pentene</i>	0.874	0.268	0.177	0.039	0.137	0.039
25	<i>X22/43b</i>	0.352	0.103	0.555	0.075	0.000	0.000
26	<i>2,2-dimethylbutane</i>	0.353	0.184	0.311	0.063	0.000	0.000
27	<i>X43/17c</i>	0.035	0.026	0.016	0.004	0.000	0.000
28	<i>cyclopentene</i>	0.063	0.019	0.059	0.016	0.003	0.000
29	<i>X17/123c</i>	0.166	0.046	0.106	0.039	0.042	0.011
30	<i>methyl tert-butyl ether</i>	0.760	0.491	0.614	0.154	0.196	0.056
31	<i>2,3-dimethylbutane, cyclopentane</i>	1.603	0.567	0.937	0.201	0.118	0.034
32	<i>2-methylpentane</i>	2.791	0.933	1.563	0.307	0.092	0.025
33	<i>X45/46b</i>	0.290	0.112	0.154	0.055	0.101	0.028
34	<i>3-methylpentane</i>	1.533	0.548	0.878	0.173	0.000	0.000
35	<i>1-hexene</i>	0.264	0.097	0.146	0.028	0.081	0.022
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.748	0.239	0.158	0.043	0.325	0.092
37	<i>X37/47b</i>	1.789	0.529	1.028	0.201	0.008	0.003
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.017	0.007	0.028	0.012	0.011	0.003
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	1.659	0.663	1.197	0.232	0.000	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.107	0.042	0.095	0.020	0.000	0.000
41	<i>benzene</i>	3.038	0.865	1.988	0.382	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	3.217	0.912	1.342	0.268	0.017	0.006
43	<i>2-methylhexane</i>	0.671	0.183	0.287	0.059	0.000	0.000
44	<i>cyclohexene</i>	0.046	0.023	0.035	0.008	0.028	0.008
45	<i>1-heptene</i>	0.624	0.176	0.256	0.051	0.039	0.011
46	<i>2,2,4-trimethylpentane</i>	1.603	0.447	0.858	0.169	0.014	0.003

Table F.16.b: Results of CMB analysis for receptor point SIMONB (Simon Str., 17.10.03, industrial area, close to Gorn workshop)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS8	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	2.191	0.601	0.591	0.122	0.036	0.011
48	1,4-cyclohexadiene	0.062	0.020	0.016	0.004	0.034	0.008
49	X210/70h	1.448	0.426	0.441	0.091	0.028	0.008
50	X210/70i	0.648	0.260	0.150	0.032	0.062	0.017
51	X210/70j	0.393	0.110	0.122	0.024	0.154	0.045
52	2,3,4-trimethylpentane	0.437	0.119	0.295	0.063	0.000	0.000
53	toluene	25.356	8.003	6.126	1.240	0.490	0.160
54	2-methylheptane	1.637	0.783	0.358	0.071	0.101	0.048
55	3-methylheptane	0.392	0.148	0.134	0.028	0.006	0.003
56	4-methylheptane, 1-methyl-1-cyclohexene	1.090	0.388	0.339	0.075	0.014	0.006
57	X211/212c	0.047	0.025	0.008	0.004	0.050	0.014
58	1-octene	1.694	0.488	0.146	0.032	0.275	0.081
59	X212/81a	4.716	1.675	0.004	0.000	7.581	2.260
60	<i>n</i> -octane	4.953	1.429	0.276	0.055	0.826	0.247
61	ethylbenzene	7.536	2.442	1.209	0.260	1.157	0.345
62	meta- and para-xylene	13.233	5.080	2.098	0.461	1.734	0.515
63	styrene	0.285	0.114	0.201	0.063	0.022	0.006
64	ortho-xylene	0.118	0.091	0.843	0.197	0.000	0.000
