

# **Spatial assessment at the regional/continental scale**

*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 (NO<sub>2</sub>) and ozone (O<sub>3</sub>) at the regional scale. 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, in which both the European scale, as well as the regional background to urban areas has been 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 European scale maps, including the regional background to urban areas. 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 Background

The urban air quality is determined by sources within and outside the city. The regional background contributions, i.e. all concentrations not resulting from local urban emissions, can make up a significant part of the total concentrations in a city. For O<sub>3</sub> the regional 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 NO<sub>2</sub> the regional background levels are generally lower than the urban concentrations, though regional background levels can be high in more polluted agglomerations. The regional background contributions can only be estimated using measurements outside of the city or by regional scale models.

## 1.2 Aim

The main aim of this document is to recommend methodologies that will lead to improved spatial assessment of PM, NO<sub>2</sub> and O<sub>3</sub> at the regional scale for use as regional background to urban areas, but also as concentration fields over Europe as a whole. 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 pollutants such as PM, NO<sub>2</sub> and O<sub>3</sub> can be used for a variety of applications. This document focuses mainly on assessment of regional air quality, i.e. for compliance with EU directives (EC 1996, EC 1999, EC 2002) and the AQ-assessment to come to the regional background data for the AQ-assessment at the urban/agglomerate scale. Although the recommendations for these two main aspects are often the same, it is still useful to make this distinction. When applying spatial assessment to the EU directives temporal information is required as annual, daily and hourly mean values, dependent on the pollutant. To perform these studies for urban areas regional background concentrations have to be available on the same temporal scale.

## 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, NO<sub>2</sub> and O<sub>3</sub> at the regional scale***

Within this topic a number of methods and issues for carrying out this assessment are treated which include:

- *Monitoring*
- *Modelling*
- *Combining models and monitoring*
- *Emissions*
- *Uncertainty analysis*

Each of these chapters is subsequently divided into particular relevant aspects of the different methodologies and recommendations on these are given at 3 levels of complexity, those being:

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

The main application area, that of compliance with EU directives, is the focus of these chapters but the recommendations given might also be relevant to other applications, such as population exposure and

source apportionment. These are addressed separately, where appropriate, but in general cover the same methodologies

Throughout the document recommendations are given in *italics* and coloured *blue* with supporting text in normal font. Where recommendations are specific for one of the compounds PM, NO<sub>2</sub> or O<sub>3</sub>, this is clearly indicated. If not, the recommendations are general for all the three compounds.

Throughout the report we refer to the recommendation report for the urban scale. That report contains a lot of detailed considerations that are valid for both the urban and regional application, independent of the scale. Also, 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, NO<sub>2</sub> and O<sub>3</sub>. These compounds have been selected since they are of primary concern to many areas and 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, NO<sub>2</sub> or O<sub>3</sub> 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 NO<sub>2</sub> also have a primary part resulting from direct emissions from particular sources. The occurrence of NO<sub>2</sub> and O<sub>3</sub> 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 directly 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 the particles is a strong function of the chemical composition of the PM as well as the physical properties of the particles. 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 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 PM<sub>10</sub> (and PM<sub>2.5</sub>) mass: 1 or 24 hourly averages
  - for NO<sub>2</sub> and O<sub>3</sub>: hourly averages
- Estimation of the spatial extent of exceedences
- 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 design of the air quality monitoring network basically involves determining the number of stations and their location, and monitoring methods, with a view to the objectives, costs and available resources. For a basic overview of the recommendations regarding 'monitoring' (network design, methods and QAQC) we refer to the urban scale document. Here we list a number of specific recommendations for the regional application.

