Technical report No 11

Guidance report on preliminary assessment under EC air quality directives

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January 1998

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Cover design: Rolf Kuchling, EEA

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Acknowledgements

The guidance report was produced by JRC-ERLAP and the EEA European Topic Centre on Air Quality (ETC-AQ), with support from the European Topic Centre on Air Emissions (ETC-AEM). Joint project leaders were Roel van Aalst (ETC-AQ) and Emile de Saeger (JRC-ERLAP).

The task was supervised by Lynne Edwards (DGXI) and Gordon McInnes (EEA). The contact person in the European Commission was Pierre Hecq. Dick van den Hout, consultant for the Commission in air quality matters, has been involved in the work. A meeting with experts from some Member States provided valuable input. We also thank national representatives and other participants in the Steering Group meeting of National Experts on Air Quality and its Working Groups for useful comments and contributions.

Summary

Under Council Directive 96/62/EC on Air Quality Assessment and Management, Member States are required to assess air quality throughout their territory. The requirements for those assessments depend on the nature of the area and the levels of air pollution, in relation to limit values as defined in Daughter Directives. In Article 5 it is stated that Member States which do not have representative measurements of the levels of pollutants for all zones and agglomerations shall undertake series of representative measurements, surveys or assessments in order to have the data available in time for implementation of the Daughter Directives.

In this report, guidance is provided on undertaking an assessment of air pollution levels as required by Article 5. It is recommended to use information from three main assessment methods: measurements, emission inventories, and modelling. Information on measurement methods concentrates on indicative measurements, for the case where data from representative monitoring are not available or incomplete. For emissions, information is provided on the CORINAIR methodology; some information is also provided for some pollutants currently not covered in CORINAIR, such as PM10. Guidance is also provided on selecting and using models for the calculation of air pollution levels from the emissions, and comparing the results with measurements.

It is strongly recommended to estimate total uncertainty of the results for each assessment method, and for the result as a whole.

This guidance focuses on those pollutants for which Daughter Directives have been proposed in 1997, viz. SO_2, NO_2/NO, particulate matter (PM10) and lead.

It is recommended that the results obtained from these assessment methods be presented as maps, where the spatial extent of an area exceeding limit values, or requiring a certain assessment methodology, can be easily seen. The total uncertainty in the result of the assessment may be compared to the margins taken into consideration to account for the inter-annual variation of the air pollution levels.

The current report will need updating and supplementing in the coming years, as experience in the Member States in this area develops further. Clearly further guidance will be needed for the preparation of air quality assessments under Article 6 of the Directive, for example, on the optimised and representative siting of measuring stations.

1. Introduction

The Framework Directive on ambient air quality assessment and management (96/62/EC)[1] was adopted by the European Council in September 1996. The four objectives of the Framework Directive (FWD) are to:

- define and establish objectives for ambient air pollution in the Community designed to avoid, prevent and reduce harmful effects on human health and the environment as a whole;

- assess ambient air quality in Member States on the basis of common methods and criteria;

- obtain adequate information on ambient air quality and ensure that it is made available to the public inter alia by means of alert thresholds;

- maintain ambient air quality where it is good and improve it in other cases.

The FWD obliges the European Commission to present proposals to Council for further legislation which will fill in the basic structure which the FWD establishes. The first such proposals (on sulphur dioxide, nitrogen dioxide, particulate matter and lead) were adopted by the Commission for presentation to Council on 8 October 1997. Other proposals are now in preparation.

The Commission is being assisted in the technical work leading to proposals by a number of small Working Groups on individual pollutants. These Working Groups are generally chaired by experts from Member States, with further experts from up to 5 Member States, plus others from the World Health Organization, industry and NGOs. They report to a Steering Group including all Member States, industry, NGOs and others.

During the Steering Group Meeting of 8-9 February 1996 it was agreed that technical guidance should be developed to assist the competent authorities in implementing the FWD and subsequent daughter legislation. This document is the first step in the development of such guidance.

Good air quality assessment is key to implementation of the FWD and daughter legislation. Articles 5 and 6 set out basic assessment requirements.

Article 6 deals with ongoing assessment requirements under the Directive once limit values have been set in daughter legislation. Member States must divide their territory into zones (an agglomeration is a special type of zone). Ongoing assessment requirements are related to the levels of pollution within the zones.