65	alpha-pinene	3.799	1.821	0.154	0.063	0.482	0.143
66	<i>n</i> -propylbenzene	0.255	0.087	0.173	0.051	0.039	0.011
67	4-ethyltoluene	0.143	0.072	0.087	0.028	0.000	0.000
68	X67/145c	0.091	0.036	0.134	0.043	0.014	0.003
69	X88/120c	0.081	0.030	0.150	0.051	0.000	0.000
70	1,3,5-trimethylbenzene	0.078	0.088	0.173	0.063	0.000	0.000
71	<i>n</i> -decane	0.077	0.024	0.071	0.032	0.000	0.000
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.351	0.140	0.492	0.189	0.000	0.000
73	X213/86b	0.022	0.009	0.016	0.004	0.000	0.000
74	1,2,3-trimethylbenzene	0.030	0.010	0.055	0.024	0.000	0.000
75	1,2,3,4-tetramethylbenzene	0.006	0.002	0.004	0.000	0.000	0.000
76	acetone	4.777	1.117	1.047	0.642	2.565	1.047
77	methyl acetate	1.125	0.232	0.102	0.035	0.230	0.157
78	ethyl acetate	0.397	0.096	0.063	0.028	0.174	0.048
79	methanol	0.839	0.210	0.028	0.008	0.359	0.381
80	2-butanone	0.142	0.062	0.051	0.020	0.106	0.025
81	isopropyl acetate	0.070	0.019	0.028	0.020	0.017	0.008
82	2-propanol	0.136	0.070	0.114	0.043	0.076	0.056
83	ethanol	7.199	2.393	0.248	0.197	0.812	0.437
84	propyl acetate	0.711	0.405	0.047	0.043	0.333	0.319
85	isobutyl acetate	0.135	0.032	0.020	0.004	0.022	0.006
86	4-methyl-2-pentanone	0.150	0.206	0.020	0.032	0.036	0.008
87	2-butanol	0.153	0.118	0.059	0.032	0.045	0.036
88	1-propanol	0.014	0.004	0.012	0.004	0.014	0.006
89	butyl acetate	1.047	0.423	0.035	0.020	2.414	1.989
90	2-hexanone	0.235	0.264	0.020	0.020	0.076	0.025
91	1-butanol	0.132	0.060	0.032	0.012	0.261	0.087
92	cyclohexanone	0.076	0.016	0.028	0.008	0.028	0.025
	Σ NMVOC	124.128	10.938	39.367	2.909	28.007	3.639

names of unknown compounds are explained in table E.1 in Annex E

Table F.17.a: Results of CMB analysis for receptor point SIMONM (Simon Str., 17.10.03, industrial area, close to Gorn workshop)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS8	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.914	0.439	0.244	0.080	0.106	0.030
2	<i>propane</i>	1.271	0.599	0.254	0.164	0.078	0.022
3	<i>propadiene</i>	0.011	0.003	0.010	0.010	0.000	0.000
4	<i>propyne</i>	0.004	0.003	0.005	0.010	0.000	0.000
5	<i>X5/13a</i>	0.004	0.003	0.015	0.010	0.000	0.000
6	<i>2-methylpropane</i>	1.246	0.640	0.348	0.109	0.027	0.007
7	<i>1-butene, 2-methylpropene</i>	1.538	0.518	0.940	0.254	0.262	0.074
8	<i>1,3-butadiene</i>	0.075	0.033	0.060	0.015	0.005	0.002
9	<i>n-butane</i>	2.759	2.293	0.532	0.174	0.043	0.012
10	<i>trans-2-butene</i>	0.190	0.134	0.075	0.020	0.006	0.002
11	<i>1-butyne</i>	0.024	0.013	0.010	0.005	0.001	0.001
12	<i>cis-2-butene</i>	0.178	0.132	0.070	0.020	0.004	0.002
13	<i>X12/18d</i>	0.621	0.660	0.070	0.025	0.012	0.003
14	<i>3-methyl-1-butene</i>	0.145	0.070	0.104	0.020	0.003	0.001
15	<i>X18/25a</i>	0.097	0.084	0.095	0.035	0.004	0.001