### a) Basic requirements

*The minimum requirement for obtaining regional background values from measurements is:*

- *Hourly, daily and annual mean concentrations taken from at least 1 regional background station in the vicinity of the urban area.*

*The regional background station should be well placed in the region of the city, to represent the concentrations in the air entering the city from outside. 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 (see below).*

*It is recommended to select sites for long-term use, i.e. sites where large changes in its surrounding are not expected.*

*It is recommended to measure all components that are measured in the urbanised area.*

*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.*

### b) Best practice recommendations

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

- *The recommended number of regional background stations required for calculating regional background concentrations is 3, surrounding the urban area. These 3 stations should be selected based on the most appropriate upwind direction.*
- *O<sub>3</sub> concentrations during stable periods are often reduced close to the surface due to a lack of mixing and depletion through deposition processes. The available O<sub>3</sub> in an urban area may actually be significantly higher, due to enhanced vertical mixing in urban regions, than the regional O<sub>3</sub> 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.*

*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 10x10 km<sup>2</sup> area, the station must be located such that it also represents the average concentration of the 10x10 km<sup>2</sup> 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.*

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

### **c) Scientific recommendations**

*As a further step towards advanced characterisation of PM and ozone formation, it is recommended to monitor aerosol composition and precursor gases (VOC profiles, NO and NO<sub>2</sub>, NH<sub>3</sub>, SO<sub>2</sub>). 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 and its precursors.*

## 3. Modelling

The following chapter looks at a number of aspects of modelling, in regard to the assessment of PM, NO<sub>2</sub> and O<sub>3</sub> at the regional scale. The objective of modelling for spatial assessment, and other applications, 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.

Important aspects of modelling addressed in the following chapter sections include the resolution required, meteorology, 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 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](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 at the regional scale in Europe and include the following general model types

- Eulerian
- Lagrangian

Nowadays regional scale models tend to be Eulerian type models that calculate average concentrations on grids with typical grid sizes of around 5-50 km and an extent anywhere from 300 to 4000 km. Lagrangian type models, that follow air parcels over urban areas, are also a variety of regional scale models that can be applied.

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](http://www.harmo.org)). The US EPA also has a well documented modelling inventory and support centre ([www.epa.gov/oar/oaqps/modeling.html](http://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 addresses general model requirements including the spatial and temporal resolution of these models.

#### a) Basic requirements

For compliance with EU directives hourly means are the minimum temporal resolution required for assessment of NO<sub>2</sub> and O<sub>3</sub>. For PM<sub>10</sub> daily mean is the minimum temporal resolution required. For PM<sub>2.5</sub> annual means are sufficient.

*The temporal resolution of the model should be appropriate to the application. For daily mean concentrations a model really requires an hourly temporal resolution. Any model being applied to assess exceedances of the EU directives thus requires a temporal resolution of 1 hour.*

The spatial resolution of models will also vary from application to application. However, as long range transport has to be resolved the size of the domain should be large enough to describe these phenomena or appropriate boundary conditions should be used.

*The recommended spatial resolution for a regional scale Eulerian model, that calculates background concentrations, is approximately 50 km or lower.*

*Eulerian models applied to the regional scale should 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. Also for NO<sub>2</sub> and O<sub>3</sub> the appropriate chemistry and deposition*

*processes should be taken into account. As far as possible the use of simplified screening models, with highly empirical parametrisations, should be avoided*

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

- Hourly, daily and annual mean concentrations taken from the grid position upwind of the urban area.*
- PM and NO<sub>2</sub> 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.*

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.*

*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, including those for the regional background, 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)*

*On top of the basis requirements formulated above, it is recommended to use evaluated and validated operational Eulerian models for the regional scale. Over the last years a number of international model intercomparison studies have been performed. It is to be preferred to use models that have taken part in these intercomparison studies, or models that can be shown to have a comparable model performance to the operational models which have participated in the intercomparison studies.*

The problem of double counting –using boundary conditions for regional background to urban areas which include the emission contribution of the urban area-can be addressed in two ways. The first, and most straightforward way is the use of a model hierarchy where nested urban models are used inside regional/continental models. Both one-way and two way nesting will avoid the problem of double counting.

The second option is to derive the regional boundary conditions at a large distance from the city, say over an area around the city of about 300 x 300 km<sup>2</sup>. In this way the city emissions will in general be a small fraction (<10 % or so) from the total emissions in the larger area.