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[1] OJ.L296, 21.11.96, p55

Article 5 deals with initial identification of the levels of pollution within a zone so that Member States can determine what the ongoing requirements are likely to be. It states that:

> *Member States which do not have representative measurements of the levels of pollutants for all zones and agglomerations shall undertake series of representative measurements, surveys or assessments in order to have the data available in time for implementation of the legislation referred to in Article 4.(1).*[1]

This means that Member States should have sufficient information by the time that legislation setting limit values is implemented with which to identify those agglomerations and other zones on which most attention should be concentrated.

The document deals with the question of how to decide whether information which is already available provides a sufficient basis for making these decisions, and, if not, how best to acquire such information.

It does not deal directly with assessment techniques to support optimisation of permanent monitoring networks, although information acquired during preliminary assessment should be useful for this purpose. Nor does it deal with issues of ongoing assessment under Article 6 of the Directive. It is expected that further guidance will be developed on these topics and on other aspects of implementing the legislation.

In chapter 2 of this report, a general outline of the assessment procedure under article 5 and its documentation, reporting and updating is provided. In chapters 3, 4 and 5, methodology and information are provided on preliminary measurements, on the assessment of human activities and emissions, and on modelling of concentration levels. In these chapters, emphasis will be on four pollutants (SO_2, NO_2, particulate matter (PM10), and lead) for which a Daughter Directive is being developed first. However, the methodology is intended to be useful also for other pollutants, to be included in forthcoming Daughter Directives. In these chapters, no specific methods are prescribed; rather, alternative methods and tools are given and recommendations are provided, and it is expected that Member States will exchange expertise and experience in this area, on the basis of which this document may be updated regularly. In chapter 6, the recommended specification for the assessments is provided. In chapter 7, the procedure for reporting, documenting and updating the assessments is described in more detail.

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[1] i.e. legislation setting limit values.

2. General outline of the procedure

Central to the procedure recommended in this report is the production, for each zone, of one or more maps of the entire zone. On these maps, all areas of exceedance or near-exceedance in the zone for quantities, for which limit values have been set in the Directives, should be clearly indicated. Such quantities may be annual average concentrations, percentiles, or other statistical concentration or deposition quantities. In some cases, Member States may find it more practical to develop a statistical overview of occurrence of exceedances and near-exceedances in the entire zone as an alternative to a detailed map. The requirement of the FWD for maps to be provided as part of formal action plans for improving air quality should however be borne in mind.

Although this report does not deal directly with the location of measuring stations for ongoing assessment, maps will be useful also for this purpose.

Unlike previous EC legislation on air quality the FWD envisages the use of tools other than measurement to provide the full picture needed to underpin successful air quality management. Article 2 defines "assessment" as "any method used to measure, calculate, predict or estimate the level of a pollutant in ambient air". Three main assessment methods or tools can be used singly or in combination for preliminary air quality assessment:

- preliminary air quality measurements;
- air emission inventories;
- air pollution modelling.

Preliminary air quality measurements (preliminary in the sense that these measurements do not serve to demonstrate compliance with Article 6 of the FWD) are used to explore air quality, particularly at those places where exceedances are to be expected, and/or emission information is inadequate.
Air emissions inventories provide comprehensive information on sources and their emissions and emission fluxes in the entire zone. This enables a first estimate of areas at risk of exceeding limit and target values.
Air pollution modelling serves to relate air quality to emissions in a quantitative sense, and provides a better basis for describing areas of exceedance in the entire zone. It also provides additional essential information for the management of the air quality in the zone, as required under the FWD.

All three methods or tools provide information with inherent uncertainty. By uncertainty we mean a quantitative measure of the most likely possible deviation of the value from the "true" value. See the text box below which defines some relevant concepts in this context.

Measurements - apart from sampling and analysis errors - may introduce major uncertainties if stations are not representative, meaning that air quality in the surroundings differs substantially from air quality at the station, or that concentrations vary appreciably in time while the measurements have only limited time coverage.