16	<i>X18/25b</i>	0.173	0.061	0.124	0.035	0.011	0.003
17	<i>X18/25d</i>	3.823	3.635	2.382	0.567	0.378	0.107
18	<i>2-methylbutane</i>	2.649	0.751	2.451	0.726	0.084	0.024
19	<i>X25/19c</i>	1.903	1.000	0.224	0.045	0.042	0.012
20	<i>1-pentene</i>	0.362	0.127	0.438	0.095	0.008	0.003
21	<i>n-pentane, 2-methyl-1-butene</i>	1.864	0.636	2.615	0.557	0.000	0.000
22	<i>2-methyl-1,3-butadiene</i>	0.156	0.047	0.810	0.204	0.000	0.000
23	<i>trans-2-pentene</i>	0.189	0.109	0.462	0.109	0.000	0.000
24	<i>cis-2-pentene</i>	0.583	0.172	0.224	0.050	0.024	0.007
25	<i>X22/43b</i>	0.415	0.139	0.701	0.095	0.000	0.000
26	<i>2,2-dimethylbutane</i>	0.318	0.092	0.393	0.080	0.000	0.000
27	<i>X43/17c</i>	0.016	0.005	0.020	0.005	0.000	0.000
28	<i>cyclopentene</i>	0.107	0.059	0.075	0.020	0.001	0.000
29	<i>X17/123c</i>	0.124	0.096	0.134	0.050	0.007	0.002
30	<i>methyl tert-butyl ether</i>	1.702	0.738	0.776	0.194	0.035	0.010
31	<i>2,3-dimethylbutane, cyclopentane</i>	1.635	0.492	1.183	0.254	0.021	0.006
32	<i>2-methylpentane</i>	2.269	0.672	1.974	0.388	0.016	0.004
33	<i>X45/46b</i>	0.508	0.301	0.194	0.070	0.018	0.005
34	<i>3-methylpentane</i>	1.271	0.377	1.109	0.219	0.000	0.000
35	<i>1-hexene</i>	0.208	0.058	0.184	0.035	0.014	0.004
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.777	0.254	0.199	0.055	0.057	0.016
37	<i>X37/47b</i>	1.296	0.384	1.298	0.254	0.002	0.001
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.021	0.024	0.035	0.015	0.002	0.001
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	1.308	0.390	1.511	0.293	0.000	0.000
40	<i>2,3-dimethyl-2-butene</i>	0.077	0.021	0.119	0.025	0.000	0.000
41	<i>benzene</i>	2.318	0.655	2.511	0.482	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	2.296	0.688	1.695	0.338	0.003	0.001
43	<i>2-methylhexane</i>	0.453	0.133	0.363	0.075	0.000	0.000
44	<i>cyclohexene</i>	0.079	0.025	0.045	0.010	0.005	0.002
45	<i>1-heptene</i>	0.434	0.119	0.323	0.065	0.007	0.002
46	<i>2,2,4-trimethylpentane</i>	1.068	0.329	1.084	0.214	0.003	0.001

Table F.17.b: Results of CMB analysis for receptor point SIMONM (Simon Str., 17.10.03, industrial area, close to Gorn workshop)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS8	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	1.366	0.413	0.746	0.154	0.006	0.002
48	1,4-cyclohexadiene	0.049	0.026	0.020	0.005	0.006	0.002
49	X210/70h	0.960	0.300	0.557	0.114	0.005	0.002
50	X210/70i	0.392	0.136	0.189	0.040	0.011	0.003
51	X210/70j	0.265	0.134	0.154	0.030	0.027	0.008
52	2,3,4-trimethylpentane	0.248	0.101	0.373	0.080	0.000	0.000
53	toluene	9.641	2.702	7.736	1.566	0.086	0.028
54	2-methylheptane	0.644	0.265	0.452	0.090	0.018	0.008
55	3-methylheptane	0.135	0.043	0.169	0.035	0.001	0.001
56	4-methylheptane, 1-methyl-1-cyclohexene	0.501	0.153	0.428	0.095	0.003	0.001