In that case the modelled regional boundary values from a specific regional model can be used as input to another type of urban model. Examples of this approach can be found in the City-Delta study. This second option can only be applied in case the urban model for the specific city can be enlarged to cover the larger 300 x 300 km<sup>2</sup> domain. When such an “enlarged urban model” is not available than

model output of the regional model could be used closer to the city, by analysing the modelled concentrations in the grids surrounding the city using the wind direction in these grids to derive up and down wind modelled concentration levels.

*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 regional 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 regional 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.*

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

### **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 heterogeneous 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.*

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

*Many regional models currently appear to underestimate NO<sub>2</sub> concentrations (van Loon et al, 2004) and so their value as regional background is questionable. The need for improved process descriptions, particularly in the vertical exchange, in these models is clear.*

*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.*

*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*

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

## 3.2 Meteorology

Meteorological input data and models are an essential part of any air quality model. The data are either prognostic via NWP-models, and diagnostic, via observations. The model performances for air quality do not lead to a clear preference for one of the two possibilities.

Mesoscale NWP models (e.g. WRF, MM5) 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.

Further information on meteorological data will come out of the new COST Action 728 “Enhancing meso-scale meteorological modelling capabilities for air pollution and dispersion applications”, at [www.cost728.org](http://www.cost728.org).

### a) Basic requirements

*It is recommended to evaluate the meteorological input data against observations for the region of interest.*

*Meteorological fields should be sequential with a temporal resolution of 1-3 hours for assessment of peak conditions and daily mean concentrations.*

*It is recommended to minimise the required interpolation of meteorological data to the model grid as much as possible. A good start is to adopt the vertical resolution of the NWP model.*

### b) Best practice recommendations

*In complex terrain a nesting approach using a mesoscale model is recommended.*

*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 urban meteorological data into mesoscale models should be further researched.*

*Improved schemes for addressing the effect of 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.*

*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.*

*One aspect for the improvement of dispersion in models is the improved parameterisation of horizontal diffusion, particularly important under low wind speed conditions.*

### 3.3. Emissions

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 chapter outlines several general recommendations of good practice for emission input on the regional scale. More detailed information on emissions is contained in the cross cutting issue report on emissions Air4EU – M1. General information on emission data generation can be found as well in (Friedrich & Reis; 2004) and (Moussiopoulos; 2003).

#### a) Basic requirements

*CORINAIR/EMEP should form the basis for the used anthropogenic emissions, but with a finer grid resolution and hourly time resolution.*

The significance of biogenic/natural sources (for e.g. sea salt, isoprene) depends on pollutant (e.g. NMVOC, PM<sub>10</sub>) and local conditions such as vegetation, soils, temperature and humidity. Biogenic/natural emissions mainly originate from remote non-urban areas but may have a significant impact on air quality in densely populated areas.

*Biogenic/natural sources are significant for the ambient air concentrations and should be taken in to account.*

#### b) Best practice recommendations

*When using regional models as boundary conditions for urban scale models the consistency between urban scale and regional scale emissions should be checked.*

*Uncertainty of emissions should be incorporated in the AQ-assessment*

#### c) Scientific recommendations

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.*

*An independent review process for regional emissions should be set-up, like in IPCC.*

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, it is recommended to use the availability of monitoring data and the application of a regional 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).*

*If possible, validation of emissions should be complemented by inverse modelling. Also source apportionment can be used to further assess the inventory and used emission factors.*

## Case study: Data assimilation for Europe I

### **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, O<sub>3</sub> and NO<sub>2</sub> 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 PM<sub>10</sub>. The determination of the regional background by observations is also problematic since it can be difficult to assess to what extent regional background stations are influenced by the city emissions themselves, resulting in the problem of double counting.