Emission inventories can be incomplete or may be based on inaccurate or inappropriate emission factors or activity figures.
Models may produce uncertain results either due to uncertainty in input such as meteorological quantities or emission data, or because of improper description or calculation of atmospheric processes and the resulting concentrations.

These assessment uncertainties can be reduced if information from all three methods is available. In order to judge the overall uncertainty in the assessment result, it is necessary to quantify and document uncertainties for each of the assessment methods.

As the FWD and Daughter Directives are implemented, the air quality is expected to change over the years for a variety of reasons. These include changes in human activity patterns (city growth, traffic increase, industrial production), technological developments (penetration of three-way catalyst, industrial abatement technology, etc.), and air quality management. Therefore, it is important to re-assess air quality on a regular basis, or if specific reasons suggest that this should be done. In chapter 7, recommendations are made for the updating procedure.

Some definitions of the concepts of Uncertainty, Verification and Validation (from the EMEP/CORINAIR Atmospheric Emissions Inventories Guidebook)

The following definitions of key terms are provided to promote common usage in the context of this guidance.

Accuracy	Accuracy is a measure of the truth of a measurement or estimate. The term accuracy is often used to describe data quality objectives for inventory data, however, accuracy is hard to establish in inventory development efforts since the truth for any specific emission rate or emissions magnitude is rarely known.
Precision	The term precision is used to express the repeatability of multiple measurements of the same event. In experimental applications a measurement or measurement technique could have high precision but low accuracy. The term precision is also used to describe the exactness of a measurement. The term precision is not well suited for use in emissions inventory development.
Confidence	The term confidence is used to represent trust in a measurement or estimate. Many of the activities discussed in this chapter are designed to increase the confidence that inventory developers and inventory users have in the databases. Having confidence in inventory estimates does not make those estimates accurate or precise, but will help to develop a consensus that the data can be applied to problem solving.
Reliability	Reliability is trustworthiness, authenticity or consistency. In the context of emissions inventories reliability and confidence are closely linked. If the approaches and data sources used in an inventory development project are considered reliable, then users will have an acceptable degree of confidence in the emissions data developed from those techniques.
Uncertainty	Uncertainty is a statistical term that is used to represent the degree of accuracy and precision of data. It often expresses the range of possible values of a parameter or a measurement around a mean or preferred value.
Validation	Validation is the establishment of sound approach and foundation. The legal use of validation is to give an official confirmation or approval of an act or product. Validation is an alternate term for the concept of verification as used in this context.
Verification	The term verification is used to indicate truth or to confirm accuracy and is used in this chapter to represent the ultimate reliability, and credibility of the data reported.

3. Preliminary measurements

3.1. Introduction

This chapter summarises methods for obtaining a preliminary overview of the air quality situation in a zone by measurements, in the case that no previous assessment is available. These measurements are not intended to control compliance of limit values under Article 6 of the FWD, but rather are screening techniques meant to determine what compliance measurements and other assessments are needed to comply to EC legislation. The results of preliminary measurements can be complemented with an assessment of emission sources and modelling to obtain a full picture of the air quality in a zone, as measurements are inherently limited in their representativeness in space and time.

3.2. Measuring strategy

A measuring strategy depends on the objectives of the monitoring, and the pollutants to be assessed. For the relevant air quality parameters (concentration of pollutants and associated averaging time), we need to specify where, how, and how often measurements should be taken. The measuring effort will be dependent on:

- the variation of pollutant concentrations in space and time;
- the availability of supplementary information;
- the accuracy of the estimate, that is required.

It is possible to derive, in quantitative terms, a measuring strategy from this information. However, this is not always practicable, as the required accuracy is often not specified, and the variation of the pollutant in space and time may not be sufficiently well known. In this guidance report, the following approach is proposed:

1. Estimate the levels and spatial variation of the quantity from existing measurements in the zone, or in similar situations elsewhere, or from emission inventories and model calculations.

   Where measurements are being used as the basis of the assessment:

2. Design a measuring strategy for assessing the spatial distribution of pollutants, the pollutant levels in areas with highest concentrations and in background locations.
3. Carry out measurements with appropriate methods, with a frequency and over a period of time as specified below.
4. Calculate from the measurement results estimates of the relevant air quality statistics.
5. Estimate the uncertainty of the measured estimates, taking into account the accuracy of the individual measurements, station representativeness, and variability of the pollutant in space and time.

