

Spatial assessment in urban areas

and its application for

compliance with EU directives and population exposure to ambient air

Summary

This document has been compiled within the FP6 project Air4EU as a guidance document for the spatial assessment of particulate matter (PM), nitrogen dioxide (NO₂) and ozone (O₃) in urban areas. It provides recommendations on basic requirements, best practices and further scientific research in regard to this topic. The major application area addressed is spatial assessment for compliance with EU directives though other applications, such as population exposure and source apportionment, are also addressed. Recommendations are provided for the various methodologies used to achieve spatial assessment including monitoring, modelling and methods for combining models and monitoring. A number of particular issues are also dealt with such as emissions and uncertainty analysis. The intended result of the spatial assessment and uncertainty analysis described here is the production of maps. The recommendations are intended as guidance for authorities involved in the spatial assessment of air quality at city, national and European level. They are intended to aid good assessment practice and to highlight areas that require further development.

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1. Introduction

1.1 Aim

The main aim of this document is to recommend methodologies that will lead to improved spatial assessment of PM, NO₂ and O₃ in urban areas. The document deals with methods and issues relevant to this topic. Emphasis is placed on the combined use of both monitoring and modelling.

1.2 Applications and scales

Spatial assessment of urban pollutants such as PM, NO₂ and O₃ can be used for a variety of applications. This document focuses mainly on assessment for compliance with EU directives (EC 1996, EC 1999, EC 2002) and the forthcoming legislation (EC 2005a, EC 2005b) but assessment can also be used for other applications such as population exposure as well as any number of air quality management applications such as source apportionment or scenario calculations.

When applying spatial assessment to the EU directives temporal information is required as annual, daily and hourly mean values, dependent on the pollutant. Spatial assessment can also be used to assess potential population exposure that, depending on the exposure methodology used, may require hourly mean values for all compounds. Impact assessment studies, especially screening type studies, may not require more than annual temporal resolution.

The required spatial resolution of assessment may vary but, in principle, both compliance and exposure calculations in urban areas require spatial resolutions ranging from meters, to assess hotspots, to kilometres, for an overall spatial assessment.

1.3 Structure of this document

As outlined in the 'Overview and structure' document (Air4EU – D6.2, Part I), each recommendation topic has been structured to provide access to the individual recommendations provided. This structure can be seen in the table of contents but is reiterated here for clarity.

The recommendations within this particular document are all relevant to the topic:

Spatial assessment of PM, NO₂ and O₃ in urban areas

Within this topic three distinctly different methods for carrying out this assessment are treated. These are:

- *Monitoring*
- *Modelling*
- *Combining models and monitoring*

These methods are presented as separate chapters within this document. In addition one particular issue is addressed separately, that being uncertainty analysis.

Each of these chapters is divided into a number of relevant aspects related to the different methodologies (e.g. for modelling this will include meteorology, emissions, chemistry, etc.) and recommendations on these are given at 3 levels of complexity, those being:

- a) Basic requirements*
- b) Best practice recommendations*
- c) Scientific recommendations*

Throughout the document recommendations are given in ***blue italics*** with supporting text in normal font. Where recommendations are specific for one of the compounds PM, NO₂ or O₃, this is clearly indicated. If not, the recommendations are general for all the three compounds.

In addition to the recommendations presented a number of case studies, designed to test and demonstrate some of the recommendations, have been carried out (See the case study summary document, Air4EU – D7.2). Results from the case studies are included in the most relevant methodology chapter.

Reference is made throughout the document to a number of other related Air4EU reports, see the Air4EU reference section at the end of this document for a complete overview. These reports include background reports leading up to this final set of recommendations, the individual and summary case study reports, reports on the mapping tool and a number of cross cutting issue milestone reports covering specific issues.

1.4 Compounds addressed

As previously stated the compounds addressed in this document are PM, NO₂ or O₃. These compounds have been selected since they are of primary concern to many cities dealing with air quality problems within Europe. For specific regions other compounds may also be of interest, such as benzene, but many of the recommendations given here are not directly compound specific and can thus be applied to other compounds.

None of PM, NO₂ or O₃ are solely primary compounds. Their occurrence in the atmosphere is partly a result of their formation due to chemical reactions between precursor gases. PM and NO₂ also have a primary part resulting from direct emissions from particular sources. The occurrence of NO₂ and O₃ is linked, as they take part in reactions between each other. Recommendations regarding one of them, thus, often entail taking account of the other.

PM is not a single pollutant. Its mass includes a mixture of many pollutants in a complex multiphase system. Particles can be 'primary' in the sense that they are emitted as particles from the source, or they can be secondary, meaning that they are produced in the atmosphere from gaseous precursors. Aerosol particles vary in size from a few nanometers for particles just produced from the gas phase, to tens of micrometers for coarse particles produced by mechanical processes. The chemical composition of the aerosol varies as a function of size. Also the physical properties of particles vary widely with size and composition. All of these properties vary with the relative humidity of the air (Tørseth and Hov, 2003). The health effect of particles is a strong function of their chemical composition and physical properties. It is also well known that PM is the sum of contributions from a variety of sources, each with its own chemical and physical characteristics.

2. Monitoring

The objective of monitoring for AQ assessment in relation to the EU air quality limit values for PM is to provide the following:

- A set of annual time series of concentration levels, of basic averaging time corresponding to the requirements of the directives:
 - for PM₁₀ (and PM_{2.5}) mass: 1 or 24 hourly averages
 - for NO₂ and O₃: hourly averages
- Estimation of the spatial extent of exceedences (including exceedences in hot spots)
- Estimation of the population exposure in ambient air (not including indoor exposure).

In connection with modelling, the objective of monitoring is to provide input data for the evaluation and validation of air quality models.

The recommendations regarding 'monitoring' are structured in three sections:

- Network design
- Monitoring methods
- Data quality control and assurance (QA/QC)

In the *basic requirement* level of 'monitoring', it is understood that the assessment is made mainly from monitored air pollution data, and modelling is not carried out in earnest. Still, even at this level one should have an eye on the requirements for the location of stations that are to be used for evaluation of the performance of dispersion models.

In the *best practice recommendations* level, it is understood that although assessment can be based solely on the monitoring part, which is improved from the *basic* level, monitoring is used more actively for

model evaluation and validation. It is also used in combination with modelling to provide a better assessment.

In the *scientific recommendations* level, it is understood that there are a number of aspects of modelling that require further research to improve both monitoring methods and monitoring practices.

2.1 Network design

a) Basic requirements

The design of the network should comply with the basic requirement in the AQ Directives for NO₂, O₃ and PM (EC 1999; EC 2002). The Directives specify requirements regarding:

- *The number of stations according to the size (population) of the city*
- *The type of stations, and an indication of number of each type. On definition of type of stations, see the Exchange of Information Council Decision 97/101/EC (EC 1997)*
- *The location of stations*
 - *macro-location: monitoring in areas of typical and high/maximum exposure*
 - *micro-location: location of shelter and inlet relative to nearby sources and nearby obstacles*
- *The reference monitoring method*

The location of monitoring sites

The Directives provide general guidelines. The actual selection should be carried out based upon careful consideration of where stations should be located relative to areas of residence, traffic, industry or commerce (see chapter 2.4 on representativeness of monitoring data). In the typical city, as the traffic intensity is highest towards the central city areas, this should be covered by a station (high-exposure area). In some cities, industrial areas may be hot spot/high-exposure areas to be covered, too. Residential areas in central districts should also be covered.

In regard to design of an urban AQ monitoring network, it is recommended to consult the following references:

- *Air4EU cross cutting issue report on representativeness (Air4EU – M3)*
- *A Topic Note developed under the EU Research project 'INTEGAIRE': (<http://www.integaire.org/indexuk.html>) (go to: Good Practice database/ Assessment/ How to design Urban monitoring networks).*
- *The report 'Guidance to assessment under the EU AQ Directives', (<http://ec.europa.eu/environment/air/pdf/guidanceunderairquality.pdf>), the process described there for selecting the locations of the number of stations available/needed according to the Directive*
- *The 'Guidance report on Preliminary Assessment under EC Air Quality Directives' (<http://reports.eea.europa.eu/TEC11a/en/tech11.pdf>)*

As examples it is recommended to study the monitoring network designs in cities with established networks (Cities such as Athens, Berlin, Brussels, London, Paris, Prague, Rome and Wien have a large number of stations, up to 25, and can be contacted regarding their procedures and considerations on network design).

It is recommended to locate, if possible, stations in pairs: an urban background station and a hot-spot station (traffic or industrial) in the same area, to enhance the use of the data (see under 'Best practice recommendations', regarding also the need for triplet stations, including also a rural background station near the city).

It is recommended to select sites for long-term use, i.e. sites where large changes in traffic/infrastructure/urban development are not expected (see under 'Best practice

recommendations' below, regarding enhanced networks, for considerations regarding locating such stations).

It is recommended to locate the stations such that they may also be used in combination with modelling, either for validation purposes or use in other applications such as establishment of source/receptor relations.

If only sparse prior information and data regarding the emissions and/or concentration distribution is available, it is recommended to carry out a pre-screening study to collect the data needed to locate the stations. A mobile laboratory with automated equipment and/or passive samplers are recommended for this type of survey. Some guidance is given in e.g. EEA's 'Guidance report on preliminary assessment under EC air quality directives', Chapters 3.4 and 3.5 (<http://reports.eea.europa.eu/TEC11a/en/tech11.pdf>).

Combination of pollution compounds at stations

It is usually required to monitor a number of pollutants, e.g. PM, NO_x, NO₂, Ozone, benzene and sometimes CO and SO₂, dependent upon the type of city and its sources. For cost effectiveness and analysis of the data this is usually carried out at the same site but any number of combinations are possible, e.g. Ozone is often not measured at hotspot sites.

It is recommended to measure both PM₁₀ and PM_{2.5} at as many stations as possible.

It is also recommended to measure NO_x and NO₂ at the PM stations, in some cases also SO₂ when industrial sources are prominent in the area, to enhance the use of the data, e.g. in terms of indicating which sources are dominating at the station.

Monitoring of meteorological parameters

Meteorological data representative of the central urban areas is necessary for enhanced use of the pollution concentration data, e.g. to help explain temporal variations of the pollutants (hourly, daily, annual), and to indicate source areas influencing a station.

It is recommended to have at least one meteorological monitoring station in the central part of the city, giving hourly data for wind speed and direction, temperature and preferably also a parameter giving the vertical stability, either temperature gradient, radiation or direct measurement of turbulent fluxes. Existing meteorological stations operated by meteorological services and/or airport authorities should be evaluated regarding their suitability and representativeness for central and residential areas in the city.

b) Best practice recommendations

The Directives prescribe minimum requirements to the monitoring network (in regard to the number of stations and their types). A sufficiently detailed assessment of concentration variations and gradients in a city most often requires a larger number of stations, or combination of monitoring with modelling.

The urban air pollution concentrations include significant contributions from sources outside the city (near and far), which creates an extra-urban background concentration. For PM this 'regional' concentration level is often significant, and for ozone it is dominant. The average urban concentrations again provides a background concentration for the levels that are found in streets and other hot-spot locations. Thus, a proper urban air quality monitoring network should include both extra-urban, urban background and hot-spot stations. See the ETC/ACC technical report (Eerens et al.; 2005, chapter 4) for an overview of typical scale contributions in European cities.

Enhanced network

*It is recommended to **enhance the network** with more stations, in order to improve the assessment.*

When locating the additional stations, the following needs should be considered:

There is a need for at least one well placed regional background station in the region of the city, to represent the concentrations in the air entering the city from outside. The difference between the regional and urban background represents the contribution of city sources to the urban background. This is relevant to city authorities to develop action plans and programmes to control urban emission sources. When it is not possible to select one location

that gives representative concentrations in the incoming air, for all the important wind directions, more than one regional background station should be considered.

NO₂ is different to PM since it is, to a large extent, the result of the chemical reaction between the primary emission of NO, from combustion sources, and the available O₃, advected into the urban region. As such NO₂ is not just the result of emissions but also of the availability of O₃ and this may vary over the urban area, depending on the spatial distribution of NO emissions, on meteorological parameters (e.g. temperature and sunshine), on emissions of other organic compounds and on the physical extent of the urban region. Both production and depletion of O₃ can take place.

A station with O₃ and NO_x monitors should also be considered at a downwind location (representing the areas that may experience locally produced ozone).

There is a need for the monitoring network to give as good a basis as possible for calculating the population exposure distribution, which is required for health effect assessments. This implies that the network should cover and represent the main areas where the population is exposed to high air pollution levels (urban centres and residential areas).

There is a need for stations suitable for evaluating and validating dispersion models. Such locations must comply with special requirements. Their location must be representative of an area that corresponds to the spatial resolution of the dispersion model. For instance:

- for a grid model that calculates average concentrations on a 1 km² area, the station must be located such that it also represents the average concentration of the 1 km² area surrounding it. The model also represents the concentration at a certain height, or rather, the average value of a layer of air of a given height (e.g. the lowest 30 m of the atmosphere). The combination of the location and height of the air inlet for the instruments must also be chosen so as to represent a similar average value, height-wise.*
- for a sub-grid model, e.g. a line source model which calculates the concentrations near streets/roads, the station location must reflect the situation which is represented by the model. Typically, such a model gives the concentrations for an idealised type of street/building configuration (e.g. continuous building facades of similar height on both sides along the street section and away from influence of complicating effects such as intersections (CFD models also exist which can calculate concentrations for more complex configurations)).*

*Consider the need to monitor **meteorological parameters** at more than one station, dependent upon the topography of the city, so that the wind conditions near each monitoring station is known.*

***Traffic data** should be monitored in the streets where monitoring stations are located. The traffic parameters should include average speed and number of vehicles (per hour) in each of several types (light duty, (sub(weight)classes of) heavy duty vehicles, buses, and possibly more classes such as taxis, if they represent a special vehicle type in terms of fuel use).*

Enhanced monitoring program for PM

As stated in the introduction to the monitoring section above, the composition of the PM mass is the key to assessing the source contributions to PM as well as to the evaluation of the potential specific health effects. The main chemical species in PM_{2.5} and PM₁₀ include:

- Elemental carbon, (EC) which originates as primary particles from combustion of fuels, fossil and non-fossil
- Organic carbon, (OC) which originates from primary and secondary formed particles from fuel combustion
- Inorganic ions, of which the most abundant are sulphate, nitrate and chloride combined with their an-ions ammonium, hydrogen, sodium and calcium, formed from gaseous precursors, mainly SO₂, NO_x and NH₃
- Minerals, mainly from suspended dust, natural or man-made

- Water from atmospheric humidity
- Heavy metals, those of health significance include e.g. Cd, Pb, Cu, Zn, As, Cr, Ni. Some of these may point to contributions from specific industrial sources.

References to the significance of PM speciation in assessment of PM and its health effects, and to methods for assessing contributions from sources based upon such PM speciation, can be found in

- EU CAFÉ: 'Second positional paper on Particle matter', Chapter 2.5 and Annex 5.
(http://ec.europa.eu/environment/air/cafe/pdf/working_groups/2nd_position_paper_pm.pdf)
- EMEP: A number of documents pertaining to the 'EMEP monitoring strategy for particulate matter' (http://www.nilu.no/projects/ccc/pm_strategy.html), the 'EMEP Manual for Sampling and Analysis' (<http://www.nilu.no/projects/ccc/manual/>) and 'The EMEP monitoring strategy 2004-2009' (Tørseth and Hov; 2003, chapter 7.5).
- WHO: 'Health risks from particulate matter from long-range transboundary air pollution' (<http://www.euro.who.int/document/E88189.pdf>)

*To support a 1st assessment of source contributions to PM mass, it is recommended to do some basic **chemical speciation of PM**. Samples of particles on filters should be analysed for the main compounds, in order of diminishing importance:*

- *Main inorganic ions (sulphate, nitrate, ammonium)*
- *Sea salt (if located close to coast)*
- *Carbon species, EC and OC, Black carbon (BC) which is a proxy for EC*
- *Mineral dust: Silicon (Si)*
- *Heavy metals: Cadmium (Cd) and Lead (Pb)*

Chemical analysis should be done on a number of 24-hour PM samples, such that the results can be said to be representative of the period covered. Source contributions differ between seasons, so analysis should be done on a number of samples per season of interest.

Determination of chemical species obviously requires manual sampling of particles on filters. If PM mass is determined in the network in question using automated methods, then additional equipment, i.e. filter samplers (see below) must be used in addition to speciate the PM.

Sampling of PM for chemical speciation requires careful consideration of the sampling needs, especially in terms of the amount of mass needed on the filter for an accurate analysis. Determination of many species may require that several samplers need to be used in parallel. Candidate samplers need to be evaluated in terms of their quality, especially related to the requirement to equivalence with reference samplers.

***The contribution from non-exhaust particles** should be measured at least at one station pair (urban background and traffic station), by hourly monitoring of PM₁₀ and PM_{2.5} at both stations (see the case study on non-exhaust PM emissions, Air4EU – CS 7.1.2).*

c) Scientific recommendations

PM

Data from a monitoring network is used to assess the concentrations and their variation at the station locations. When combined with meteorological data, it is possible to some extent to indicate which source areas (as indicated by wind directions) give dominating contributions to the concentration levels. Through the methods of 'source apportionment' (SA), PM monitoring data can also be used to assess source sector contributions to PM concentrations in a statistical manner. These methods give a very valuable addition to the apportionment of sources that can be derived using dispersion models based upon emissions inventories. These two methods of assessing source contributions are

complementary. The statistical method can be used to evaluate the quality and completeness of the emissions inventory (see also chapter 4.4 and the case study on source apportionment in Oslo, Air4EU – CS D7.1.5).