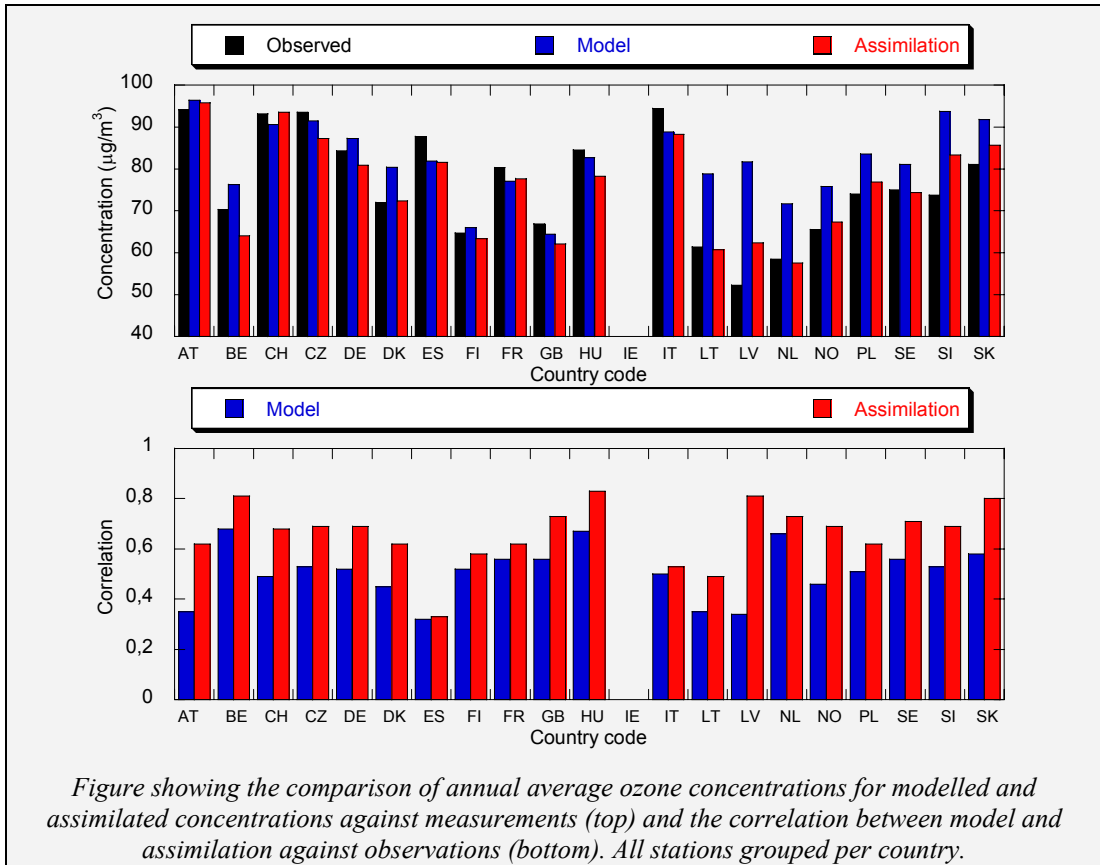
The AIR4EU project has recognised that determining, in a reliable way, regional background concentrations is one of the major drawbacks cities are facing and so AIR4EU has developed a method to prepare background concentrations through innovative data assimilation methods.

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 O<sub>3</sub>, PM<sub>10</sub>, PM<sub>2.5</sub> and NO<sub>2</sub>, 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 km<sup>2</sup>, and for time periods of years. Examples have been made for the year 2003 for PM<sub>10</sub> and O<sub>3</sub>. 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 km<sup>2</sup> is represented.
- To improve especially PM<sub>10</sub> 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.



## Case study: Data assimilation for Europe II

### Basic data assimilation: application to the European scale ( Air4EU-CS D7.1.13)

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. The complexity of such methods limits their application to research institutes, making them less accessible to authorities that require such maps. A methodology already developed for the production of European maps based on annual mean model and monitoring statistics is applied in this case study. The assimilation method investigated uses linear regression analysis combined with residual kriging of the observed-modelled residual. The methodology is further applied to daily mean model fields and monitoring data to assess the differences between assimilation using annual or daily statistics for PM<sub>10</sub>. The quality of the two different methods is assessed using the cross validation RMSE and by producing uncertainty maps. Maps showing the annual mean, the 36th highest daily mean percentile value and the number of exceedance days for PM<sub>10</sub> are produced using both methods.