57	X211/212c	0.006	0.009	0.010	0.005	0.009	0.003
58	1-octene	1.078	0.500	0.184	0.040	0.048	0.014
59	X212/81a	0.789	0.783	0.005	0.000	1.333	0.398
60	<i>n</i> -octane	1.824	1.509	0.348	0.070	0.145	0.043
61	ethylbenzene	2.865	1.136	1.526	0.328	0.203	0.061
62	meta- and para-xylene	5.975	3.712	2.650	0.582	0.305	0.091
63	styrene	0.182	0.055	0.254	0.080	0.004	0.001
64	ortho-xylene	0.327	0.471	1.064	0.249	0.000	0.000
65	alpha-pinene	2.614	2.153	0.194	0.080	0.085	0.025
66	<i>n</i> -propylbenzene	0.160	0.070	0.219	0.065	0.007	0.002
67	4-ethyltoluene	0.366	0.100	0.109	0.035	0.000	0.000
68	X67/145c	0.446	0.602	0.169	0.055	0.003	0.001
69	X88/120c	0.485	0.100	0.189	0.065	0.000	0.000
70	1,3,5-trimethylbenzene	0.335	0.100	0.219	0.080	0.000	0.000
71	<i>n</i> -decane	0.248	0.100	0.090	0.040	0.000	0.000
72	1,2,4-trimethylbenzene, tetrabutylbenzene	1.256	1.000	0.622	0.239	0.000	0.000
73	X213/86b	0.070	0.010	0.020	0.005	0.000	0.000
74	1,2,3-trimethylbenzene	0.116	0.145	0.070	0.030	0.000	0.000
75	1,2,3,4-tetramethylbenzene	0.003	0.001	0.005	0.000	0.000	0.000
76	acetone	10.165	7.219	1.323	0.810	0.451	0.184
77	methyl acetate	0.536	0.264	0.129	0.045	0.040	0.028
78	ethyl acetate	0.583	0.520	0.080	0.035	0.031	0.008
79	methanol	1.315	0.371	0.035	0.010	0.063	0.067
80	2-butanone	0.107	0.091	0.065	0.025	0.019	0.004
81	isopropyl acetate	0.110	0.076	0.035	0.025	0.003	0.002
82	2-propanol	0.120	0.049	0.144	0.055	0.013	0.010
83	ethanol	1.501	0.542	0.313	0.249	0.143	0.077
84	propyl acetate	0.927	0.858	0.060	0.055	0.059	0.056
85	isobutyl acetate	0.091	0.019	0.025	0.005	0.004	0.001
86	4-methyl-2-pentanone	0.005	0.001	0.025	0.040	0.006	0.002
87	2-butanol	0.109	0.024	0.075	0.040	0.008	0.006
88	1-propanol	0.016	0.008	0.015	0.005	0.003	0.001
89	butyl acetate	0.184	0.212	0.045	0.025	0.425	0.350
90	2-hexanone	0.015	0.008	0.025	0.025	0.013	0.004
91	1-butanol	0.047	0.020	0.040	0.015	0.046	0.015
92	cyclohexanone	0.056	0.024	0.035	0.010	0.005	0.004
	Σ NMVOC	88.706	10.966	49.719	2.930	4.926	1.798

names of unknown compounds are explained in table E.1 in Annex E

Table F.18.a: Results of CMB analysis for receptor point VIEHOF (Viehhof Str., 04.09.02, industrial area, close to Conrads solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS4	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
1	<i>propene</i>	0.280	0.041	0.163	0.053	0.097	0.016
2	<i>propane</i>	0.283	0.069	0.170	0.110	0.090	0.023
3	<i>propadiene</i>	0.002	0.002	0.007	0.007	0.000	0.000
4	<i>propyne</i>	0.002	0.003	0.003	0.007	0.000	0.000
5	<i>X5/13a</i>	0.010	0.004	0.010	0.007	0.000	0.000
6	<i>2-methylpropane</i>	0.535	0.079	0.233	0.073	0.310	0.049
7	<i>1-butene, 2-methylpropene</i>	0.900	0.150	0.629	0.170	0.148	0.025