*It is recommended to carry out proper **Source Apportionment (SA)** studies using receptor models, by sampling PM at, at least, one of the stations according to SA procedures. Source apportionment studies involve rather extensive chemical characterisation of a number of PM samples (a significant step further than the speciation under 'Best practices' above). Usually at least 40 samples from each monitoring station is suggested. The chemical species to be analysed must dominate or be specific in regard to the sources in the area, so that the analysis will produce clear source relationships. The extent of the sampling and analysis is (much) larger than for the speciation analysis under the 'best practice' section. There is a wealth of literature regarding receptor models, see e.g. Watson and Chow (2004) for a review. The US EPA also provides some guidance on receptor modelling (www.epa.gov/scram001/receptorindex.htm)*

The effects of PM air pollution are to a large extent related to particle size.

*It is recommended to study the **size distribution** in the city, by measuring it at one or more locations. The study should include instrumentation that will separate the particles in size fractions like PM₁₀, PM_{2.5}, PM₁ and UFP or better. Optical counters can be used for particle numbers, while inertial impactor type instruments can provide samples of size fractions for chemical analysis.*

Advanced assessment of PM in urban areas through advanced modelling also includes the chemical formation of particles within the urban area from precursor gases.

As a further step towards advanced characterisation of PM, it is recommended to study formation of secondary particles (inorganic and organic) within the urban area. If this is to be carried out then monitoring of precursor gases (VOC profiles, NO and NO₂, NH₃, SO₂) is also required.

O₃

In large urban areas in Southern parts of Europe, ozone formation might occur. This should be assessed. It requires that ozone is monitored in areas upwind and downwind of the urban area in addition to within the urban area, as described in the 'best practices' above. Study of ozone formation would also entail a measurement programme which includes NO, NO_x, hydrocarbons (light (C₂-C₇) as well as heavier (C₈-C₁₂)) and other organic compounds (carbonyls, PAN, organic nitrates).

It is recommended to monitor such compounds according to the recommendations specified in the EMEP monitoring strategy, and measurement program 2004-2009 (Tørseth and Hov, 2003)

2.2 Monitoring methods

a) Basic requirements

For compliance with directives hourly average concentrations for NO₂ and O₃ are required. For PM₁₀ only 24 hourly averages are required, however, it is recommended even for PM to use methods with as short time averaging as possible, preferably hourly, to enhance the use of the monitored data (e.g. analyse PM concentrations as a function of wind direction and speed, traffic etc.).

It is recommended to use the reference methods, as specified in the Directive (EC 1999, Annex IX).

If these are not used, the equivalence of the methods used must be proven, using standard procedures (see EUs 'Guidance on equivalence demonstration' (http://ec.europa.eu/environment/air/pdf/equivalence_report3.pdf) and 'Equivalence test format' (http://ec.europa.eu/environment/air/pdf/test_equivalencev31004.xls) for general guidance on equivalence testing.

PM mass

A number of methods are described specifically for PM₁₀ equivalence testing and should be referred to. These include the CEN standard EN 12341 (CEN, 1998), which describes a reference method and field test procedure to demonstrate equivalence. This standard is developed for testing the equivalence of manual (filter) samplers, but it can be, and is, used for equivalence testing on automatic monitors as well. Other examples of reports from equivalence testing of PM₁₀ monitors include the 'UK Equivalence Programme for Monitoring of Particulate Matter' (http://www.airquality.co.uk/archive/reports/cat05/0606130952_UKPMEquivalence.pdf) and 'PM monitoring and intercomparison with the reference sampler in Helsinki' (http://www.fmi.fi/kuvat/FINAL_PM_report_30_1_2004.pdf).

The equivalence testing usually results in the need to correct the data from non-standard samplers/monitors with a correction factor or algorithm (CF). For data PM reported by countries to the European Commission, and stored in the AirBase data base for European air quality data hosted by the European Environment Agency (EEA) and its European Topic centre on Air Quality and Climate Change (ETC/ACC) (<http://air-climate.eionet.europa.eu/>), correction factors for individual stations and samplers are reported. ETC/ACC can provide an overview of CF(s) used by different countries, stations and samplers. However, each network should establish its own CF(s).

If the method is proven to be equivalent, it is recommended to give preference to methods that provide hourly data over the reference gravimetric method, which typically gives 24-hour averages.

PM chemical components

It is referred to e.g. the 'EMEP Manual for Sampling and Analysis' (<http://www.nilu.no/projects/ccc/manual/>) regarding recommended methods for sampling and analysis of chemical components of PM.

b) Best practice recommendations

PM

It is well known that PM samplers and monitors are affected by sampling artefacts, implying that particulate material is added or lost from the collection stage (filter or otherwise) during sampling. There is a wealth of literature of studies and summaries of results from such studies. See e.g. the ETC/ACC technical report (De Leeuw, 2005) for an overview in regard to AirBase.

When choosing instruments for sampling or monitoring of PM, it is recommended to seek advice in those studies and summaries, regarding the suitability of various samplers for the type of PM assessment one is considering.

Reference to institutions where up-to-date information can be sought includes: European Committee for Standardisation (CEN), its Technical Committee TC 264/WG 15; the US Environment Protection Agency (USEPA); WHO.

It is recommended, if possible, to measure PM both with a monitor giving hourly averages and with a sampler giving PM samples on a filter for later analysis, at least at 1-2 stations, to enhance the database for assessing source contributions.

c) Scientific recommendations

PM

The correct sampling and monitoring of PM and its chemical components is a demanding task, since all methods, manual as well as automatic, are affected by sampling errors and artefacts (loss and formation of particles on the particle collection medium, depending heavily on the chemical nature of the particles collected). Research on this topic is continually being conducted and reported. It is out of the scope of most network operators to conduct or participate in such research, although the possibilities exist to team up with consortia conducting such research, e.g in European research projects under EC DG Research's Framework Programmes.

It is recommended to keep oneself updated on this literature, through searches in databases of scientific literature.

2.3 Data quality control and assurance

Measuring the concentration of atmospheric pollutants is of primary importance in order to obtain the closest value to the reality. Nevertheless, the actual measured value is always affected by a certain amount of error due to a number of sources.

Quantifying, or establishing, the uncertainty associated to a measured value, although difficult, is strongly recommended. Detailed information can be found in the Air4EU cross cutting issue report (Air4EU – M2) on uncertainty.

The first step is to clearly define the purposes of the measurements. Examples are:

- Determine compliance with air quality standards
- Determine the highest concentration in a predefined area
- Determine the representative concentration in areas of high population density
- Determine effects of particular emitters on the ambient air concentrations
- Determine background pollution levels.

The purpose of the measurements will then lead to a set of Data Quality Objectives (DQOs), which fit that purpose. Quality assurance and control (QA/QC) assures that the measurements will meet the defined standards of quality with a stated level of confidence. It should be emphasized that the function of QA/QC is not just to achieve the highest possible data quality, in regard to the precision and accuracy of the instruments. Rather, it is a set of activities enabling the network measurements to comply with the specific DQOs for the monitoring programme.

The main parts of the Quality System are:

- **Quality assurance (QA):** the management of the activities within the system, and setting of overall objectives and criteria.
- **Quality control (QC):** the procedures of the day-by-day operations and data validation.
- **Quality assessment:** the external validation of the implementation of the quality system.

Proper QA/QC ensures that data reported for a monitoring station have a stated level of accuracy and precision, a specified area of representativeness, and a sufficient time coverage, all as defined by the DQOs.

A basic description of a data quality system has been developed by EMEP (<http://www.nilu.no/projects/ccc/qa/index.htm>), by EEA in the Technical Report 'Criteria for EUROAIRNET- The EEA Air Quality Monitoring and Information Network' (Larssen et al., 1999) and in the

WHO UNEP GEMS/AIR Methodology Review Handbook Series, Volume 1, "Quality Assurance in Urban Air Quality Monitoring".

The EU Air Quality Directives (<http://www.europa.eu.int/comm/environment/air/ambient.htm>) specify Data Quality Objectives (DQOs) and certain data quality related requirements that should be used to guide the actual specification of QA/QC systems. DQO requirements are set for:

- Minimum accuracy and data capture for monitoring, as well as for modelled data, and objective estimation
- Location of monitoring stations
- Minimum number of stations e.g. in urban networks
- Reference monitoring methods

a) Basic requirements

The QA/QC system, or activities, must comply with a set of minimum requirements.

A minimum documented QA/QC system must consist of the following elements (refer to Larssen et al.; 1999, chapter 4.5.5):

- *DQO for accuracy, precision, data capture and time coverage, which must comply with the EU AQ Directives.*
- *An organisation responsible for the QA/QC system and activities.*
- *Site selection criteria. Refer e.g. to Larssen et al. (1999), its Annex 3, and to Garber et al. (2002), chapter 2.2.*
- *A documented calibration program.*
- *A data validation procedure complying with the Eol Decision (97/101/EC) (EC 1997).*

b) Best practice recommendations

The best QA/QC practice is to develop and follow a complete QA/QC plan, which includes all the three parts: quality assurance, quality control and quality assessment.

The requirements to a complete QA/QC plan have been described in the EUROAIRNET recommendations (Larssen et al., 1999; Chapter 4.5.6).

2.4 Representativeness of monitoring data

This subchapter considers recommendations on how to deal with uncertainties that result from the limited coverage of monitoring stations when performing an assessment. Further details concerning this form of representativeness can also be found in the cross-cutting issue report (Air4EU – M3). In Chapter 5.3 of this document uncertainties related to the spatial representativeness of models and monitoring are addressed, particularly in regard to model validation and data assimilation.

Well-established operational methods for quantifying representativeness uncertainties in air quality networks do not exist, and the uncertainties are often ignored. However, these uncertainties can be larger than the instrument-related uncertainties dealt with in chapter 2.3. This type of uncertainty tends to be highly dependent on the purpose of the measurements: a network adequate for one purpose (e.g. identifying limit value exceedances) may be highly inadequate for another (e.g. characterising exposure of the general population). In a similar way networks designed for model validation will not be representative for direct use for exposure calculations.

a) Basic requirements

When basing the results of assessment on monitoring data, it should be ensured that the relevant locations in the study area are sufficiently covered. In the current AQ directives for PM and NO₂ these include the hotspot locations with the highest population exposure as well as areas representative for the exposure of the general population. For O₃ this includes only areas representative for the exposure of the general population.

b) Best practice recommendations

To characterise and possibly quantify the representativeness uncertainties in a monitoring assessment it is recommended to take the following steps – **for each pollutant and each purpose of the measurements separately**. It would be wise to do this first quickly, to acquire insight, and then to elaborate where needed.

1. Decide for **which area** the assessment should be made, e.g. a city, a city district, a specific air quality zone. If there are several areas to be assessed separately, carry out the following steps for each area.
2. Estimate the main spatial characteristics of the air pollution concentration patterns in the area using the results of the monitoring network, **supplementing this** by model results or by estimates based on knowledge of emissions in the area. In particular, estimate where **peaks** exist and where **smooth patterns** can be expected.
3. Characterise for each station its site firstly by looking at the **station class** (See the annex of the 'Exchange of Information Decision' EC (1997)) and secondly at the **relative pollution level**: the severity of pollution at this station compared with all other locations within this class: is the station at one of the most polluted locations of its class in the study area (**'highest'**) or at a typical site for its class (**'average'**).
4. Taking the purpose of the assessment into account, determine which relative pollution level should be characterised: the highest, the average or both. Establish for each station class which stations in the network give the required information.
5. For each station class and relative pollution level, determine whether the available station(s) give adequate information on the relative pollution level needed. (If several stations within a class are available, estimate whether they characterise the distribution of the relative pollution level well.) If not, the information is not adequate:
 - a. Identify this as a shortcoming of the network and mention this clearly in the assessment report.
 - b. If possible, estimate which concentration range is missed by the network. This requires a priori knowledge of typical concentration ranges per station type, which can be gained from air quality reports from other authorities, preferably in the same region. Also Wilson et al (2005) gives information on the spatial variability of PM between stations. It should be remembered that the less the concentration patterns in the area are known, the less also the uncertainty related to representativeness can be known. Exact quantification of the uncertainty due to imperfect representativeness is generally out of reach. Because of this and also because the uncertainty is generally not symmetrical as in $\pm x\%$, it is recommended not to add the estimate to the instrumental uncertainty, but to describe it separately in a paragraph.

c) Scientific recommendations

In view of the severe shortcomings in comparability of European networks due to differences in coverage, further development of procedures to characterise and minimise the uncertainty ranges related to representativeness is needed.

3. Modelling

The following chapter looks at a number of aspects of modelling, in regard to the assessment of PM, NO₂ and O₃ in urban areas. The objective of modelling for spatial assessment, and other applications such as population exposure, is to provide a spatially and temporally resolved representation of air quality. In addition modelling is also required for scenario calculations to assess emission abatement strategies.

The model spatial resolution required for these assessments is dependent on the objective of the application. For population exposure and for compliance of PM₁₀, NO₂ and O₃ with EU directives then both urban and local scales need to be addressed. For PM_{2.5} the current directives require only urban scale assessments.

Important aspects of modelling addressed in the following chapter sections include the required resolution, meteorology, emission inventories, dispersion schemes, physical and chemical processes as well as interactions between modelling scales.

Air quality modelling is a complex system that requires, under most circumstances, expert knowledge for its application as well as for an understanding of the results. However, those who make use of models can use these recommendations to help better specify their requirements and understand the limitations of modelling in regard to a number of different model types and modules. Technical details of the internal workings of air quality models will not be discussed but reference to the use of a number of detailed aspects are. References and links within the text should help for more background information. The reader is referred here to the other relevant Air4EU documents (http://www.air4eu.nl/reports_products.html) that already contain a large amount of background information to these recommendations.

3.1 General model types and requirements

There are a variety of models available for calculating concentrations in urban areas and include the following general model types

- Eulerian
- Box
- Gaussian
- Lagrangian
- Empirical/statistical

Urban scale models tend to be Eulerian type models that calculate average concentrations on grids with typical grid sizes of around 0.5-2 km and grid extent anywhere from 20 to 300 km. However, steady state Gaussian models may also be used, where appropriate, and these potentially provide higher spatial resolutions. Box models are simplified urban scale models that treat the urban region as a single well mixed box and can be applied when emissions are poorly defined. Lagrangian type models, that follow air parcels over urban areas, are also a variety of urban scale model that provide similar resolutions to Eulerian models.

Local scale models can be Eulerian, in the case of computational fluid dynamic (CFD) models, but are more often parameterised models based on Gaussian, or near Gaussian, dispersion models. These are generally applied to traffic and point source emissions, which produce large local concentration gradients.

Empirical/statistical models are not process models but create a statistical link between observed concentrations and other factors, e.g. meteorology or other observations. As these do not describe the processes leading to pollutant concentrations they are usually only applicable at the site for which the statistics are developed. Some relationships developed in this way may be more universal and applicable at other sites but such models, and maps that may be produced using the relationships developed, must be dealt with cautiously.

Information on most models being used in Europe can be found on the ETC/ACC Model Documentation System (<http://pandora.meng.auth.gr/mds/gstart.php>). Another initiative to promote good modelling practise across Europe is the initiative on "Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes" (www.harmo.org). The US EPA also has a well documented modelling inventory and support centre (www.epa.gov/oar/oaqps/modeling.html) for a large number of US models that are often applied in Europe.

The following sets of recommendations address general model requirements including the spatial and temporal resolution of these models.

a) Basic requirements

The temporal resolution of models varies from application to application. For compliance with EU directives hourly means are the minimum temporal resolution required for assessment of NO₂ and O₃. For PM₁₀ daily mean is the minimum temporal resolution required. For PM_{2.5} annual means are sufficient. For population exposure (short or long term) the required temporal resolution will vary from minutes to years.

The temporal resolution of the model should be appropriate to the application. When only annual means are required then statistical Gaussian models may be suitable. For daily mean concentrations a model really requires an hourly temporal resolution. Any model being applied to assess exceedances of the EU directives, with the exception of PM_{2.5}, thus requires a temporal resolution of 1 hour.

The spatial resolution of models will also vary from application to application. For screening studies box models may be used that cover an entire city. For urban background assessment Eulerian models with grid resolutions of kilometres may be used. For Gaussian models the sampling resolution can vary dramatically.

The recommended spatial resolution for an urban scale Eulerian model, that calculates urban background concentrations, is approximately 1 km. This provides high enough resolution for emission gradients within urban areas without needing to resolve small topographic and large building features that should be described using local scale models.

In addition some basic principles apply when using models, as follows:

Atmospheric dispersion models should only be used when they are appropriate for the intended application, and their use should be justified. Thus it is very important to understand the model's limitations and apply it only to the situations that match its capabilities.

Models must always, whenever possible, be validated against observational data for the site of application (See the cross cutting issue report on uncertainty, Air4EU – M2, for details on recommended validation methods).

Model calculations should be analysed by experts before they are utilised.