The result of the case study indicates that there are differences in the maps produced using either annual or daily statistics. The most significant difference occurs in regard to the maps showing the number of exceedance days. Differences in particular areas can be as high as 30 days. However, the uncertainty in both methods has also been shown to be of a similar order, 20 – 30 days, in large regions of Europe. It is concluded in the case study that assessment maps should be produced using daily assimilated means rather than annual statistics. These maps contain more information, since observational data is often discarded from annual statistics when the temporal coverage is incomplete, and produce consistent maps in regard to percentiles and the number of exceedance days.

To demonstrate the improvements in the air quality maps, corresponding uncertainty maps are also produced. The construction of such maps aids in visualising the uncertainty in the assessment maps however methodologies for producing these maps still require further refinement. The case study supports a number of recommendations concerning combining monitoring and modelling on the European scale.

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

1. It is recommended to carry out the assimilation on the same temporal scale for which the limit values apply. For the case of PM<sub>10</sub> the assimilation should be carried out on daily mean concentrations rather than on annual statistics of the percentiles.
2. Basic assimilation methods such as linear regression, scaling or correction of bias using observations can significantly improve model assessment and their associated uncertainty.
3. Pure kriging of observational data alone can give statistically better results than models but the uncertainty in these is very high, especially far from the observations. This uncertainty far from stations is clearly reflected in the kriging parameter of sill and uncertainty maps should be used to indicate this.
4. Estimates of uncertainty and/or uncertainty maps should be co-produced with the assessment map to give a clear indication of their validity.
5. Standard deviation is a useful parameter for indicating spatial uncertainty.
6. Effort should be made to understand the sources and form of uncertainty so that the best possible uncertainty map can be produced.

## 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, regional and urban conditions etc., can only be done using well performing regional, 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 regional and 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, under uncertainty analysis, and in the cross cutting issue reports, Air4EU – M2 and M3. During a model 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 is to use monitoring data to evaluate/validate the model.

#### a) Basic requirements

*The regional model 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.*

*The models should be validated for PM<sub>x</sub> as well as its composition at 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 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 regional and 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, D4.1 and D 5.1 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 Re-sampling method (SIR).

For regional and 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 regional and urban scale model, such as e.g., emission data, meteorology (wind, stability, etc.), or boundary conditions. Which parameters to choose, generally depends on the aim of the assimilation, i.e., which parameters one wants to estimate better using available measurements.

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. Such regression models will minimise the RMSE between the air quality model and the available observations whilst preserving the spatial form of the model.*

*Regional air quality has a typical spatial variation that is similar to the distance between regional monitoring stations. Interpolation methods such as optimal interpolation and kriging, when applied solely on monitoring data, will not capture all the 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. 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.*

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 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 generally advisable to increase the interaction with the statistical communities.*

## **6. Uncertainty analysis**

### **6.1 Uncertainties in monitoring data**

For a detailed discussion on uncertainties in monitoring data we refer to the recommendation report for the urban scale. Important information for the application to the regional scale can also be found in the EMEP Manual for Sampling and Analysis' (<http://www.nilu.no/projects/ccc/manual/>).

### **6.2 Uncertainties related to representativeness**

This subchapter considers recommendations on how to deal with uncertainties that result from the limited spatial coverage of monitoring stations in an assessment and uncertainties that result when comparing or combining monitoring and modelling data.