6. Where available compare model estimates and measured estimates, and evaluate discrepancies.

Steps 2 and 3 are covered in paragraph 3.4, 3.5 and 3.6, steps 4 and 5 in paragraph 3.7. Information on emissions and models is provided in chapters 4 and 5.

A measuring strategy for preliminary assessment will concentrate on the question in which areas pollution levels exceed limit values, or the associated assessment threshold levels, as set by the Directive. For those areas, more intensive assessment as described in article 6 of the FWD will be required. The preliminary assessment should not only identify the location of maximum concentrations, but also determine the extent and the limits of the area of exceedance.

3.3. Preliminary measurement techniques

Currently used air quality measurement techniques can be sub-divided in three main categories:

Manual methods
These are the simplest and cheapest measurement methods, usually based on a sampling procedure followed by chemical analysis (or gravimetric determination for suspended particulate matter). According to the implemented sampling procedure, different manual methods can be recognised: the use of bubblers for gaseous pollutants, the diffusive sampling method for gaseous pollutants, and the collection on filters for suspended particulate matter (Black Smoke and PM10) and heavy metals measurements.

Automated methods
These currently constitute the most widespread monitoring technique in the air quality monitoring networks. The analysis of the pollutants is based on physical principles and processed electronically. Automated analysers allow for the continuous, automated, on-line and time-resolved measurement of air pollutants. The major drawback of this technique resides with the high costs for purchase and maintenance of the analysers, often resulting, as a consequence, in low network density and low spatial resolution of the measurements. Mobile laboratories equipped with automated analysers constitute a useful application of this technique as a tool for measurement campaigns at locations of interest.

Long-path optical methods, such as the Differential Optical Absorption Spectrometry (DOAS), allow for the simultaneous monitoring of various gaseous pollutants integrated over a distance of several hundreds of meters. As for the other automated methods, the long-path optical methods allow for the continuous, automated, on-line and time-resolved measurement of air pollutants.

Among these measurement techniques, screening techniques based on the use of a mobile laboratory and the diffusive sampling technique or other manual methods are of particular interest, because of their relatively low cost and their simple and fast operation, in comparison with fixed monitoring stations. Three different approaches are proposed in this chapter:

- the diffusive sampling technique (see 3.4);
- the use of a mobile laboratory in areas of maximum concentrations (see 3.5);
- the use of a mobile laboratory for grid measurements (see 3.6).

or a combination of one or more of the proposed approaches.

3.4. Use of the diffusive sampling technique

3.4.1. General methodology

The low cost and easy operation of the diffusive sampling technique make it an ideal tool for large scale air pollution surveys with a high spatial resolution (De Saeger et al.,1991,1995). A diffusive sampler is a device capable of taking gas samples from the atmosphere at a rate controlled by molecular diffusion, and which does not require the active movement of air through the sampler. The diffusive sampler consists of a tube, one end containing a sorbent which fixes the pollutant. The pollutant is sampled onto the sorbent at a rate controlled by the molecular diffusion of the pollutant gas in the air, without requiring any pump or electrical power. After exposure of the samplers over periods varying from a few days to a few weeks, the tubes are closed and returned to the laboratory for analysis. According to the type of device and the measured pollutant, analysis can be performed using different techniques, such as colorimetry, ion chromatography and others. Maps of the pollutant concentrations over the area can be obtained by interpolation of the diffusive sampler measurements (see Fig. 1: Example of Madrid - Spatial distribution of NO_2 levels determined by diffusive sampling) Diffusive samplers are today available for a large number of gaseous pollutants, such as SO_2, NO_2, O_3, CO, Benzene.

The technique is particularly suited to determine the pollutant distribution over a large area, and to assess integrated concentration levels over longer periods of time (long-term limit values). Short-term limit values can be derived from statistical data, by comparison with extended and time resolved measurement series from similar measurement locations. The proposed methodology can be used to determine areas of maximum concentration and combined with the use of a mobile laboratory as described in 3.5. In addition it may support the optimisation of monitoring networks and assessments supporting generalisation.