Semi-empirical parametric or statistical models should be recalibrated against at least a small number of field measurements, if they are to be applied to new locations.

Models are only as good as their input data, i.e. emissions, meteorology, boundary conditions, etc. and so as much attention should be given to these aspects as to the modelling itself.

b) Best practice recommendations

In addition to the basic requirements some general best practice recommendations are as follows

Models are in general complex systems and only the most basic types, e.g. steady state Gaussian models, should be used and analysed by non-experts. Most models require expert understanding of the whole modelling system before successful application.

Any model has limitations to the scope of its application and to the accuracy of its predictions. It is recommended that the uncertainty of model results should be determined, and should form an integral part of the AQ-assessment. Also the uncertainty of the separate modules and input data should be determined (see chapter 5 on uncertainty analysis)

When showing maps of air quality, uncertainty maps should also be presented.

c) Scientific recommendations

Traditionally Gaussian type models have been applied due to their simplicity and limited computer requirements. As computer capacity and speed increases more advanced models may be applied at higher and higher resolutions. Mesoscale Eulerian models are now common place and CFD models are using increasingly higher resolutions and covering larger areas.

Before new and advanced models are operationally implemented their improved value, above current simpler methods, must be well documented.

In general, there is a need for independent, quantitative review and intercomparison of the various models used.

Refinement of guidance on QA/QC for modelling should be established. A clear statement of model uncertainties is indispensable in any AQ assessment study

3.2 Meteorology

Meteorological data, and the models used to create them, are an essential part of any air quality model. Spatial and temporal meteorological fields for air quality models can be determined using local observations and interpolated using diagnostic models or can be calculated using prognostic mesoscale models coupled to larger synoptic scale models.

Diagnostic models have the advantage of real world measurements to drive the model but the disadvantage that the measurements are often spatially sparse leading to large uncertainty between measurements. Mesoscale models have the advantage that they give the best representation of the results in areas without observational data, since they reflect the processes involved, but are more complex and resource consuming. Data assimilation techniques, on the mesoscale, would combine both of these methods but are also quite resource demanding.

a) Basic requirements

Urban meteorological measurements must be representative of an area equivalent to at least the model resolution, before they should be included in diagnostic models. This means that measurements in built up areas need to be made at least twice as high as the surrounding building height. Radio towers are one possible site for such observations.

Simple diagnostic models are appropriate for generating meteorological data when annual average concentrations are to be calculated.

When using diagnostic models it is recommended to have as extensive an observational net as possible since interpolation between, or beyond, measurements with diagnostic models is quite uncertain. It is particularly important to have meteorological measurements both in- and outside the built up urban region to provide information on both areas.

Statistical meteorological fields are often sufficient for annual mean calculations, when applied to steady state dispersion models

Meteorological fields should be sequential with a temporal resolution of 1 hour for assessment of peak conditions and daily mean concentrations.

b) Best practice recommendations

In complex terrain a nesting approach for the coupling of mesoscale to local models should be used.

The use of CFD models should be limited to particular hotspots where more knowledge of the complexity of the meteorological field is required. These are complex and time consuming models and not suitable for operational urban scale assessment.

Meteorological measurements should always be made at air quality monitoring sites. This will allow a clearer analysis of model performance in light of the meteorological parameters.

c) Scientific recommendations

Currently most meteorological models do not make use of urban meteorological measurements in data assimilation as they are generally considered to be unrepresentative. The use of data assimilation of meteorological data on the urban scale should be further researched for use in urban scale assessment.

Improved schemes for addressing the effect of urban land use are required for mesoscale models.

Strong stability and weak wind conditions, that can often lead to pollution episodes, are generally poorly modelled by even advanced mesoscale models. Research into methodologies to improve this situation are required.

Direct measurements of inversion strength and depth in urban regions is extremely useful information for generating meteorological fields and further research is required to implement this operationally.

3.3 Emission data: general recommendations

A detailed sectoral emission inventory leads to the identification of major emission sources. Emission data in spatial and temporal resolution are generated in an emission model and used as input to represent the sources within atmospheric dispersion models. Accuracy of generated emission data depends on the representativeness of activity rates and emission factors used for emission calculations as well as spatial allocation data and temporal profiles. This subchapter outlines several general recommendations of good practice for emission modelling. In the following subchapter more specific recommendations for PM, NO_x and NO₂ emission modelling on urban scale are provided. More detailed information on emissions is contained in the cross cutting issue report on emissions Air4EU – M1. General information on emission data generation on urban scale can be found as well in (Friedrich & Reis; 2004) and (Moussiopoulos; 2003).

Compiling emission data usually requires a multitude of input parameters in order to model reality as accurately as possible. Data collection, data analysis and data choice are important procedures for this compilation. Quality criteria for generated emission data specifically include accuracy, completeness, consistency and comparability (IPCC; 2000). The following general recommendations mainly refer to these requirements.

a) Basic requirements

It is good practice to document and archive all information, assumptions and methodologies for emission data generation as results are often significantly affected by individual choice of these input parameters.

Emission inventories should include summaries of methods used and references to source data such that the emissions estimates are transparent and steps in their calculation may be retraced. The documentation should consist of records that are unambiguous. This is an important precondition for a constant improvement and update as well as for an uncertainty analysis/verification. Examples of specific documentation and reporting can be found in (IPCC; 2000).

A validation of emission data or a verification of source contributions by source apportionment studies is desirable but often not possible because it requires extensive project capacities. If a direct validation of emission data is not possible, results of other emission estimates as well as source apportionment studies in similar areas can be reviewed to assess the inventory and used emission factors.

A recommended possibility for verification is the 'cross-check' with other independently compiled emission datasets e.g. on regional/national scale or for similar urban areas. In addition, results of source apportionment studies in similar areas analysing source contributions based on the chemical content of ambient air concentrations inside and outside the city may allow to assess emission estimates e.g. to verify the ratio of exhaust and non-exhaust PM₁₀ from road traffic or contributions from oil, coal and wood combustion.

The assessment of uncertainties within the emission inventory is usually complicated and cannot be done with statistical methods because of possible systematic errors due to the choice of methodologies and emission factors. Nevertheless, it is always necessary to give an answer to questions about uncertainties and plausibility.

It is recommended to always carry out an uncertainty assessment and analysis for calculated emissions at least qualitatively. The EMEP/CORINAIR Guidebook (EEA; 2003) presents a default table for quality ratings that can be used for uncertainty discussion and assessment.

b) Best practice recommendations

Emission inventories should include all anthropogenic sources that may contribute significantly to the concentration in the area under investigation. Coarse estimations – if transparent – are better than to omit relevant sources even though there is no established methodology and data for an emission calculation. Internal and external reviews can help to

evaluate completeness, key sources and plausibility of source contributions. A real expert peer review calls for a systematic approach to calculate emission data.

Although harmonised methodologies often do not exist, it is recommended to discuss data choice e.g. for emission factors with external experts in order to avoid systematic errors due to the choice of inappropriate or unrepresentative values.

As far as possible and reasonable, basic data (e.g. emission factors, activity rates, temporal profiles) and methodologies applied (e.g. sectoral level of detail, spatial allocation, other assumptions) should be harmonised with already existing inventories on regional or national level.

PM

Especially with regard to fugitive particulate matter, it is recommended to include emission estimations for sources like e.g. agriculture, construction, fugitive industrial sources, road dust suspension, barbecues, smoking, fireworks etc. The cross cutting issue report on emissions (Air4EU – M1) provides some references for the quantification of these emissions.

The significance of biogenic/natural sources depends on pollutant (e.g. NMVOC, PM₁₀) and local conditions such as vegetation, soils, temperature and humidity. Biogenic/natural emissions mainly originate from non-urban areas but may have a significant impact on urban air quality as well. Usually measured regional and urban background concentrations of PM₁₀ and its chemical content are used in order to include biogenic/natural primary and secondary contributions in urban scale air quality assessment. In addition, urban biogenic/natural emissions can be calculated and included in an urban emission inventory based on land use data and methodologies similar to quantifications on regional scale (see Air4EU – M1).

It is recommended to analyse contributions from biogenic/natural sources if they are significant for the urban ambient air PM concentrations in order to distinguish anthropogenic contributions from urban sources.

A validation of calculated emission data in spatial and temporal resolution aims for an assessment of total accuracy, parameter sensitivities and source contributions. This can be done by comparing measured and modelled total concentrations for selected areas (grid cells) and by comparing source contributions calculated in the inventory with locally measured contributions derived from a source apportionment study. A combination of both methodologies will provide best feedback to improve the emission data.

It is recommended to carry out a source apportionment study for at least one selected site in order to quantify the primary emissions and to compare calculated and measured source contributions (see Chapter 2).

c) Scientific recommendations

Further harmonised methodologies for emission calculation, documentation and validation are needed.

Therefore, clear and standardised requirements and practical guidelines for quality assurance and quality control of urban emission calculations should be defined by official national/European experts and applied for urban emission estimates.

Quantitative uncertainty assessment and analysis remain a problem regarding source inventories as well as emission data in temporal and spatial resolution.

Thus, it is required to have more research activities in Europe dealing with the definition of adequate procedures for an error quantification and sensitivity analysis with regard to emission data in temporal and spatial resolution.

Differences between measured and modelled concentrations are not only a result of uncertain emission data applied but also of model uncertainties or because the monitoring data was not representative for the spatially averaged value of the grid area obtained by the model.

For air quality assessment in cities, it is recommended to use the availability of monitoring data and the application of an urban atmospheric dispersion model to evaluate/assess the emission data input for selected grid cells. A scientific spatial and temporal analysis of model

and parameter sensitivities is required and should be done in cooperation between experts/responsible persons for modelling, monitoring and emission calculations (see chapter 4.1 on model evaluation/validation).

An additional scientific methodology for emission data validation is the evaluation of calculated emission data by air pollutant flux measurements around agglomerations of emission sources, see e.g. Slemr et al.(2002) or Friedrich and Reis (2004).

3.4 Emission data: specific recommendations for PM, NO_x and NO₂ on the urban scale

The first step of generating emission data is the calculation of sectoral emissions based on source specific basic data (activity rates, emission factors and source specifications). This leads to a sectoral source and emission inventory usually as an annual emission table for the city or already subdivided into different inner urban administrative units. Calculation methodologies as well as data quality are mainly a function of data availability and data choice. Based on the emission table, a spatial mapping can be achieved by allocating source emissions to smaller geographic units/areas or cells of a model grid. Often a geographic information system (GIS) and an intersection with geographic information such as road maps, point source coordinates and land use data are used for this purpose. The cross cutting issue report (Air4EU – M1) gives more detailed information on the methodologies. Recommendations for the generation of emissions on urban/agglomerate scale are given in the following.

a) Basic requirements

Road traffic, large combustion plants, industrial activities and small residential heating are usually major emission sources in urban areas. Emissions from key source groups should be calculated based on respective activity rates and typical emission factors. Generated emission data sets should match the spatial and temporal resolution of applied atmospheric dispersion models.

It is recommended to analyse emissions of key source groups in detail and as far as possible based on site specific information on activities and emission factors.

It is recommended to reach a spatial mapping of urban emissions with a resolution that is sufficient to identify and characterise most polluted areas (e.g. 1 km x 1 km or 2 km x 2 km).

The spatial allocation of emissions should be based on point, line and area sources. It is recommended to allocate area source emissions by local statistical and land use data and to use a GIS to intersect source contributions with a model grid.

The generation of hourly or at least daily emission data in spatial resolution is recommended for urban air quality assessment. Source specific temporal profiles of the activities should be used for this purpose.

PM

It is recommended to quantify not only PM₁₀ but also PM_{2.5} emissions in order to distinguish between mechanically generated particles and particles mainly generated by combustion processes.

NO₂

It is recommended to quantify not only sum of NO_x but also primary NO₂ emissions in order to be able to assess the influence of an increasing NO₂/NO_x emissions ratio from road traffic emissions on urban air quality.

b) Best practice recommendations

Air quality assessment on urban scale requires a high spatial resolution. In order to minimise uncertainties of gridded emission data, a detailed **spatial allocation** of point and line sources should be done before intersecting with a grid.

It is recommended to generate urban emissions on the highest possible spatial resolution in order to improve the accuracy and spatial differentiation. A resolution between 250 m x 250 m and 500 m x 500 m can possibly be achieved.

It is recommended to model emissions from major roads in urban areas as line sources based on local traffic census data (automatic counting). The spatial allocation requires a digitised road net and linked mileage data.

For the inclusion of point source data, local industrial data should be used if available. EPER data can be used alternatively for major sources. In addition to the emission fluxes, information on source location (coordinates) and effective height of stacks (stack height plus plume rise) should be available for the spatial allocation.

For area sources it is recommended to use statistical data and land use data on small scale (e.g. fuel consumption or population per square of residential area).

For air quality assessment on urban scale the generation of **emission data in temporal resolution** (e.g. hourly) is required. Temporal profiles should be defined and assigned to source groups on a detailed sectoral structure.

It is recommended to use local data if possible (e.g. traffic counts, working hours in local plants, holiday seasons). Local hourly temperature data should be taken into account for sources like residential combustion plants, gasoline evaporation and vehicle cold starts.

It is recommended to use monitoring data in temporal resolution for a validation of the temporal PM emission profiles.

As far as possible, **road traffic emissions** should be calculated and modelled with a bottom-up approach based on local information. Census data from automatic counting on segments of major roads can give a rough assessment of the overall traffic volume and a differentiation in large (heavy) and small (light) vehicles.

Manual traffic counting is recommended for selected roads and episodes (typical working day, Saturday, Sunday of different seasons) in order to distinguish between several vehicle categories, to determine travel patterns and fraction of heavy-duty vehicles and to specify traffic on roads where no automatic counting is done.

Detailed emission factor data sets such as HBEFA or COPERT III (see UBA 2004, Ntziachristos and Samaras; 2000) can be used if no national expert validated emission factor database is available for the quantification of road transport emissions. Because of the different methodologies both emission factor data sets are based on, the same assumptions for vehicle category, technology and road class will lead to different results. The user has to decide which emission factors are suitable and applicable for his scope.

It is recommended to calculate vehicle emissions from road traffic based on emission factors distinguishing between road classes, vehicle categories, the fraction of diesel and gasoline engines, the distribution of EURO emission standards, vehicle speed and different driving modes such as hot and cold start.

It is recommended to discuss and harmonise data choice for emission factors with national experts.

PM

Non-exhaust emissions of particulate matter due to tyre wear, brake wear and road dust suspension should be included in urban emission inventories as they contribute significantly to the PM₁₀ concentration. Recently a new chapter within (EEA; 2003) was published that provides suitable methodologies as well as default emission factors. Other emission factors from different measurement and modelling campaigns have been published enabling estimations of non-exhaust emissions for selected driving situations (see Air4EU - M1). Contributions to ambient air concentrations in urban areas can be quantified based on monitoring data as well.

Empirical models such as the US EPA model (EPA, 2003) can only be recommended if the model parameters represent well the local conditions. It is recommended to analyse the road dust contributions in addition to emission calculations by comparing urban background monitoring data for NO_x, PM₁₀ and PM_{2.5} with monitoring data from traffic stations (see the case study on non-exhaust PM emissions, Air4EU – CS D7.1.2, and cross cutting issue report Air4EU - M1).

For **power plants and large industrial facilities**, the usage of average emission factors from literature may not reflect local characteristics, which leads to significant under- or overestimations of single source emissions.

Activities of and emissions from large plants should be included as individual point sources. Emission calculations for single point sources should be done using specific emission factors taking into account local plant and abatement technologies.

It is recommended to use for this purpose industrial data provided by plant operators that should be available from regulatory authorities. If local industrial point source data are not available, EPER can provide emissions data from major sources in the urban area under investigation (EPER; 2004)

Small combustion plants, production processes, mobile sources on side roads and industrial areas as well as the use of products (e.g. barbecues, fireworks, smoking) can contribute as key area sources to the urban emissions.

It is recommended to calculate emissions from key area sources based on a bottom-up determination of activities. Suitable information must be sought within municipal registers.

Fuel consumption of small combustion plants can be quantified using energy and sales statistics and information from energy supply companies. Type and capacity of solid fuel combustion plants can be derived from building registers that often includes information collected by chimney sweepers or administration.

Default emission factors per fuel type from (EEA; 2003) or (EPA; 1995) are recommended for emission calculations if more recent and more specific information is not available from national or regional experts (see also data for wood combustion in the cross cutting issue report on emissions, Air4EU – M1).

If emissions from an **area source group** have to be calculated with a **top-down approach**, e.g. by allocating national figures to a smaller administrative unit/area, statistical and socio-economical data should be used that correspond well to the emission causing activities. Down-scaling by simply using population data is recommended only for certain source groups such as residential product use and residential combustion.

For downscaling and spatial distribution, it is recommended to apply other useful parameters such as car registrations or fuel consumption for road traffic emissions, employment by branch, nominal production or capacity, energy consumption, fuel consumption, raw material consumption for industrial source groups or land use statistics, animal numbers and crop production for agriculture.

For a top down approach it is recommended to use available emission data from official national/regional inventories with a high sectoral resolution instead of aggregated country totals that are provided e. g. from EMEP (2004). Generally, as much local data as possible should be used.