8	<i>1,3-butadiene</i>	0.038	0.007	0.040	0.010	0.000	0.000
9	<i>n-butane</i>	0.318	0.053	0.356	0.117	0.000	0.000
10	<i>trans-2-butene</i>	0.095	0.014	0.050	0.013	0.044	0.007
11	<i>1-butyne</i>	0.012	0.002	0.007	0.003	0.002	0.000
12	<i>cis-2-butene</i>	0.078	0.011	0.047	0.013	0.025	0.005
13	<i>X12/18d</i>	0.052	0.025	0.047	0.017	0.000	0.000
14	<i>3-methyl-1-butene</i>	0.052	0.028	0.070	0.013	0.000	0.000
15	<i>X18/25a</i>	1.100	0.183	0.063	0.023	1.287	0.224
16	<i>X18/25b</i>	0.324	0.046	0.083	0.023	0.277	0.042
17	<i>X18/25d</i>	0.487	0.175	1.594	0.379	0.000	0.000
18	<i>2-methylbutane</i>	5.286	2.118	1.641	0.486	4.088	1.654
19	<i>X25/19c</i>	0.278	0.073	0.150	0.030	0.116	0.030
20	<i>1-pentene</i>	0.502	0.247	0.293	0.063	0.173	0.086
21	<i>n-pentane, 2-methyl-1-butene</i>	3.144	0.916	1.750	0.373	1.210	0.358
22	<i>2-methyl-1,3-butadiene</i>	1.738	0.525	0.542	0.136	1.337	0.411
23	<i>trans-2-pentene</i>	0.567	0.199	0.310	0.073	0.226	0.081
24	<i>cis-2-pentene</i>	0.328	0.083	0.150	0.033	0.180	0.046
25	<i>X22/43b</i>	0.832	0.309	0.469	0.063	0.314	0.118
26	<i>2,2-dimethylbutane</i>	0.442	0.111	0.263	0.053	0.146	0.037
27	<i>X43/17c</i>	0.537	0.148	0.013	0.003	0.658	0.185
28	<i>cyclopentene</i>	0.110	0.115	0.050	0.013	0.058	0.060
29	<i>X17/123c</i>	0.245	0.049	0.090	0.033	0.171	0.035
30	<i>methyl tert-butyl ether</i>	0.970	0.185	0.519	0.130	0.407	0.081
31	<i>2,3-dimethylbutane, cyclopentane</i>	1.044	0.306	0.792	0.170	0.072	0.021
32	<i>2-methylpentane</i>	1.977	0.334	1.321	0.260	0.413	0.074
33	<i>X45/46b</i>	0.922	0.158	0.130	0.047	0.959	0.173
34	<i>3-methylpentane</i>	1.132	0.192	0.742	0.146	0.261	0.046
35	<i>1-hexene</i>	0.149	0.021	0.123	0.023	0.000	0.000
36	<i>n-hexane, 2-ethyl-1-butene</i>	0.242	0.039	0.133	0.037	0.097	0.016
37	<i>X37/47b</i>	1.384	0.215	0.869	0.170	0.379	0.062
38	<i>2,3-dimethyl-1,3-butadiene</i>	0.029	0.006	0.023	0.010	0.000	0.000
39	<i>methylcyclopentane, 1-methyl-1-cyclopentene</i>	1.511	0.336	1.012	0.196	0.314	0.072
40	<i>2,3-dimethyl-2-butene</i>	0.151	0.028	0.080	0.017	0.062	0.012
41	<i>benzene</i>	2.096	0.322	1.681	0.323	0.000	0.000
42	<i>cyclohexane, 2,3-dimethylpentane, 1,3-cyclohexadiene</i>	1.826	0.309	1.135	0.226	0.517	0.092
43	<i>2-methylhexane</i>	0.351	0.053	0.243	0.050	0.062	0.009
44	<i>cyclohexene</i>	0.025	0.006	0.030	0.007	0.000	0.000
45	<i>1-heptene</i>	0.269	0.039	0.216	0.043	0.000	0.000
46	<i>2,2,4-trimethylpentane</i>	1.181	0.173	0.726	0.143	0.347	0.053

Table F.18.b: Results of CMB analysis for receptor point VIEHOF (Viehhof Str., 04.09.02, industrial area, close to Conrads solvent factory)

	compounds	measured concentration		CMB calculated concentrations			
		$\mu\text{g}/\text{m}^3$	\pm	TRAFFIC1		SOLVENTS4	