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 6.1. This type of uncertainty tends to be highly dependent on the purpose of the measurements: a network adequate for one purpose (e.g. identifying the regional background) 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 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.*

#### **b) Best practice recommendations**

*To characterise and possibly quantify the representativeness uncertainties in a monitoring assessment it is recommended to follow a procedure discussed in the urban scale recommendation report– for each pollutant and each purpose of the measurements separately.*

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

#### **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.*

*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.*

### **6.3 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.

*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.*

*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.*

*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.*

#### **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 to input parameters (initial and boundary conditions, meteorological parameters, emissions, land use and topography) is recommended, for example, using Monte Carlo approach.*

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

### 6.4 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 process of cross-validation. The most appropriate measure to indicate this is the RMSE. Comparison should be made of 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 insight into 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.*

## **6.5 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. The available parameters are 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 6.3) 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 used then cross validation can be used to spatially represent the uncertainty. This can be dealt with in a similar fashion as the methods outlined for model error

#### **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 and the number of observations is large then this approaches the standard deviation of the residuals (the same as 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.*

## **7. Concluding remarks**

Clearly there is much to be considered when carrying out air quality assessment of the regional background and concentration fields at the European scale. The list of recommended basic requirements and best practices given in this document describe a wide variety of aspects 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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### **Background reports**

Air4EU – D1.1: Inception report

Air4EU – D1.2: Mid term assessment report

Air4EU – D1.3: Final report

Air4EU – D2.1: Policy framework and requirements analysis report

Air4EU – D3.1: Review of monitoring and modelling methods at hotspot/local scale

Air4EU – D3.2: First recommendations for air quality assessment at hotspot/local scale

Air4EU – D4.1: Review of monitoring and modelling methods at urban/agglomeration scale

Air4EU – D4.2: First recommendations for air quality assessment at urban/agglomeration scale

Air4EU – D5.1: Review of monitoring and modelling methods at regional/continental scale

Air4EU – D5.2: First recommendations for air quality assessment at regional/continental scale

### **Recommendation reports**

Air4EU – D6.2: Final Recommendations for AQ assessment

Part I: Overview and structure

Part II: Spatial assessment in urban areas

Part III: Spatial assessment at local/hot spot scale

Part IV: Spatial assessment at regional/continental scale

### **Case study and mapping reports**

Air4EU – CS D7.1.1: Trend analysis of NO<sub>2</sub>/NO<sub>x</sub> and PM<sub>10</sub> exceedances of daily limit values in Rotterdam

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

- Air4EU – CS D7.1.3: Model and observation uncertainty analysis towards data assimilation on the urban scale
- Air4EU – CS D7.1.4: Data assimilation in open line source modelling
- Air4EU – CS D7.1.5: Source apportionment of particulate matter using dispersion and receptor modelling
- Air4EU – CS D7.1.6: Basic data assimilation: application to the urban scale
- Air4EU – CS D7.1.7: Comparisons of data assimilation methods at urban scale in Paris
- Air4EU – CS D7.1.8: Traffic management impact in London
- Air4EU – CS D7.1.9: Assessment of stationary source contribution to surface pollutant concentrations using a 3-D Eulerian Air Quality Model
- Air4EU – CS D7.1.10: Uncertainty in AQ assessment in London
- Air4EU – CS D7.1.11: Assessment of PM levels and contributions in the Athens region
- Air4EU – CS D7.1.12: Data assimilation with a regional scale model: homogenous regional background for city assessment
- Air4EU – CS D7.1.13: Basic data assimilation: application to the European scale
- Air4EU – CS D7.1.14: Assessment of model uncertainty for PM10 and NO2
- Air4EU – D6.1: Protocols for implementation of case studies
- Air4EU – D7.2: Summary report of case studies
- Air4EU – D7.3: Air4EU mapping tool: description and user guide
- Air4EU – D7.4: Air4EU mapping tool: URL: [www.air4eumaps.info](http://www.air4eumaps.info)

#### **Cross cutting issue milestone reports**

- Air4EU – M1: Emissions and data needs
- Air4EU – M2: Uncertainty of models and modelling
- Air4EU – M3: Representativeness of model outputs and monitoring data
- Air4EU – M4: Scale interactions
- Air4EU – M5: Data assimilation