Monitoring data of regional and urban background stations as well as local traffic stations can be combined and analysed following e.g. the approach of Lenschow et al.; (2001). A comparison of regional background concentrations with urban concentrations leads to urban source contributions. If urban background concentrations are compared to local concentrations near major roads, contributions from local road traffic can be estimated and compared to model results. Methods and applications of urban source apportionment studies were extensively studied within the EU project SAPPHIRE (www.gees.bham.ac.uk/research/sapphire/).

PM

As mentioned before, PM source apportionment studies are recommended to compare background concentrations of primary particulate matter from urban sources – distinguishing between major source contributions based on the chemical content and the particle sizes - with modelled source contributions within the urban area.

It is recommended to distinguish at least between exhaust and non-exhaust emissions from road traffic, solid fuel combustion processes and significant industrial processes by using appropriate tracers (EC, OC or BC and particles smaller 1 µm for combustion derived

particles (mainly road traffic), selected elements (e.g. Si, Na, Cl, Ca, K, Fe for suspension of road dust or other mineral sources), organic compounds (e.g. Polycyclic Aromatic Hydrocarbons (PAHs) for incomplete combustion, levoglucosan for wood combustion, cholesterol for meat cooking).

The development of **action plans and strategies** to reduce urban emissions requires **trend scenarios** in addition to emission inventories for previous years. National trend scenarios can be taken e.g. from CAFÉ baselines (IIASA 2004) or national experts. Prognosis studies for specific source groups on a regional scale might exist that should be taken into account. This information can be used for urban or local trend scenarios as well.

In addition to that, it is recommended to include into scenario calculations also urban/local conditions, which may change the emission situation in the future (e.g. changes in road network, land use, industrial structure).

c) Scientific recommendations

For a realistic representation of urban traffic emissions, real world driving conditions are essential. Topography (road slopes), acceleration, ambient temperatures, traffic flow on minor and major roads and the vehicle load of heavy duty vehicles are aspects to be considered.

Hence, it is recommended to derive and use (real-world) emission factors that depend on traffic situations rather than just on one parameter such as average speed. This should be based on data from dynamometer measurements for different vehicle types, engine loads and driving conditions (real world driving cycles).

A systematic verification of vehicle emission factors used in Europe is required in order to assess their reliability and improve accuracy.

PM

The quantification of fugitive PM emissions (e.g. from agriculture, construction, material handling, industrial vents, barbecues and road dust suspension) remains a problem due to insufficient information about activity rates, specific emissions and influencing parameters/mechanisms.

Therefore, it is recommended to further examine fugitive PM emissions, to carry out more size selective measurements at typical sites and a systematic analysis and determination of model parameters.

In general, there is the need for additional emission measurements focussing on PM₁₀, PM_{2.5} as well as finer fractions and the chemical content of specific emissions relevant for urban areas.

Hence, it is recommended to identify and further examine significant emission sources in a systematic way in order to better characterise source contributions and their potential significance regarding health impacts in urban areas.

Emission measurements should always be associated with an uncertainty analysis and an accurate determination of activity rates of the sources under consideration in order to be able to derive usable emission factors (emission per unit activity).

Due to the obligation to develop action plans and programmes to control urban emission sources city authorities need approved information to assess possible abatement measures on urban scale.

It is recommended to carry out a systematic analysis of the impact of technical and non-technical measures such as low emission zones, improving traffic flows, speed limits, gas engines or particle traps for public transport, street sweeping etc. on PM_x emissions in urban areas.

Case study: Non-exhaust PM emissions in Rome, London, Oslo and Rotterdam

Assessment of non-exhaust PM by road traffic in urban areas (Air4EU – CS D7.1.2)

A method, developed in the European Topic Centre Air Quality and Climate Change project “Street Emission Ceilings”, was used to assess non-exhaust emissions of PM (PM₁₀ and PM_{2.5}) by road traffic. The method applies hourly monitoring data of NO_x and PM (PM₁₀ and PM_{2.5}, or fine and coarse fraction of PM₁₀) collected at a station pair: an urban background location and street/traffic monitoring station nearby. The method involves calculating the difference in concentrations, on an hourly basis, between the street station and the urban background station, and subsequently the ratio between the increments of PM fine and coarse fraction relative to the NO_x increment. This is presented on an hourly basis (average hourly variation across the day). An estimate of the non-exhaust contribution to PM is arrived at by assuming the coarse PM fraction represents the non-exhaust, and the fine (PM_{2.5}) fraction represents the exhaust particles. This analysis is carried out for winter and summer periods, and for work days and weekend days separately. This allows to consider the influence of heavy duty vehicles (HDV) to the non-exhaust PM (the HDV fraction of the traffic flow is usually considerably less during weekends), and also provides basis for looking at the seasonal variations in non-exhaust PM (important for conditions in Northern Europe/Scandinavia where studded tyres may be used).

The method is demonstrated for annual data in Rome, London, Oslo and Rotterdam. The case study shows that the method can be used to estimate non-exhaust PM, defined as the coarse PM fraction. Prerequisites are that the urban background station of the station pair is representative for the background pollutant situation at the traffic site, and that the monitoring is carried out with strict QA/QC procedures limiting the measurement uncertainty of the data, especially regarding the zero level calibration of the monitors. The method does not distinguish between suspension of road dust, tyre wear and brake wear particles, unless additional data are available (such as elemental composition, or EFs for tyre and brake wear particles). In addition, non-exhaust emissions for Rome were calculated based on literature and local traffic census data in order to verify if abrasion processes and re-suspension of road dust may be responsible for the difference in PM/NO_x ratio between concentration increments and traffic emissions. The results show that non-exhaust emissions are likely to be the missing source dominating the PM/NO_x ratio

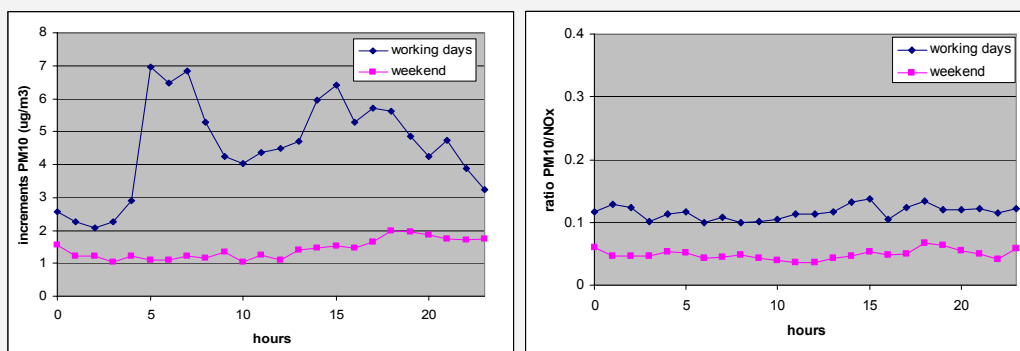


Figure showing the local contribution (Increments) to PM10 (left) and to the ratio PM10/NO_x for a traffic site in Rotterdam as a function of time of day. Blue are working days, and pink are weekends.

3.5 Dispersion and transport

Meteorological models provide the required input for the transport and dispersion of emitted pollutants. These two processes are essentially the same for all compounds even though the chemical or physical processes may differ between them. E.g. O₃ chemistry and deposition is quite different to PM chemistry and deposition but their transport and dispersion are treated in the same way within all models.

The treatment of transport and dispersion differs between model types. Gaussian steady state models generally assume a spatially constant wind field and ignore dispersion in the wind direction, i.e. the slender plume approximation. More advanced Gaussian and non-Gaussian models may improve on this but still rely to a large extent on spatially homogenous wind fields. Urban scale Eulerian models, which make use of spatially varying wind fields, often have well developed schemes for advection and vertical dispersion but not for horizontal dispersion. Urban scale box models simplify dispersion to a well mixed layer beneath the mixing height. CFD models can produce complex wind and turbulence fields for hot spot calculations but require large computing resources.

a) Basic requirements

Box models

- *Box models for urban areas may be used when emission data are incomplete or only available on a coarse grid. They should only be used for screening applications and preliminary policy analysis. At a basic level they can be used to supply urban background concentrations for local scale modelling.*
- *Box models for street canyons may be used when calculating annual mean concentrations but are not suitable for hourly means.*

Gaussian models

- *Gaussian models may be used for urban scale assessment if the terrain is reasonably homogenous. When meteorological fields become more complex, due to terrain or land use inhomogeneities, then Eulerian models should be used.*
- *Gaussian models are suitable for screening purposes when generating urban air quality maps. They are recommended for long-term applications when applied to the urban scale or for hourly calculations where meteorology is spatially homogenous.*
- *Steady state Gaussian models can be used for hourly calculations over short distances, distances less than the distance travelled in one hour, under most conditions assuming that building effects do not significantly alter the transport fields.*

Eulerian models

- *Eulerian models used for basic urban background calculations may be single or multiple layered. Multiple layered dispersion parameterisations should be based on at least K theory.*

b) Best practice recommendations

Gaussian models

- *When dealing with less homogenous meteorological conditions other Gaussian type models, such as segmented plume or puff models, may be appropriate for use with point sources.*
- *Point source subgrid models should include non-Gaussian effects of skewness in the turbulence profiles.*
- *Gaussian models used for the calculation of hourly concentrations near traffic sources in street canyons should contain parameterisations of the street canyon meteorology, e.g. OSPM (Berkowicz, 2000).*

- *Stability should be assessed using similarity theory rather than traditional stability classes.*

Eulerian models

- *The vertical resolution of a Eulerian model may have significant influence on the near surface concentrations, depending on the height of the emission sources. The sensitivity of Eulerian models to vertical resolution should be assessed for the differing source categories.*

c) Scientific recommendations

Non-Gaussian models that take account of vertically varying wind speed and turbulence should be further researched to establish their use in operational dispersion modelling.

When modelling near road dispersion of traffic emissions more research is required to establish the effect of traffic induced turbulence on the initial dispersion of these pollutants.

More research is required to improve models and their turbulence schemes under low wind speed and highly stable conditions.

Lagrangian particle models, that calculate concentrations from point or line sources based on the release of a large ensemble of model particles, are most appropriate for dispersion and transport calculations in complex meteorological conditions, e.g. GRAL (Öttl et al., 2001). However these models are usually too time consuming for operational application but hybrid systems, such as HYSPLIT (Draxler, 2003) may be applicable.

One aspect for the improvement of dispersion in models is the improved parameterisation of horizontal diffusion. This is true for both Gaussian and Eulerian models and particularly important under low wind speed conditions.

The initial dispersion of emissions in urban areas, such as those from domestic heating and from traffic, is not well defined in many models. Further research is required to establish these distributions.

Ensemble modelling, using a range of models, may be an appropriate method for establishing improved urban scale assessments (e.g. Cuvelier et al., 2007)

3.6 Chemistry and aerosol processes

In regard to modelling, the largest difference between the compounds of PM, NO₂ and O₃ lies in the description of the chemical and physical processes that lead to their formation and removal. For NO₂ and O₃ chemical processes are the most significant. These processes vary hugely on time scale. The faster processes, which quickly convert NO into NO₂ through photochemical reactions with O₃, will dominate during daytime on the local and urban scale.

Formation and removal of PM, on the other hand, generally occurs on time scales larger than those of significance on the urban scale, with the exception of wash out which has a significant effect.

Chemical and aerosol processes can be described at several levels of complexity. The simplest level is the use of direct empirical relationships, e.g. that can convert NO_x emissions to NO₂ values (Derwent and Middleton, 1996). The next level are simplified steady state schemes, for example the photochemical steady state NO_x / O_x scheme and the Ozone limiting method (OLM) (Cole and Summerhays, 1979). Simple non-steady state schemes also exist, e.g. the discrete parcel method (DPM) from Benson (1984). These simplified schemes are those applied to Gaussian models. Further to these Eulerian models can make use of more complex time varying chemical schemes that can contain any number of compounds.

PM₁₀

a) Basic requirements

On the local and urban scale the influence of chemistry, secondary particle formation and aerosol dynamics on the total mass of the particles is limited. As such a model may neglect these processes as a good first estimate and treat PM as a totally inert species.

b) Best practice recommendations

The approximation described under 'basic requirements' above will be less correct in southern latitudes and during summer periods. However, there is still a large uncertainty in

many of the aerosol processes relevant to particle growth and formation and it is not recommended to include these processes in urban scale models.

It is recommended that Eulerian models applied to large urban regions take into account the influence of chemistry, through the formation of sulphates and nitrates, on the total PM mass as well as the deposition processes.

Gaussian models for point and line sources should include both dry and wet deposition processes.

c) Scientific recommendations

There are still a large number of uncertainties in many of the aerosol processes and continued research is required to improve these. This includes the formation of secondary organic aerosols as well as the heterogenous effects associated with water solubility and particle growth.

Up to now most assessments are confined to particle mass concentrations, which are less variable within the local urban scale. However, particle numbers can vary by many orders of magnitude within these scales. As such it is not expected that particle number concentrations, if these are to be calculated, can be assessed using the same methodologies as for particle mass.

NO₂ and O₃

NO_x emissions (NO+ NO₂) from traffic and other combustion sources are dominated by NO (~90%). The conversion of NO to NO₂ on short time scales is dominated by the photochemical reactions between NO, NO₂ and O₃. In an urban setting these reactions will reach equilibrium on time scales less than an hour. Even so, other reactions involving various hydrocarbons can also significantly affect the production of NO₂ and O₃ on these short time scales.

The most complex chemical models involving NO₂ and O₃ can contain 100's, if not 1000's, of reactions but most of these occur on timescales much larger than those found on the local and urban scales. Most of the chemical schemes thus applied in urban areas are simplified versions of these. Even so, chemical equilibrium is not approached for even the simplest of these chemical schemes on the local scale and so local and urban scales will require different approaches.

It should be noted that the introduction of reactive species into Gaussian models requires estimates of 'effective' concentrations for the reactions calculations. Non-linear chemical processes are not compatible with the linear Gaussian model.

a) Basic requirements

For screening purposes and longer-term averages, locally deduced empirical relationships for determining NO₂ based on NO_x concentrations can be used, e.g. (Derwent and Middleton, 1996).

For urban background calculations the photostationary state relationship may be used but should not be applied to local scales.

Ozone limiting method (OLM) generally over predicts NO₂, makes assumptions concerning the availability of O₃ and assumes stationarity. It is not recommended for general use.

b) Best practice recommendations

For local scale modelling the discrete parcel method (DPM), e.g. Benson (1984), which takes into account non-stationarity and the basic photochemical reactions, is recommended as the best analytical technique.

The photostationary state relationship is not suitable for local scale modelling, as equilibrium will not be reached, and should not be used on this scale. However, this may be applied on the urban scale when no information is available concerning other reactive species.

For hourly or peak values of the pollutants NO₂ and O₃, models with simplified chemical reaction schemes, e.g. generic reaction set GRS (Venkatram et al., 1994) can be used for both local and urban scale modelling.

More complete chemical schemes, similar to those applied in regional scale models, are preferred for use on urban scales, in combination with Eulerian models, if emissions and rural background concentrations of the other relevant reactive species is known.

c) Scientific recommendations

A detailed comparison of different chemistry schemes relevant to local scales is needed to identify the merits and limitations as well as the applications of the various approaches.

3.7 Rural background contributions

The rural background contributions, i.e. all concentrations not resulting from local urban emissions, can make up a significant part of the total concentrations. For O₃ the rural background levels are generally higher than the urban levels, for PM urban contributions are often of the same order as the regional contributions and for NO₂ the rural background levels are generally lower than the urban concentrations, though regional background levels can be high in more polluted agglomerations. The rural background contributions can only be estimated using measurements outside of the city or by regional scale models.

When using regional models, or rural observations, it is important to be aware of 'double counting'. This is when the results of emissions from the urban area are effectively counted twice. With observations this can occur when rural background concentrations are taken from rural stations downwind of the urban region. With models this can occur when regional and urban scale models, which both in principle contain the same emissions, are not responsibly combined, e.g. different meteorological fields in the two different models.

a) Basic requirements

The minimum requirement for obtaining rural background values from measurements is:

- *Hourly, daily and annual mean concentrations taken from at least 1 rural background station in the vicinity of the urban area.*
- *If more than one station is available then wind direction should be used to determine the most appropriate upwind station. This may be based on weighted averages dependent on the wind vector.*

The minimum requirement for obtaining rural background values from regional models is:

- *Hourly, daily and annual mean concentrations taken from the grid position upwind of the urban area.*
- *PM and NO₂ bias is common in regional models as most models currently underestimate these 2 compounds. The model should be either validated or adjusted, through data assimilation, to account for this bias.*

b) Best practice recommendations

When using observational data from rural background stations the following best practices apply:

- *The recommended number of rural background stations required for calculating rural background concentrations is 3, surrounding the urban area. These 3 stations should be selected based on the most appropriate upwind direction.*
- *Hourly average values are always preferred, including meteorological data, for a clearer understanding of the transport processes*
- *O₃ concentrations during stable periods are often reduced close to the surface due to a lack of mixing and depletion through deposition processes. The available O₃ in an urban area may actually be significantly higher, due to enhanced mixing in urban regions, than the rural O₃ measurement indicates. There is no simple method for accounting for this, apart from using daily means or running means, but the user should be aware of this.*

When using regional models as boundary conditions for urban scale models the following best practices apply:

- *When meteorology is consistent between the regional and urban scale model then boundary conditions can be spatially interpolated directly from the regional model. When this is not the case then the urban model domain should be expanded to be significantly larger than the urban region so that no 'double counting' takes place.*
- *As an alternative, when meteorology is not consistent between regional and urban models, the boundary conditions can be taken from the upwind side of the regional model*
- *Nesting, where larger and smaller scale models directly interact with one another (be it one or two way nesting) is highly recommended as a consistent methodology for including rural background concentrations into an urban scale model*
- *The use of data assimilation, to improve upon the bias of current regional models, is recommended to improve rural background concentrations used for assessment*
- *The chemical schemes and compounds should correspond as closely as possible to each other when regional and urban scale models are nested.*

c) Scientific recommendations

Many regional models currently underestimate PM concentrations and so their value as rural background is questionable. The need for improved emission inventories and process descriptions in these models is clear.