				$\mu\text{g}/\text{m}^3$	\pm	$\mu\text{g}/\text{m}^3$	\pm
47	<i>n</i> -heptane	1.033	0.154	0.499	0.103	0.517	0.081
48	1,4-cyclohexadiene	0.009	0.002	0.013	0.003	0.000	0.000
49	X210/70h	0.581	0.085	0.373	0.077	0.146	0.023
50	X210/70i	0.215	0.031	0.127	0.027	0.074	0.012
51	X210/70j	0.125	0.020	0.103	0.020	0.000	0.000
52	2,3,4-trimethylpentane	0.430	0.062	0.250	0.053	0.150	0.023
53	toluene	7.844	1.132	5.178	1.048	1.744	0.268
54	2-methylheptane	0.516	0.082	0.303	0.060	0.176	0.030
55	3-methylheptane	0.154	0.022	0.113	0.023	0.016	0.002
56	4-methylheptane, 1-methyl-1-cyclohexene	0.392	0.056	0.286	0.063	0.044	0.007
57	X211/212c	0.006	0.004	0.007	0.003	0.000	0.000
58	1-octene	0.157	0.092	0.123	0.027	0.002	0.002
59	X212/81a	0.005	0.005	0.003	0.000	0.002	0.002
60	<i>n</i> -octane	0.357	0.055	0.233	0.047	0.086	0.014
61	ethylbenzene	2.139	0.326	1.022	0.220	1.090	0.176
62	meta- and para-xylene	4.558	0.830	1.774	0.389	2.961	0.561
63	styrene	0.158	0.044	0.170	0.053	0.000	0.000
64	ortho-xylene	1.387	0.309	0.712	0.166	0.628	0.143
65	alpha-pinene	0.130	0.019	0.130	0.053	0.000	0.000
66	<i>n</i> -propylbenzene	0.161	0.058	0.146	0.043	0.000	0.000
67	4-ethyltoluene	0.128	0.031	0.073	0.023	0.049	0.012
68	X67/145c	0.114	0.050	0.113	0.037	0.000	0.000
69	X88/120c	0.101	0.021	0.127	0.043	0.000	0.000
70	1,3,5-trimethylbenzene	0.167	0.076	0.146	0.053	0.000	0.000
71	<i>n</i> -decane	0.042	0.017	0.060	0.027	0.000	0.000
72	1,2,4-trimethylbenzene, tetrabutylbenzene	0.352	0.139	0.416	0.160	0.000	0.000
73	X213/86b	0.027	0.005	0.013	0.003	0.014	0.002
74	1,2,3-trimethylbenzene	0.037	0.010	0.047	0.020	0.000	0.000
75	1,2,3,4-tetramethylbenzene	0.006	0.006	0.003	0.000	0.002	0.002
76	acetone	0.718	0.311	0.885	0.542	0.000	0.000
77	methyl acetate	0.077	0.085	0.087	0.030	0.000	0.000
78	ethyl acetate	0.011	0.002	0.053	0.023	0.000	0.000
79	methanol	0.012	0.005	0.023	0.007	0.000	0.000
80	2-butanone	0.072	0.042	0.043	0.017	0.025	0.014
81	isopropyl acetate	0.081	0.018	0.023	0.017	0.065	0.014
82	2-propanol	0.045	0.019	0.097	0.037	0.000	0.000
83	ethanol	0.493	0.106	0.210	0.166	0.291	0.065
84	propyl acetate	0.039	0.022	0.040	0.037	0.000	0.000
85	isobutyl acetate	0.018	0.005	0.017	0.003	0.000	0.000
86	4-methyl-2-pentanone	0.012	0.003	0.017	0.027	0.000	0.000
87	2-butanol	0.028	0.007	0.050	0.027	0.000	0.000
88	1-propanol	0.007	0.010	0.010	0.003	0.000	0.000
89	butyl acetate	0.131	0.139	0.030	0.017	0.116	0.122
90	2-hexanone	0.004	0.002	0.017	0.017	0.000	0.000
91	1-butanol	0.075	0.016	0.027	0.010	0.051	0.012
92	cyclohexanone	0.007	0.002	0.023	0.007	0.000	0.000
	Σ NMVOC	56.989	3.008	33.278	1.791	23.097	2.042

names of unknown compounds are explained in table E.1 in Annex E

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