Many regional models currently appear to underestimate NO₂ concentrations (van Loon et al, 2004) and so their value as rural background is questionable. The need for improved process descriptions, particularly in the vertical exchange, in these models is clear.

Case study: Homogenous regional background concentrations for Europe

Data assimilation with a regional scale model: homogenous regional background for city assessment (Air4EU –CS D7.1.12)

In the context of implementing the European air quality legislation and aiming to maintain the limit values for the regulated pollutants PM, O₃ and NO₂ cities strive to identify abatement measures to limit emissions from mobile and stationary sources. In this context it is of importance to differentiate, as precisely as possible, between air quality concentrations caused by sources within the city and regional background concentrations. To assess the latter is much more difficult since local authorities normally do not have enough information available (e.g. emission inventories) to assess the background concentrations through model runs. In addition, the models used often have a limited model performance, especially in the case of PM₁₀. The determination of the regional background by observations is also problematic since it can be difficult to assess to what extent rural background stations are influenced by the city emissions themselves, resulting in the problem of double counting.

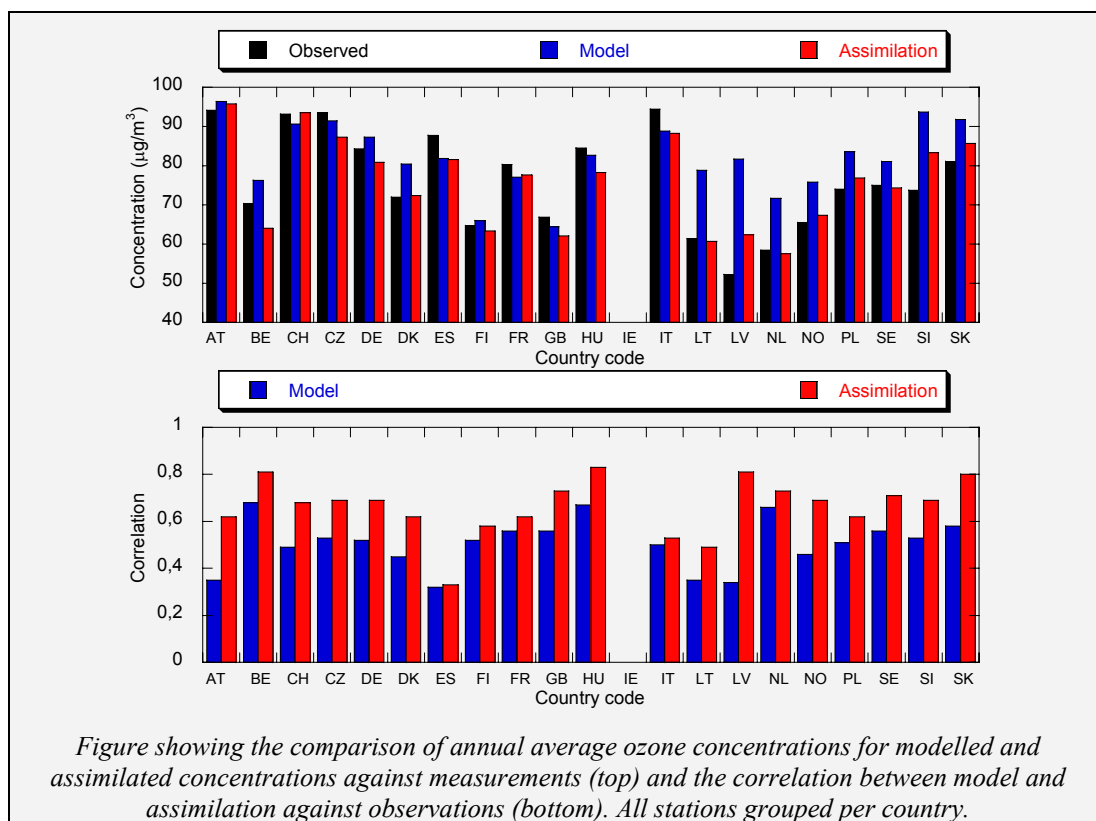
The AIR4EU project has recognised that determining, in a reliable way, regional background concentrations is one of the major drawbacks cities are facing and so AIR4EU has developed a method to prepare background concentrations through innovative data assimilation methods.

The method developed consists of the CTM LOTOS-EUROS coupled with the data assimilation method Ensemble Kalman Filtering. This system can combine observations of the species O₃, PM₁₀, PM_{2.5} and NO₂, and also of other species if wanted, with modelled concentrations of these species. The results are consistent air quality fields over Europe, on an hourly/daily averaged basis, and on a grid resolution currently of about 15 x 15 km², and for time periods of years. Examples have been made for the year 2003 for PM₁₀ and O₃. The assimilated fields have a reduced uncertainty relative to the uncertainty of the observations, or the uncertainty of the modelling separately. These fields can be used to provide regional background concentrations as well as to provide air quality fields for air quality assessment over Europe.

In principle, because the system is operational, these background concentrations can be made available and can be used by city users and others

Based on the experience gained in this case study we recommend:

- To use the produced background conditions in combination with a high resolution urban model in which the city including the area around the city of about 300 x 300 km² is represented.
- To improve especially PM₁₀ modelling to try to remove the consistent underestimation
- To try to clean the data from the AIRBASE network and/or concisely assess the quality of the data. This would be very beneficial for validation and probably future assimilation experiments.
- To launch a study to address the impact of the developed system on cities air quality assessment using a detailed city scale model.



3.8 Interactions between modelling scales

Most models are developed to deal with a limited spatial scale. This is a requirement strongly determined by both computational cost and availability of data. However it is often necessary to calculate concentrations on a variety of scales. Rural background contributions to urban scale modelling, see chapter 3.7 above, is an example of scale interaction from large to small scales.

When calculating exceedances or human exposure in an urban area it is necessary to include both the urban scale and the local scale in the model calculations. This can be done by coupling urban and local scale models together. There are two different approaches to this. The first is 'nesting' where particular local regions, within the urban area, are selected and Eulerian type models, e.g. CFD models, are coupled to the urban scale model. The other is the use of 'subgrid' models that are employed to improve resolution near particular emission sources such as major roads and stacks. Subgrid models often employed are Gaussian type line and point source models.

Double counting of emissions is one aspect of scale interactions that should be addressed in any model system. This occurs when the same emissions, e.g. from a road, is placed within both the urban scale Eulerian model and the subgrid model. If the contributions from both subgrid and Eulerian model are added together then double counting of emissions will occur. This tends to be negligible near the source, where the subgrid model will dominate, but can be substantial further from the source.

More detailed information on the interaction between model scales and rural background contributions is contained in the Air4EU Milestone report (Air4EU - M4) on scale interactions.

a) Basic requirements

When subgrid models are used then PM may be treated as a passive pollutant.

When subgrid models are used NO_2 must be calculated using one of the chemical schemes detailed in chapter 3.6.

b) Best practice recommendations

When carrying out assessment in urban areas with Eulerian models some form of subgrid model must be employed to address strong gradients near traffic and industrial sources.

When subgrid Gaussian line source models are employed within a Eulerian urban background model the effect of double counting on modelled concentrations can be approximated by

$$\text{Double Counting}\% \approx \frac{L}{\Delta X} \frac{\sigma_z}{h_{mix}} \times 100.$$

Where L is the road segment length, ΔX is the grid width, σ_z is the Gaussian vertical distribution parameter and h_{mix} is the mixing height of the boundary layer. This formula indicates that double counting is most likely when line sources are long and when mixing heights are low. Since σ_z increases with distance so too does the relative effect of double counting.

Double counting of emissions may be a problem when using subgrid models. An assessment of the influence of double counting on the results should be made.

Modelling systems that avoid double counting should be employed where possible.

c) Scientific recommendations

Almost all subgrid and nested model systems employ one way nesting, i.e information from the larger scale is provided for the smaller scale.

It is recommended that methods for two way nesting for subgrid models be investigated further. In regard to PM and NO₂ such models may be required to better describe effective emissions into the urban scale grid when transformation processes are important.

Plume-in-grid models, particularly those that contain photochemical reactions, are still not sufficiently developed or tested for operational applications and further research is required on these.

Methodologies for upscaling subgrid models, i.e. inclusion of subgrid model fluxes into Eulerian grids, still needs further research to identify the best operational method for doing this.

Model resolution needed in an assessment depends on the application and pollutants concerned. Because of the lack of highly resolved spatial and temporal input data and the limitations of model formulation, more research is needed to examine the proper model resolution for different applications (Air4EU – CS D7.1.9)

Case study: Stationary source contribution in SE England

Assessment of stationary source contribution to surface pollutant concentrations using a 3-D Eulerian Air Quality Model (Air4EU – CS D7.1.9)

Conventionally stationary source emissions are evaluated using dispersion models in the near-field, with background concentrations provided from measurements. Usually one ground-level upwind monitoring site is used to describe the composition of the background air coming into a region of a stationary source. Long-range deposition from stationary sources is treated by assuming the stationary source makes up part of the emissions within a grid square. More strict emission controls are already in place, or will be in place for most major European stationary sources, which would tend to focus attention on the interaction of stationary sources, in combination with other sources, rather than the behaviour of a single source on its own. The complex nature of the problem which is governed by multipollutant and multiscale interactions and coupling between atmospheric chemistry and dynamics suggest that improved methods are needed. This case study demonstrates the use of a 3-D Eulerian air quality model-CMAQ to estimate the contribution of UK stationary point source emissions to ground level pollution levels focusing on the uncertainty related to model resolution. The investigated area is the Southeast of England. Twenty-two monitoring stations with observation on O₃ and NO₂ are available within the studied domain. The model was assessed using statistical parameters including correlation coefficient, fractional bias, root mean squared error, normalized standard deviation and fraction of predictions within a factor of 2 of observations. Results indicate that the CMAQ model has better performance for O₃ than for NO₂. For NO₂ fine-resolution simulation presents better statistic scores. The performance of the model for ground-level O₃ was not improved when the horizontal grid spacing was reduced. The contribution of UK point sources to ground level O₃ and NO₂ concentrations in the presence of other sources, i.e. area, traffic and biogenic, was assessed using sensitivity analysis where emissions from UK point sources were removed. The dependence of results on model resolutions was discussed.

The following recommendations resulting from the case study can be identified.

- When an assessment involves complex interactions among multi-pollutant and multi-scales more advanced models should be used. 3-D Eulerian air quality models, such as CMAQ, are able to give valuable information on magnitude of point source contributions, and their spatial distribution. This information can help end users to identify the most affected area and the most important pollutant to regulate.
- When a model is applied to a new study area, a thorough evaluation should be performed and model performance should be documented. Both qualitative and quantitative methods should be used to get a full picture of model performance before its regulatory use
- Model resolution needed in an assessment depends on the application and pollutants concerned. Because of the lack of highly resolved spatial and temporal input data and the limitations of model formulation, more research is needed to examine the proper model resolution for different applications

Case study: Assessment of PM in Athens

Assessment of PM levels and contributions in the Athens region (Air4EU – CS D7.1.11)

Efficient Air Quality Management is based on a detailed and accurate air quality assessment where the relative source contribution is identified and, if possible, quantified. Therefore, in this case study, a combination of monitoring and modelling methods was employed, in order to derive information on current and future Athens air quality respectively. The study focused mainly on PM₁₀ because of their recognised health impacts and the increased scientific interest they recently have received.

The current air quality in Athens was analysed using measurements, by collecting and comparing urban and suburban PM₁₀ data for the years 2001-2003. In this way, the prevailing trends during this short time period have been revealed and they were then connected through the modelling studies with the main contributing sources, thus indicating the appropriate emission reduction strategy. The data demonstrated an increase of PM₁₀ annual values, mainly in the urban but also in the suburban stations, between 2001 and 2002, while a decrease was observed between the years 2002 and 2003. However, the number of PM₁₀ exceedances relative to the 2005 EU limit was significantly reduced between 2001 and 2002, as well as in some cases between 2002 and 2003. The emissions indicated that road transport was the main source contributing to NO_x and CO concentrations, whereas the industry sector was mainly responsible for PM and SO₂ emissions.

In this case study, scale interactions were considered by combining three different scale models, from the regional down to the local scale. Also, aspects of scale interaction are examined by a sensitivity analysis of the model to two different boundary condition datasets (meteorological and initial/lateral concentrations). Background/natural emissions are also taken into account in the case study modelling simulations. Emission reduction scenarios were successfully employed in the Athens case study, and with their use the most appropriate control strategies were identified in order to achieve compliance with EU legislation.

In chapter 3.4 of this document, it is recommended that non-exhaust emissions of particulate matter due to tyre wear, brake wear and road dust suspension should be included in urban emission inventories as they contribute significantly to the PM₁₀ concentration. Although the US EPA resuspension model has often been criticised for overestimating emissions, data availability made it the model of choice in this case study. Therefore, if the application of a resuspension model is considered necessary, the user should consider the high input data requirements of most relevant methodologies.

3.9 Population exposure

Dependent on the methodology employed and the needs of the calculation, population exposure can be carried out at a variety of levels. In general, population exposure is dealt with as the 'potential' exposure. The following is indicative:

a) Basic requirements

The most straightforward methodology for assessing population exposure is to combine spatially distributed population density maps with concentration maps. E.g. if a map showing the spatial extent of exceedance and the population density is available then a similar map can be constructed by taking the intersection of these maps. The spatial resolution of both model and population density defines the final spatial resolution of the combined maps.

b) Best practice recommendations

When population distribution is well known, in terms of high-resolution population density maps or home address data, then more advanced methods for population exposure can be applied. This entails the use of subgrid modelling to reflect local air quality concentrations near hotspots within the urban region.

It is strongly recommended that potential population exposure calculations take into account high-resolution population density data near major roads and other hotspots. To achieve this local scale models are required and thus subgrid models must be implemented in the modelling scheme.

c) Scientific recommendations

There are a number of more advanced methods for assessing the total population exposure based on the mobility of populations, indoor exposure calculations and activity data. These methods are more complex and require a large and varied dataset of concentration data as well as a statistically significant activity data

It is recommended that these methods be further investigated and properly validated to assess their improvement of population exposure calculations above the static methods described above.

3.10 Modelling source contributions

Models are very useful tools for assessing the contribution of various sources to the total concentration. Models allow any number of scenarios based on the removal or addition of sources or on changed emission scenarios. One of the most widely used applications of models in this regard is for carrying out impact assessment studies whenever new developments are proposed, be they changes in traffic flows or the building of new industrial plants. Used in this fashion, models are predictive and cannot be corroborated by observations. Other methods that use source apportionment from monitoring data as well as models, chapter 4.4, can be used to obtain independent checks of the model estimated source contributions.

a) Basic requirements

There is a long history for the use of Gaussian type models for impact assessments from industrial stack emissions. Any one of a number of widely used models may be employed for an impact assessment, keeping in mind that the results are most reliable when the terrain is homogenous.

When dealing with non-reactive pollutants on urban scales, e.g. PM, then source contributions from particular emission sectors or areas can be calculated simply by modelling that single source. For reactive pollutants such as NO₂ all other sources must be included in the calculation since the impact of each source cannot be linearly summed (Air4EU – CS D7.1.9).

b) Best practice recommendations

Some estimate of the uncertainty should be provided with any impact assessment.

If models are used to determine source contributions and to assess abatement scenarios then it is highly recommended that some form of independent check be made, usually

through source apportionment by monitoring, to assess if the model is correctly proportioning the sources.

Some applications can be quite complex, e.g. multiple interactive sources with reactive chemistry. The complexity of the situation should be reflected in the model applied. Gaussian models generally cannot deal with interacting sources such as multiple stacks and urban regions and so typically Eulerian CTM models need to be applied to assess source impacts (Air4EU – CS D7.1.9).

4. Combining modelling and monitoring

Measurements provide the most direct information on pollution conditions (at least at the measurement sites), but they cannot be used to explain the relationships between sources and ambient pollution, which is necessary if surveillance programmes are to be used for other purposes than merely reporting the present conditions. Proper interpretation of the measurements in terms of source-receptor relationships, meteorological conditions, emissions, urban conditions etc., can only be done using well performing urban and local dispersion models. It should be stressed, however, that neither measurements nor models on their own can provide all the information needed in conducting a good AQ assessment at the urban scale. In fact, both measurements and modelled concentrations contain relevant information about the air quality patterns and their behaviour. Consequently, using only measurements or models, and not both, for AQ assessment, should be avoided.

Combining model results with measurements reduces uncertainties inherent in both, and is strongly recommended in order to achieve a better depiction of the real situation in the area of interest.

The most common method for combining modelling and monitoring is to use monitoring data to evaluate/validate the model. The actual process of evaluation/validation is discussed in more detail in chapter 5.1, under uncertainty analysis, and in the cross cutting issue reports, Air4EU – M2 and M3. During a models development, and its further application, the evaluation processes should indicate deficiencies in the model. Improvement of the process description in the model based on the comparison with observations is an essential part of any model development activity. However, there is always a danger that models become 'tuned' to their validation data when this is limited.

Any model used for assessment should have been validated under a number of varied conditions and at a number of varied sites.

The so-called 'inverse' modelling used in emission determination procedures, which typically uses receptor site species and dispersion data to estimate emission rates, is another application for integration of monitoring and modelling. This form of combination has been addressed in the Air4EU case study Air4EU – CS D7.1.5.

4.1 Model evaluation/validation

The most common method for combining modelling and monitoring on urban and local scale problems is to use monitoring data to evaluate/validate the model.

a) Basic requirements

The models used in AQ assessment should have some form of published evaluation or validation assessment available, and/or should be recognised as fit for the purpose of application.

When measurements are not available in the assessment region then the model should have been well validated at a number of other, but similar, sites.

Expert assessment of the evaluation/validation is always required.

b) Best practice recommendations

The models used for assessment should be well validated at a number of different locations within the assessment area.

c) Scientific recommendations

Understanding properly the relationship between a given model and a set of observations is generally a complex issue. Although much work has been done in this area resulting in different recommended statistical evaluation parameters, and evaluation kits and procedures such as the BOOT program and the ASTM procedures etc., more research on how to evaluate models properly is still needed.

Sensitivity analysis of model response to uncertainties in input data using Monte Carlo ensemble methods is one research area that could well be studied further.

It is generally advisable to increase the interaction with the statistical communities to further advance methodologies.

4.2 Data assimilation

Combining monitoring and modelling can also be done using different techniques of data assimilation. The purpose of such techniques is to adjust the resulting model fields or model parameters with monitoring data to achieve a better fit with the measured concentrations.

A number of data assimilation techniques are available. Some data assimilation methods have already been applied at the urban scale with good results, though few, if any, have been carried out on the local scale, see the Air4EU background reports Air4EU – D3.1 and D4.1 for a review of current methods. Available methods include the simpler linear regression models, Kriging and Optimal interpolation (OI) methods. Other more advanced techniques are also available, such as the 3D-Var, 4D-Var, Kalman filters such as the Ensemble Kalman filter (EnKF) and the Reduced Rank Kalman Filter (RR-KF) methods, smoother versions of the same methods (EnKS and RR-KS) using measurements over a time interval, and Monte Carlo Markov Chain methods such as the recently developed Sequential Importance Resampling method (SIR).

For urban scale models there are many ways to select the data assimilation parameters. If the model is a 3D Eulerian grid model, one could choose as model 'parameters' the vector of all 3D grid cell concentrations. The data assimilation procedure will then directly adjust these concentrations in order to better fit with the measurements. Alternatively, the parameters could be chosen among input parameters to the urban scale model, such as e.g., urban emission data, meteorology (wind, stability, etc.), or boundary conditions such as the regional scale background concentrations etc. Which parameters to choose, generally depends on the aim of the assimilation, i.e., which parameters one wants to estimate better using available measurements.

In addition to a Eulerian grid model, an urban scale model may also include subgrid models such as an open road or street canyon model for dealing with dispersion close to specific roads or streets. Input parameters to the subgrid model, like local emissions, wind speed and direction, local dispersion conditions etc., could then be added to the list of data assimilation parameters, and estimated as part of the data assimilation procedure, if there are one or more monitoring sites influenced by such sources. Also, if pollution from industry stacks etc. influences the air quality level at the monitoring sites, parameters characterizing the variability of such sources should be added as well.

The following set of recommendations on data assimilation reflect some of the more basic methods and general considerations when applying data assimilation. More detailed information on data assimilation is contained in the Air4EU Milestone report (Air4EU – M5) on data assimilation.

a) Basic requirements

At a basic level data assimilation is not always possible since the number of available, or suitable, sites for carrying out data assimilation may be very limited. If this is the case then data assimilation should not be implemented.

When model results are poor, in relation to the evaluation process, or with strong bias then it is not recommended to carry out data assimilation but rather to improve the model description.

When a number of measurement stations are available then a robust and simple method of data assimilation is to create a linear regression model, based on the air quality model. The regression should take into account background concentrations, which may or may not be part of the model itself. Such regression models will minimise the RMSE between the air quality model and the available observations whilst preserving the spatial form of the model.

Urban air quality has a typical spatial variation that is much higher than the distance between monitoring stations when local scale sources are included. Interpolation methods such as optimal interpolation and kriging, when applied solely on monitoring data, will not capture this variation. These methods should only be applied in combination with models that can represent the spatial variation.

For all data assimilation purposes the spatial representativeness of the model and observations should match as closely as possible.

b) Best practice recommendations

When selecting parameters to be used in the data assimilation procedure, focus should be on those parameters which are most uncertain, and for which measurements will be most useful. Parameters which are uncertain, but for which model output concentrations will not be very sensitive, should not be included in the data assimilation procedure. Thus one should be selective and parsimonious in order not to over-fit the model to the measurements. In this respect data assimilation is very similar to the classical problem of parameter estimation in statistics.

Before using more sophisticated techniques of data assimilation it is of vital importance that the model is thoroughly evaluated and validated locally, using local input data and measurements. This part of the work should not be underestimated, as it often forms the key to success in combining monitoring and modelling. Ideally, the model should show little or no bias as compared to the measurements. Most of the above mentioned data assimilation methods work best if there are little or no bias between the model and the measurements. There should also be a reasonable good time correlation between the two before attempting to use such methods.

PM

It is perhaps easiest to apply data assimilation first to $PM_{2.5}$ rather than PM_{10} , since there are generally more sources to PM_{10} , and thus more difficult to model PM_{10} than $PM_{2.5}$.

NO₂ and O₃

It is perhaps easiest to apply data assimilation first on inert or nearly inert species such as NO_x ($NO + NO_2$) or O_x ($NO_2 + O_3$), before working with more reactive species such as NO_2 and O_3 .

Data assimilation methods applied to NO_2 or O_3 should use relevant information from other related chemical species when carrying out the assimilation. For example, it is not recommended to assimilate only O_3 data into a chemical model for calculating O_3 concentrations; NO_2 , NO and other hydrocarbons should also be included since they directly influence the O_3 concentrations

One should also bear in mind that typically in data assimilation only about ¼ of the work involves the selection or development of a particular method or technique of data assimilation, while the remaining ¾ part of the work is typically spent working with the model itself and with the monitoring data, in order to improve the model and to understand the relationship between the model and the measured concentrations

c) Scientific recommendations

It is generally recommended that more research is done to improve understanding of how to best apply existing methods of data assimilation when we have many model input parameters and relatively few observations, as is typically the case for urban scale air pollution modelling.

More research is required into how to best characterize and estimate the representativeness of point-like observations compared to spatial averages from grid models.

It is important to study the advantages and disadvantages of different data assimilation methods as applied on the urban scale when it comes to cost of computation and accuracy of results. Most data assimilation methods assume that the model and observation errors have Gaussian probability distributions. If this is not the case, due to different non-linear processes taking place in the urban environment such as aerosol-chemistry processes, it is important to study further the eventual improvements of using other methods of data

assimilation that do not depend on such Gaussian assumptions, such as the class of Markov Chain Monte Carlo methods.

It is generally advisable to increase the interaction with the statistical communities.

Case study: Data assimilation in Prague

Basic data assimilation methods: application to the urban scale (Air4EU- CS D7.1.6)

There are a number of methodologies available for combining monitoring and modelling data that will lead to the production of maps showing air quality. Many of these are complex applications involving data assimilation techniques that will require direct interaction between model calculations and observational data. Often the complexity of such methods limits their application to research institutes, making them inaccessible to city authorities that require such maps. This case study looks at a number of 'off line' methods for combining maps of annual means, calculated using a Gaussian statistical model, with monitoring data. The application area is the city of Prague where 12 monitoring stations with measurements of the pollutants PM₁₀, SO₂ and NO₂ are available. The methods investigated include regression analysis, kriging, kriging of the observed-modelled residual and Bayesian assimilation. The quality of the assimilation method is assessed using the cross validation RMSE.

The results of the study show that all of the assimilation methods for this application can provide improved maps of air quality with the following recommendations:

- Regression analysis is the simplest and most effective method for improving the assessment maps and their associated uncertainty.
- At least 10 measurement sites, of similar spatial representativeness to the model resolution, should be available for confidence in the regression analysis.
- Small improvements in the assessment maps, near observational sites, can be achieved through residual kriging or through Bayesian assimilation.
- To demonstrate the improvements in the air quality maps, corresponding uncertainty maps should be produced along with maps.
- It is important to have good regional background measurements and/or model fields for assessment purposes

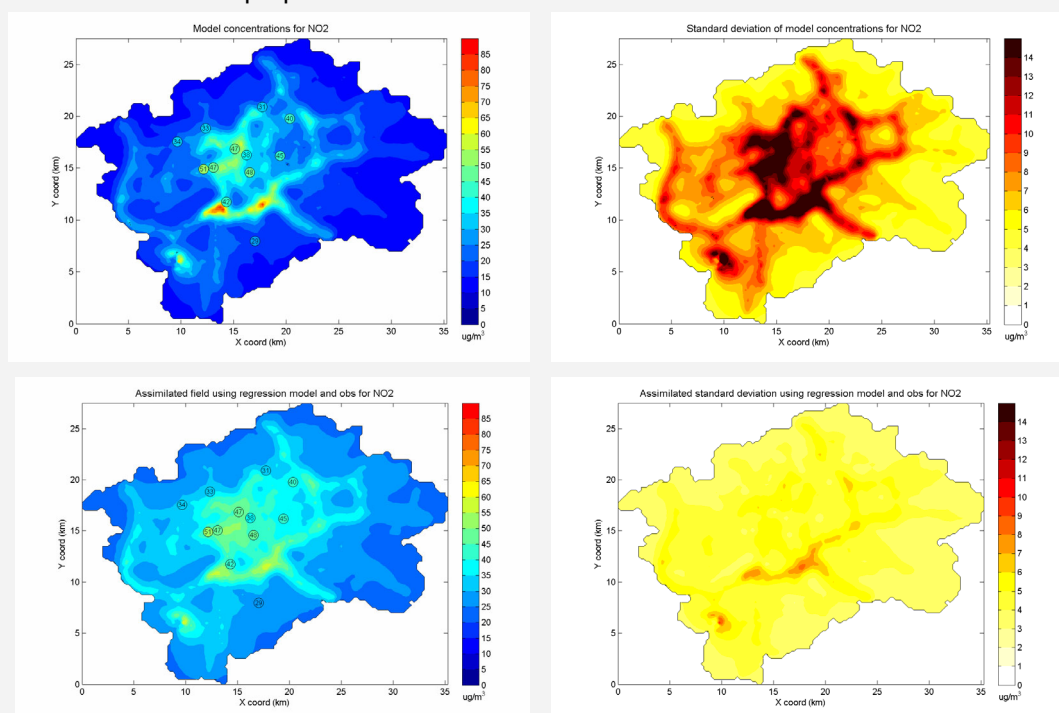


Figure showing the annual mean NO₂ concentrations for Prague, left, along with the uncertainty, right, displayed as standard deviation. The original model calculations for Prague from ATEM are shown, top, before data assimilation and after data assimilation, bottom, using a Bayesian combination of kriged observed fields and model regression. The estimated uncertainty in the NO₂ field is reduced by almost a factor of 2 and overall NO₂ levels have been reduced slightly.

Case study: Data assimilation in Paris

Comparisons of data assimilation methods at the urban scale in Paris (Air4EU – CS D7.1.7)

Air quality assessment can be performed using a monitoring network, an integrated mesoscale modelling system and/or data assimilation techniques, which couple observations and simulations. In this case study two data assimilation methods, currently used in AIRPARIF, are assessed. The two methods are anisotropic statistical interpolation (SI) and innovation intrinsic Kriging. These methods are applied to the POLLUX system outputs for daily air quality index mapping. In this case study, we aimed for two objectives: first, to extend the assimilation processes to the new ESMERALDA forecast system and secondly, to make an evaluation of the 2 techniques for ozone.

The two methods are compared using cross validation RMSE as well as standard deviation maps which have also been plotted. These maps allow us to visualize the spatial distribution of ozone concentration uncertainties for the two data assimilation methods. This case study provided a better understanding of the SI and Kriging data assimilation methods. Moreover, data assimilation seems to be a very promising tool for AIRPARIF needs:

The results of the case study indicate that:

- For annual air quality assessment, assimilated concentration patterns are significantly more reliable than the model outputs
- The use of these annual concentrations with the associated uncertainties will allow us to define risk assessment for limit value exceedances.
- Assimilation can also be used as a powerful tool to establish the relevance of some stations or to determine areas where monitoring stations should be needed.
- Concerning the differences between methods, we can say that innovative Kriging seems to be a better method near measurement points while Statistical Interpolation is better further away. Nevertheless, some additional work should be undertaken to compare precisely the two methods.
- The case study showed us that it is absolutely necessary to have sound mathematical and scientific knowledge to make correct use of these methods. For such algorithm implementation, statistical knowledge is essential, especially the variogram and covariance matrix concepts.

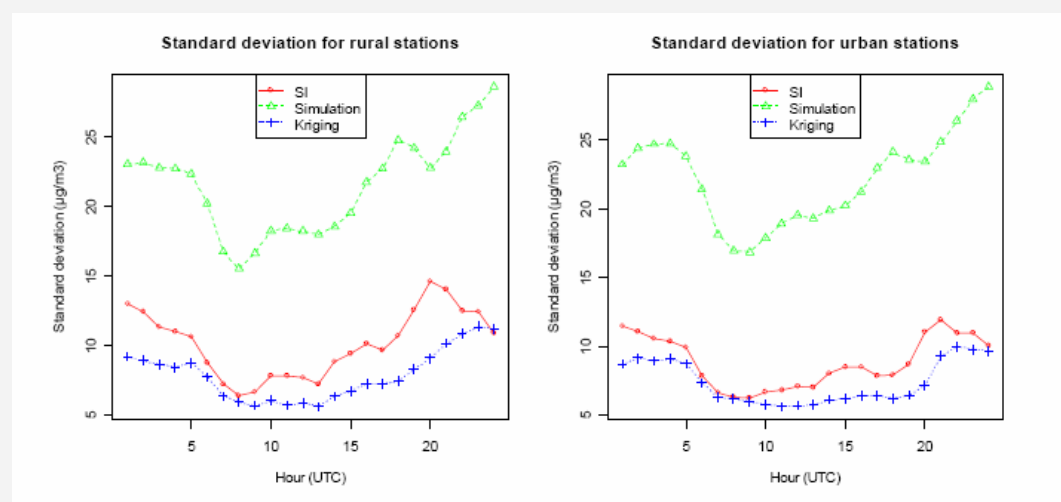


Figure. Hourly Standard deviation plots - Analyses and Simulation plots on average on urban stations and rural stations. SI in red, simulation in green and Kriging in blue.

Case study: Local scale data assimilation in Oslo

Data assimilation in open road line source modelling

In this case study we have investigated how an open road line source model can be improved by using local (roadside) air quality (AQ) observations. Available data from the site Nordbysletta close to Oslo, Norway is used. The site is ideal for this study since it is a relatively flat area containing a single 800 m long 4-lane roadway with traffic. Air quality observations at the site consist of measured hourly average concentrations of NO_x , NO_2 and PM_{10} , at three stations in different distances from the road, during a 4 months period (January-April 2002). During the same period, hourly average background concentrations of the same species, together with O_3 , were measured at a station on the opposite side of the road. Hourly data for local meteorology and traffic counting were also available.

The line source model used in the case study is the WORM model (Weak Wind Open Road Model), which is a newly developed integrated Gaussian line source model at NILU. The model uses a preprocessor based on Monin-Obukhov similarity theory to calculate derived meteorological parameters such as horizontal and vertical turbulence intensity, Lagrangian timescale and mixing height using local observations of temperature gradient, wind speed and direction. The model incorporates some new features compared to traditional Gaussian line source models. First it uses a new numerical procedure for calculating integrated concentrations in receptor points, based on Gaussian quadrature, which is highly accurate, also in situations when the wind blows parallel to the road. It also contains a new formula for calculating the growth of the horizontal plume spread, which takes into account plume meandering at low wind speeds. The meandering parameters in this formulation are taken from the GRAL (Graz Lagrangian) dispersion model.

We decided to focus on NO_x in this case study since this is simpler to model than NO_2 and PM_{10} . There are e.g., no photochemical reactions involved in the modelling of NO_x locally as compared to NO_2 where the transition of NO to NO_2 as a function of distance from the road has to be taken into account. It is also much easier to estimate emissions of this compound than to estimate emissions of PM_{10} , especially during springtime in Norway due to the heavy re-suspension of road dust. Local traffic counting data of light and heavy duty vehicles were used to estimate emissions of NO_x from the road traffic accurately on an hourly basis. In addition observed background concentrations of NO_x were subtracted from the measured concentrations at the three roadside stations, in order to produce net observations that could be compared directly with the modelled concentrations at the stations. Further improvement of the model could then be focused on the meteorological input parameters.

After careful investigation of the importance and uncertainty of different meteorological parameters it was decided to focus on horizontal diffusivity and initial size of plume as two of the most important parameters in modelling pollutants from roads. Data assimilation was then used on an hourly basis in order to estimate these parameters using the available AQ observations. It was decided to use one station and leave the other two stations for checking any model improvement. As assimilation method we have used the SIR (Sequential Importance Resampling) method. In this method, ensembles of 2500 NO_x concentrations values were calculated at each station and for each hour during the period, based on randomly perturbing the meteorological parameters according to a given Bayesian prior probability density function (PDF). Corresponding posterior PDFs were calculated by multiplying the prior PDFs with Gaussian likelihood functions assuming that observations of NO_x have a relative measurement error standard deviation equal to 5%. The parameters were finally estimated as the mean values of the posterior PDFs.

The results show that using AQ observations at one roadside station reduces the meteorological uncertainty and improves the model concentration results significantly at the other two independent stations, especially regarding the high percentiles of the model concentration distribution. The case study supported recommendations concerning:

- AQ monitoring is important in order to properly evaluate and validate local scale AQ models
- One of the benefits of having more observations is reduced model uncertainty
- Input data should be used as variables in the data assimilation procedure for local scale models rather than directly interpolating the model output concentrations
- Focus should generally be on model variables which are uncertain and for which the model output concentration is most sensitive
- Sequential Monte Carlo methods (particle filters) such as the SIR-method can be used for performing data assimilation at the local scale

4.3 Optimisation of monitoring networks using models and data assimilation

Data assimilation can also be used to evaluate different monitoring networks with the aim of optimizing the network with respect to a given set of criteria. This should first start by addressing the purpose of the monitoring network, and for what reasons one wants to combine monitoring and modelling. One example could be to check compliance with the limit values, e.g., that all concentrations in an area are below a certain threshold. Another example could be to estimate the degree of pollution exposure and health hazard for the population living in the area etc. When the purpose of the monitoring network and the combination of monitoring and modelling is clear, an evaluation of fitness for purpose of a combination of an urban scale AQ model, a given monitoring network, and a given data assimilation technique, may guide us in selecting an optimal monitoring network to best solve the specific problem.

a) Basic requirements

The use of data assimilation for network design is an advanced methodology and so no basic requirements are recommended. The recommendations on network design given in chapter 2.1 above will in practice form a general set of constraints on the number and possible placements of monitoring stations in an urban environment.

The optimisation of the network design discussed in chapter 2.1 should be performed as the basic requirement.

b) Best practice recommendations

In order to evaluate a given monitoring network, pseudo measurements may be more advantageous to use than real measurements. Pseudo measurements are synthetic measurements produced by first running the urban scale AQ model to produce a conceived set of 'true' concentrations for the area, and then for each measurement point to use Monte Carlo random draw procedures to simulate deviations from these true concentrations in the form of measurement errors. Typical errors of model input data and/or model physics etc. can then be introduced in the urban AQ model, and assimilated concentrations produced, based on using the set of pseudo measurements.

Since the 'true' concentrations are assumed known, one may easily check how close the assimilated concentrations comes to the true concentrations, and thus check the fitness of the current monitoring network with respect to the given set of criteria. This may be repeated and compared for different configurations of the monitoring network, which may then form part of an iterative procedure for optimising the network.

In order to position stations to be representative of the urban background it is preferred that measurements are conducted with monitoring stations placed at open spaces within cities, such as parks, school playgrounds, etc., as a city-wide measurement of pollution. However, monitoring planned in this way may not sufficiently capture the spatial variation of urban pollutants, as the local flow field and pollutant dispersion is strongly controlled by the surrounding building shape and street geometry.

These small scale effects have to be considered in order to assess how representative the monitoring data of an urban site are for the entire city. A general approach for assessing monitoring data representativeness is based on using CFD modelling, combined with a statistical analysis of routine monitoring data (Scaperdas and Colvile, 1999).

c) Scientific recommendations

Currently monitoring networks are not designed for optimising assessment through data assimilation techniques. Research is generally needed to understand better the role that different monitoring network configurations have on the statistical inferences drawn from the results of applying air quality models and data assimilation techniques on the urban scale. Here again increased interaction with the statistical communities is recommended.

4.4 Source apportionment using models and monitoring

Identifying the sources that lead to poor air quality is an important aspect of assessment, particularly in regard to abatement strategies for improving air quality. Source apportionment can be carried out to some extent using only monitoring data. Simple methods, such as those described in Air4EU – CS D7.1.1, can make use of monitoring data to identify urban and regional contributions for PM as well as identifying contributions to NO₂ that come from the chemical reaction with O₃. In a similar fashion local and urban contributions may be identified using pairs or triplets, see Chapter 2 of this document and the non-exhaust PM case study (Air4EU – CS D7.1.2).

It is also possible to use more advanced monitoring methods for PM, since it is a multi-component compound, that analyse the individual chemical species of PM (Chapter 2.2). From this analysis, known as receptor modelling, the source apportionment can be applied and the relative contributions from a number of sources can be identified. This methodology is limited as it provides the contributions at the site of measurement but cannot give information on the actual emissions.

By combining dispersion models with receptor models it is possible to estimate emission strengths, providing verification of emission rates and identifying the absolute contributions of the various sources to ambient air quality (Air4EU – CS D7.1.5).

a) Basic requirements

Identification of source contributions using monitoring data is recommended as a basic screening method, e.g. Air4EU – CS D7.1.2.

b) Best practice recommendations

The application of receptor models, based on both gaseous and particulate compounds, should be carried out. This will require both a monitoring campaign and an analysis period. Expert support is required for such campaigns (see chapter 2.2).

Receptor models should be compared with air quality modelling to assess their differences and similarities. If there are significant differences then these must be assessed and explained.

The uncertainty in both receptor modelling and air quality modelling must be assessed for any comparison between the two methodologies.

c) Scientific recommendations

Inverse modelling methods, that include data assimilation, can be used to determine emission rates. This technique is complex and its application to urban areas has been limited. This area of research should be developed further.

Case study: Source apportionment of PM in Oslo

Source Apportionment of Particulate Matter in Air using Dispersion and Receptor Models (Air4EU – CS D7.1.5)

A source apportionment study has been performed for Oslo. In this case study, the quality of the emission inventory for particulates (PM_{2.5} and PM₁₀) was assessed. This assessment was performed by comparing source apportionment estimates from a dispersion model, using this inventory, with source apportionment estimates from a receptor model.

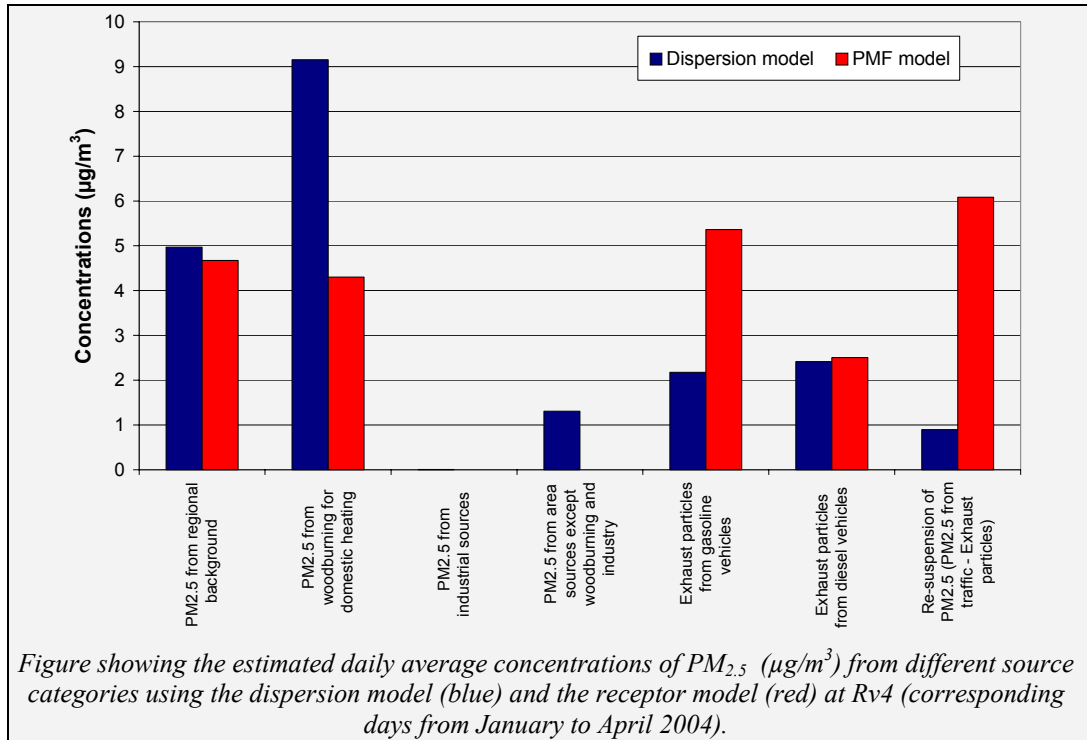
The study is based on data from a measurement campaign performed from January to April 2004 in Oslo. In that campaign the chemical contents of both PM₁₀ and PM_{2.5} from filter samples was analysed. With these data as input, Positive Matrix Factorization (PMF) receptor modelling was applied to detect and quantify the various source contributions. For the same observational period and site, we performed emission and dispersion model calculations using the Air Quality Management system AirQUIS (www.airquis.com).

The emission inventory assessment was performed by comparing the estimated source contributions of a number of different source categories, for both the PMF model and the dispersion model. The results identified gaps and weaknesses in the emission inventory and in the receptor model results. Particularly for contributions from wood burning and traffic, we observed large deviations between the two methodologies. For the example of domestic wood burning, the dispersion model estimated an average PM_{2.5} contribution that was twice as large as the contribution estimated by the receptor model. On the other hand, the receptor model estimated source contributions for traffic-induced suspension that were 7 times higher than the dispersion model estimates. On the average however, the deviation between the model estimated and measured PM_{2.5} was only 13%.

Based on the results, we improved the emission inventory for individual source categories and calculated new PM₁₀ and PM_{2.5} estimates for Oslo using the dispersion model. PM₁₀ and PM_{2.5} concentrations were compared with measurements at three other stations to evaluate the improvements of the updated inventory. The analysis showed an improvement in the dispersion estimated concentrations for PM_{2.5} for all these three stations. For PM₁₀, however, the analysis revealed no improvements in the results.

The following recommendations based on the case study are made:

- Receptor modelling can be used to provide information on the various sources contributing to urban air quality.
- It is important in air quality assessment be able to differentiate between the various sources, e.g. traffic, heating, long range transport, and to be able to model each source type well. This is especially important when planning abatement scenarios.
- Receptor modelling in combination with dispersion modelling provides an independent assessment of emission inventories for PM and is a highly recommended method.
- It is recommended that more than one monitoring site be used for the receptor modelling.
- An assessment of both model and receptor model uncertainties is required for a meaningful comparison of the results
- Results from receptor model analysis can be used to improve the assessment by adjustment of emission rates but the improvement needs to be independently checked.
- The methodology has been shown to work best for non-local sources, e.g. domestic heating rather than traffic.



5. Uncertainty analysis

In chapter 2.3 quality assurance and control (QA/QC) of monitoring data is presented. In this Chapter uncertainty related to other aspects of monitoring and modelling are discussed. These include concepts such as:

- uncertainties in modelling
- uncertainties when combining monitoring and modelling
- spatial representativeness of monitoring and modelling data
- mapping of uncertainties

5.1 Uncertainties in modelling

The uncertainty concept is one of the crucial points of Quality Assurance/Quality Control (QA/QC) procedures that should provide quantitative information about the modelling precision, identifying the uncertainty sources and their potential reduction. The present European legislation defines the Modelling Quality Objectives as an acceptability measure, to guarantee good model performance and reliable modelling results for decision makers. However, a practical application of these requirements and interpretation of the uncertainty analysis results based on the recommended methodology is ambiguous, and in some cases incomprehensible for non-expert users. The development of a consistent procedure for the uncertainty evaluation is still a challenge for the scientific community.

The following recommendations are proposed to estimate the total model uncertainty. The different steps should be addressed according to the end users needs. More detailed information on the application of the referred procedure can be found in the Milestone Report 6.5.

a) Basic requirements

The first point that needs to be defined is the purpose of the uncertainty estimation process. If the goal is to estimate the quality of the model itself then data error could be omitted, but if the modelling results will be used as support for political decision, the total model uncertainty is essential, and the information about uncertainties associated with modelling results will be as important as the modelling results themselves.

An assessment of known model error or estimated uncertainty is always required when modelling results are presented.

Another issue refers to the effective communication of model uncertainties to decision makers, so that model outputs can be correctly interpreted.

For the application of the Quality Objectives of the Air Quality Framework Directive it is recommended to use the alternative model error Relative Percentile Error (RPE) when dealing with percentiles. For annual means, the Quality Objectives requirements of the EU Directives are unambiguous. A distinction between a paired-in-time and an unpaired-in-time intercomparison, or between the relative percentile error and the relative maximum error is not necessary. Thus both RPE and RME (relative maximum error) are compatible for annual means and should be applied in that context.

For the estimation of the Total Model Uncertainty it is recommended to use the following statistical parameters: correlation coefficient, fractional bias and normalized standard deviation.

Presentation of a qualitative (e.g., graphical) and a quantitative (e.g., statistical) analysis of model results against measured values from the air quality network should be made.

b) Best practice recommendations

Stochastic variability

In order to improve model performance, it is necessary to investigate the contribution of the different components of total model uncertainty. The contribution of stochastic variations in the total model uncertainty should be examined separately, since it cannot be reduced.

To analyse the uncertainty related to variability it is recommended to filter out stochastic processes from the monitoring data based on spectral analysis and the quantification of model uncertainty without the influence of stochastic variations.

It is recommended that the analysis of the stochastic contribution to uncertainty be taken into account when assessment is based on hourly means but this is not required for annual means.

c) Scientific recommendations

Analysis of intrinsic model uncertainty

For a complete knowledge of the components of total model uncertainty it is recommended to perform a sensitivity analysis and/or model intercomparison to evaluate the different model modules (Chemical mechanisms, physical parameterisations and numerical algorithms) to determine intrinsic model uncertainty.

For the estimation of uncertainty related to input data a sensitivity analysis (based for e.g. on Monte Carlo simulations) to input parameters (like initial and boundary conditions, meteorological parameters, emissions, land use and topography) is recommended.

An appropriate measure for intrinsic model uncertainty and input data uncertainty is the standard deviation and normalised bias of the results of sensitivity tests.

Case study: Model uncertainty in Berlin

Berlin case study report: assessment of modelling uncertainties (Air4EU – CS D7.1.14)

The uncertainty concept is one of the crucial points of Quality Assurance/Quality Control (QA/QC) procedures that should provide quantitative information about the modelling precision, identifying the uncertainty sources and their potential reduction. The present European legislation defines the Modelling Quality Objectives as an acceptability measure, to guarantee good model performance and reliable modelling results for decision makers. However, a practical application of these requirements and interpretation of the uncertainty analysis results based on the recommended methodology is ambiguous, and in some cases incomprehensible for non-expert users. The development of a consistent procedure for uncertainty evaluation is still a challenge for the scientific community.

The aim of this case study is to provide an example of the methodology described in the cross cutting report regarding the estimation of air quality modelling uncertainty (Air4EU-M2). An uncertainty analysis was performed on the modelling results of the Berlin case, concerning both urban and hot spot scales for the main critical pollutants. According to the basic Air4EU recommendations the estimation of total model uncertainty will be determined through comparison between model predictions and air quality observations, based on the Air Quality Framework Directive (FWD) settlements and on statistical parameters. The referred recommendations consider three levels of application adaptable to end-users needs, goals and ability. The first level is a simple qualitative analysis. The estimation of total model uncertainty based on statistical parameters and on FWD settlements is covered by the second level. In order to improve model performance, it is necessary to investigate the contribution of the different components of total model uncertainty. Therefore, the third level details the total model uncertainty, through the estimation of its different components. The variability is addressed as a first step. The contribution of stochastic variations in the total model uncertainty should be examined separately, since it cannot be reduced. For a more complete evaluation, sensitivity analysis to model and input parameters should also be performed. This sequence of recommendations should be regarded in these three levels of complexity and could be applied by end-users according to their desire and need of detail.

For the Berlin case study the second level of recommendations is applied. The alternative model error RPE (Relative Percentile Error) will be considered to estimate model uncertainty, corresponding to the allowed number of exceedances of the limit value normalized by the observation. The Berlin case study is composed by two different model scale approaches. First of all, simulations were performed with the RCG model over the urban area of Berlin, with 4x4 km² grid resolution. The Gaussian multi-source dispersion model IMMISnet was used for the local scale modelling simulations over Berlin. The modelling and monitoring data were provided by the Senat Berlin for the year 2002 and for the pollutants PM₁₀ and NO₂. The uncertainty estimation methodology described was applied separately for each numerical model scale application.

Results of the first step point to the fulfilment of the modelling acceptability criteria defined in the FWD, for all the analysed pollutants for the urban scale and partially for NO₂, at the local scale. For the same scale and for PM₁₀ most of the RPE values determined are above the modelling quality objective of 50%. In the second step, the statistical analysis, comprising a set of parameters, gave information about the ability of the model to predict the tendency of observed values (r), relative and absolute errors on the simulation of average and peak observed concentrations (RMSE and NMSE), and type of errors (Bias). This analysis shows that the urban scale model is able to predict concentrations for the Berlin case with correlation factors higher than 0.8 for O₃ and for PM₁₀. For the local scale, the averaged correlation factor is 0.48 and 0.51 for NO₂ and PM₁₀ pollutants, respectively, indicating that the model is not able to simulate correctly the physical processes involved in the dispersion of the referred pollutants. Besides that, the models average error shows no significant discrepancies between model values and observed data. At the urban scale the Bias shows no model tendency for some pollutants, suggesting that local phenomena could be responsible for model errors at each specific monitoring site, but a clear model

overestimation for PM_{10} is observed. The uncertainty spatial mapping showed that all the analysed indicators are adequate to perform the spatial representation of the uncertainty. Considering that the basic level of recommendations is completed for this case study, it is recommended for future work to investigate the stochastic contribution to the total model uncertainty and to perform a sensitivity analysis or model intercomparison to evaluate the different model modules.

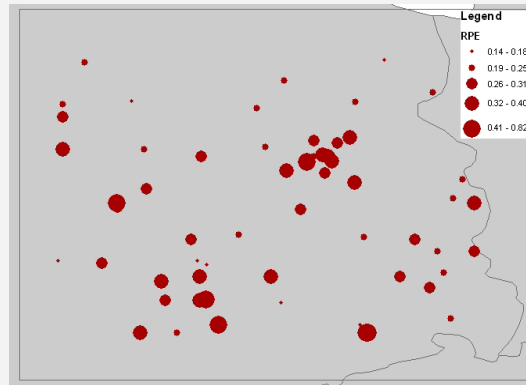


Figure. Mapping of RPE of O_3 simulation (concerning the 26th maximum 8h running average percentile) with the RGC model over the Berlin regional domain (11-15° W of longitude and 51-53.5° N of latitude) with 4x4 km² resolution grid. The size of the dots represents the magnitude of RPE.

5.2 Assessment of uncertainties when combining monitoring and modelling

The major aim of combining monitoring and modelling is to reduce the uncertainty in the final spatial assessment. There is no guarantee that carrying out such a combination will improve the spatial assessment so this must always be assessed. The assessment of this is confounded by the fact that the 'true' value will always remain unknown since both monitoring and models have intrinsic uncertainties.

When monitoring is assimilated then improvement in the assessment field is likely to occur in the vicinity of the monitoring site but its improvement elsewhere is uncertain. To assess this cross-validation techniques are commonly used in which one, or several, observations are excluded from the assimilation. These excluded observations are then used to verify the results. When simpler methods of data assimilation are used, e.g. kriging and optimal interpolation, then cross-validation using rotating exclusion can be used since these methods are not normally computationally expensive. When more complex methods, such as 4Dvar are applied then cross-validation can be carried out with a subset of excluded monitoring stations.

a) Basic requirements

When assessing the uncertainty when combining monitoring and models it is recommended to treat the observations as 'true', especially in regard to the EU directives which are based on monitoring as the 'true' state of the atmosphere.

Optimal interpolation and kriging methods all generate their own intrinsic uncertainties based on the spatial variance. These quantities should be used to indicate the spatial distribution of the uncertainty.

b) Best practice recommendations

The recommended technique for assessing uncertainty when using data assimilation is the processes of cross-validation. The most appropriate measure to indicate this is the RMSE. Comparison should be made before and after the assimilation.

When assessing the uncertainty when combining monitoring and models it is recommended to treat the observations as having their own uncertainty. If this cannot be established then best estimates should be used.

Bayesian methods for calculating the uncertainties should be applied.

Ensemble methods of data assimilation provide information on the uncertainty of the assimilated fields. The standard deviation of the ensemble should be used as a spatial indication of uncertainty.

Consistency between cross-validation and ensemble estimates of uncertainty should be assessed when both methods are available.

c) Scientific recommendations

There is a significant gap in the understanding of spatial representativeness and its effect on monitoring uncertainty. This needs to be addressed before more meaningful uncertainty assessment using data assimilation can be carried out.

Bias in models, particularly for PM, remains a problem in regard to assimilation techniques since most of these techniques are applicable only when there is little or no bias present. Bias is best dealt with by improvement of the model, rather than adaptation of the assimilation method.

5.3 Spatial representativeness of monitoring and modelling data

This subchapter considers recommendations on how to deal with uncertainties related to the spatial representativeness of air quality, particularly when comparing or combining monitoring and modelling data. Due to the difficulties of establishing the spatial variation of air quality on all scales this aspect of uncertainty is rarely dealt with in a quantitative way but needs to be considered whenever monitoring and modelling data are to be compared.

a) Basic requirements

When comparing or combining monitoring data with modelling data it is important that both the spatial and temporal representativeness of the two data sets matches as closely as possible.

The uncertainty associated with both the model and monitoring spatial representativeness is dependent not just on spatial parameters but also on the temporal averaging time. E.g. for measurements or modelling in street canyons annual mean values will be representative for the whole street canyon, as apposed to hourly mean data that are representative for only that spot. This should be taken into consideration when assessing the spatial representativeness of a measurement or model result.

b) Best practice recommendations

It is also possible to assess the spatial representativeness of observations by examining their spatial co-variance. Such methodologies are commonly used when determining variograms for kriging interpolation and can also be applied to assess the uncertainty, related to representativeness, of measurements when used for data assimilation purposes. This, however, generally requires a dense network of stations.

When spatial representativeness needs to be better defined, e.g. for the placement of permanent monitoring stations, then this may be assessed on the local and urban scale by placement of a dense network of passive samplers. The results however will be dependent on the averaging period.

Spatial representativeness on the local scale may be assessed by the use of CFD models. The use of these models requires expert support.

c) Scientific recommendations

The spatial representativeness of monitoring data is poorly defined for almost all applications. More research is required to improve this situation, especially in regard to data assimilation techniques which require knowledge of this.

Case study: Uncertainty analysis in Oslo

Model and observation uncertainty analysis towards data assimilation on the urban scale (Air4EU – CS D7.1.3)

In this case study an uncertainty analysis towards the ultimate aim of using data assimilation for combining an urban grid model with urban background air quality (AQ) observations in Oslo has been performed.

The model considered is the 22 x 18 km² Eulerian grid model AirQUIS/EPISODE which is a well established air pollution dispersion model for the city of Oslo. The current urban background AQ observations consists of hourly and daily average values of NO₂, PM₁₀ and PM_{2.5} at the three urban background stations Aker hospital, Sofienberg park and Skøyen in Oslo during the period February-March 2004. The emphasis of the study is to analyse the involved errors and uncertainties related to the model and the observations during this period as a necessary precursor step for using data assimilation. Special emphasis has been put on analysing representativeness errors arising when comparing point like observations with gridded model averages, since this kind of error becomes much more important than the pure observation (instrument) error when comparing grid averages with point values.

A model evaluation was first performed for the two-months period comparing hourly concentrations of NO₂ and daily mean values of PM₁₀ and PM_{2.5} with corresponding model calculated values. The results of the evaluation show reasonable good agreement between the model and the hourly and daily observations. Best agreement is found for NO₂ and PM_{2.5}. The agreement is poorer for PM₁₀ which is mainly due to traffic induced re-suspension of road dust, common in Oslo during the spring period each year.

An uncertainty analysis was then performed based on analysing ratios of modelled and observed concentrations at the different stations. Such ratios and their mean values have been found (theoretically) to be linked with model, observation and representativeness errors and their standard deviations. Based on the calculated ratios at the different stations and for the different compounds, corresponding values of model and representativeness standard deviations have been estimated. Representativeness error standard deviations have also been estimated separately based on comparing different grid resolution averages. Although it is difficult to determine the correct value for each of the above mentioned errors in the present study, the theoretical relationship can be used to find the correct value of the combined observation and representativeness standard deviations if the degree of model uncertainty is given. The correct level of the latter should, in our view, always ideally be found using model ensemble perturbations.

Maps of model uncertainties in the form of gridded standard deviation fields for each of the three compounds NO₂, PM₁₀ and PM_{2.5} have been calculated for 1 March 2004, which was the day during the winter period of 2003/2004 with the highest levels of air pollution. In addition probabilities of exceedances (POE) of limit values have been calculated as a map for each of the three compounds for this day. Calculating POE values based on model uncertainties represents in our view a more robust approach for checking compliance with limit values than simply checking whether a given model calculated value is above or below a certain limit.

The small number of available urban background stations (only 1-2 depending on compound) makes it in general difficult to use data assimilation as a technique for improving urban grid modelling in Oslo at the present stage, except perhaps in areas close to the monitoring stations. Ideally we believe that at least 8-10 monitoring stations should be available as urban background stations in Oslo to perform such data assimilation. In order to find an optimal placement of stations, simulations should be performed to test the suitability of different monitoring network configurations. This was unfortunately not possible to do within the scope of the current case study.

This case study supported the following recommendations

- AQ monitoring is important in order to properly evaluate and validate urban scale AQ models

- One of the benefits of having more observations is reduced model uncertainty
- There is a general need for more urban background stations in order to perform proper data assimilation at the urban scale
- It is very important to address representativeness error when comparing grid model values with point like observations
- Representativeness error standard deviations could be several times larger than pure observation (instrument) error standard deviations even for grid cell sizes as small as $1 \times 1 \text{ km}^2$
- It is important to include proper representativeness error standard deviations in the data assimilation procedure in order to have the right balance with the model error standard deviations
- Averages of ratios of modelled and observed concentrations contains valuable information for checking the correct balance between the model and the representativeness error standard deviations
- Model error standard deviations should be calculated using model ensemble perturbations

5.4 Spatial mapping of uncertainties

There are a number of uncertainty parameters available that can be spatially represented using maps, and these should accompany any assessment maps. Nevertheless, the available parameters will be dependent on the methodology used to produce the maps and on the application of the maps.

Interpolating model errors between monitoring sites

When the model error for annual means and daily average percentiles are required for directive purposes then the most relevant parameter is RPE for daily or hourly averages and RME for annual means (as proposed in Chapter 5.1) evaluated at monitoring sites. Such point like assessments can be spatially interpolated to create maps from the given values through

- Direct spatial interpolation of the model errors through kriging or some other interpolation method
- Creating a regression model, based on model concentrations, for the error field
- Calculating the normalised RMSE of these values and apply this as a representative uncertainty
- When both local and urban scale models are involved in the model assessment then the error from these can be treated separately using any of the methods described above.

However, since model error is only known at the observational sites any interpolation of the error values between sites must be addressed with caution. For the application of the interpolation method is necessary to guarantee a good spatial coverage of the study domain by the air quality network. In case of deficient spatial coverage it is recommended to use point representation instead of spatial interpolation. The error analysis must first be interpreted as model uncertainty, e.g. by calculating the RMSE of the values or assuming the error to be representative of model variability.

Model uncertainty from sensitivity assessment

When intrinsic model uncertainty is required then the results from ensemble runs and sensitivity analysis can be directly mapped using the fractional bias and standard deviation. No interpolation is required as these parameters can be assessed on the spatial grid

Model uncertainty from data assimilation

When data assimilation techniques that involve ensemble methods are used then the results can be directly mapped using the estimated standard deviation. No interpolation is required as these parameters are assessed on the spatial grid.

When data assimilation is applied cross validation can also be used to spatially represent the uncertainty. This can be dealt with in a similar fashion to the methods outlined for model error, Chapter 5.1. For complex data assimilation methods cross validation of individual stations is not realistic due to computing demands and this cannot be used.

a) Basic requirements

When there is limited information concerning the model error, i.e. few or no observations available, then mapping of uncertainty can be carried out by a 'best estimate', based on other information available. This should be applied to the assessment map as a relative uncertainty, e.g. 20%, which should be representative of the expected standard deviation.

When more information is available concerning the model error, e.g. more sites, then the RMSE from these sites can be used as indicative of the uncertainty and used as a constant relative, or absolute, uncertainty for the mapping.

When plotting contour or gridded maps using colour coding it is recommended to use a contour spacing that reflects the estimated uncertainty, e.g. using a rounded value of the standard deviation as the contour spacing, as this provides a good visual indication of the uncertainty of the mapped result.

When representing the model error based on point assessments, e.g. RME or RPE, then it is not recommended to spatially interpolate the error when there is not a sufficiently high density of station available.

b) Best practice recommendations

When model fields consist of both urban and local scale models then the individual uncertainties of the models and their contribution to the total air quality assessment should be assessed and included in the spatial distribution of model uncertainty.

When data assimilation techniques are used that provide their own uncertainty estimates, e.g. kriging and ensemble methods, then the variance or standard deviations should be used to represent uncertainty in a map.

When regression is applied as a data assimilation technique then the 'prediction interval' can be used to provide an assessment of the typical uncertainty. When the system is unbiased then this approaches the standard deviation of the regression residuals and is equivalent to the RMSE of the regression model.

Sensitivity analysis using ensemble modelling, based on estimated uncertainties in the input and model parameters, should be used to create maps of intrinsic model uncertainty.

c) Scientific recommendations

Uncertainty mapping is currently not carried out for most air quality assessments. The methodologies described here still require further assessment to establish them as operational methodologies.

Other methods of using uncertainty in maps, such as the probability of exceedence, should be further investigated to assess their usefulness as uncertainty indicators.

Case study: Uncertainty assessment in London and SE England

Uncertainty in AQ assessment in London (Air4EU – CS D7.1.10)

Case studies illustrating typical approaches to air quality management assessment in the U.K. are presented, for comparison purposes with other approaches applied in Europe. The assessment of uncertainty in air quality models is outlined, based on Monte Carlo simulations. Examples of increasingly complex spatial concentration patterns are presented. It is argued that the uncertainty should be presented wherever possible. However is not always practical, or useful, to present the uncertainty in detail in all situations, especially very complex ones and simplifications are necessary, which should be determined by the decision being made. For example emission reduction strategies can be evaluated using a spatial aggregation of the weighted exceedence of concentration, or probability of exceedence, over the region of interest, rather than detailed mapping of every region of potential exceedence. It is concluded that the treatment of uncertainty depends on the regulatory framework and approaches towards uncertainty mapping should be viewed in this context.

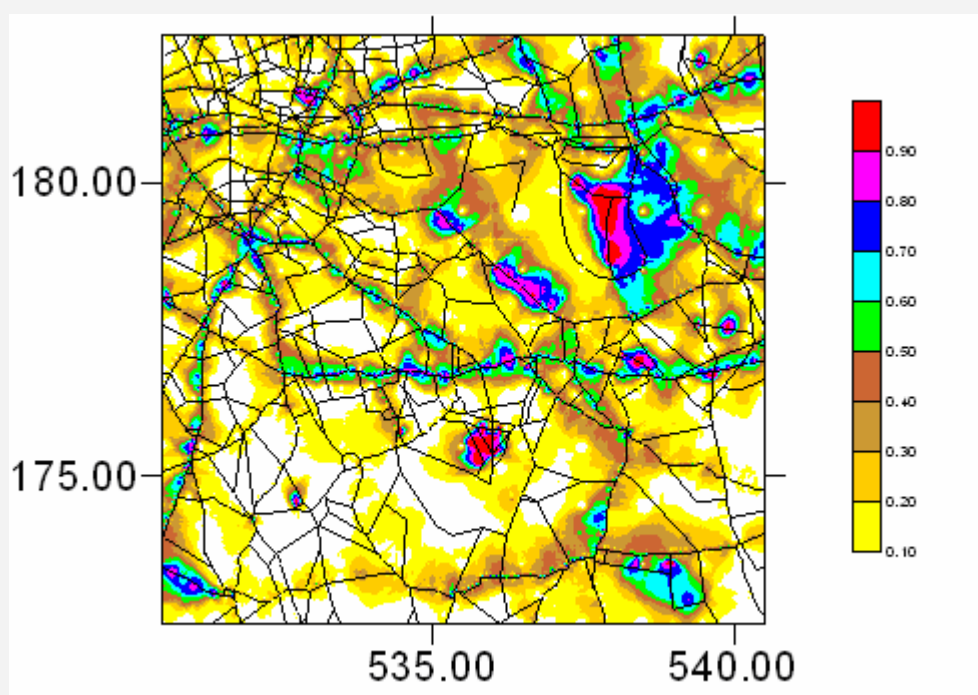


Figure. A sample probability of exceedence map for part of the city of London. Values near to 1 suggest a high likelihood of exceedence whilst values close to 0 indicate very low likelihood.

6. Concluding remarks

Clearly there is much to be considered when carrying out air quality assessment for urban areas. The list of recommended basic requirements and best practices given in this document, which number more than 250 separate recommendations, describe a wide variety of issues that need to be considered when carrying out such assessment. However, there are always real world limitations that will not allow all of the best practice recommendations to be carried out, nor indeed some of the basic requirements. Despite this, this document should serve as a guide to give both city users of air quality assessments and the institutes carrying them out an overview of the many methods, of varying quality or effectiveness, available. These recommendations are intended to steer decisions that need to be made in how assessment is carried out, from monitoring network design and modelling applications through to their eventual combination. This will not only achieve the best assessment of air quality but will also improve the understanding of the causes and effects that lead to the current and future air quality situation.

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