When applying this methodology in the case of a preliminary assessment, the following steps are proposed:

1. Establish the location of the main emission sources from an assessment of emission sources.
2. Construct a grid over the area under investigation taking into account the density of the sampling sites specified in the data quality requirements.
3. Select for each cell of the grid a location representative of the background pollution level in that cell, that is not directly influenced by local pollution sources.

4. If necessary, select additional sampling sites in the vicinity of important pollution sources (hot spots such as roads with heavy traffic, industrial sources).
5. Install the samplers over the area and expose them over a representative time period taking into account the minimum time coverage specified in the data quality requirements included in this guidance.
6. In support of the QA/QC of the measurements, it is recommended to install duplicate/triplicate samplers in a limited number of sites in order to assess the reproducibility of the measurements. Unexposed samplers should be kept during the period of exposure for assessing the sampler blank value.
7. Perform the analysis of the diffusive samplers in the laboratory and calculate the pollution levels for each particular site.
8. Calculate the distribution of the pollution levels by interpolation of the measurements made in each grid cell. The measurements performed in the vicinity of sources (hot spots) are not necessarily representative of a larger area, and should in that case not be included in the interpolation calculations.
9. Make a graphical presentation of the pollutant in map form. Concentrations measured at hot spots are indicated on the map.
10. Estimate percentile values by comparison with extended and time resolved measurement series from similar measurement locations.
11. Compare the obtained measurement results with the limit values of the directive and select the appropriate assessment regime.

It should be noted that diffusive samplers are very cost effective, but that their implementation on a large scale may be labour intensive and hence costly. They can however also be a useful tool when used less intensively in conjunction with other assessment methods.

Other manual measurement techniques, such as bubblers (total acidity, Thorin and TCM method for SO_2, Saltzmann method for NO_2), can be used as an alternative to the diffusive sampling technique, in particular when the number of samplers to be implemented is low. The methodology proposed for the diffusive sampling technique applies in that case also for bubblers.

3.4.2. Data quality requirements

When performing diffusive sampling campaigns, the following data quality requirements are proposed. These data quality objectives are only indicative, and may be strengthened where possible.

- Maximum uncertainty of the measurements: ±30% (for single measurements and a 95% confidence interval averaged over the reference period and at the level of the limit value, taking into account errors of calibration, sampling efficiency, analytical performances and the effect of environmental parameters). The measurements should be supported by an adequate QA/QC programme during the period of the campaigns, and the quality of the measurements should be fully documented.

  It should be noted that the diffusive sampling technique is still coping with a lack of harmonised validation data. The current state of the art of the technique however has shown that the required uncertainty level (± 30%) can be met for SO2 and

NO2, provided that the measurements be supported by an adequate QA/QC programme. The European Committee for Standardisation (CEN - Technical Committee 264 - Working Group 11) is currently developing requirements and test methods for the implementation of the diffusive sampling technique (CEN,1996).

- Siting criteria and number of samplers: The diffusive samplers should be installed at those sites where the limit values apply (kerbside, urban background, rural background, etc.). The density of the sampling sites essentially depends on the spatial variability of the pollution levels, and hence may vary with type of pollutant, source distribution, local orography and meteorology.

  In the case of those agglomerations for which an intensive measurement campaign is undertaken, it is proposed to install a number of samplers equal to 15 times the initial number of measurement stations required for mandatory measurements (Ni). This would result in a number of 30 samplers for agglomerations with a population of 250.000 inhabitants, of 60 samplers for agglomerations with a population number of 1.000.000 inhabitants and of 150 samplers for an agglomeration of 6.000.000 inhabitants (see Daughter Directive proposal for SO_2, PM10, NO_2 and Pb). The sampler density may vary in function of the emission sources configuration, and it is good practice to increase the sampler density in city centers with respect to the outskirts (see Fig. 2: Example of Athens - Construction of the measurement grid). Additional samplers would be installed at a representative sample of hot spots, such as along busy roads and crossings, as well as in the surroundings of industrial pollution sources, in particular if they are likely to affect local pollution levels. A limited number of samplers should be installed at the periphery of the area under investigation, in order to assess the impact of adjacent areas.

In other cases (industrial zones, rural background), the number of stations should be sufficient to determine the extent of pollution and exposure.

- Minimum time coverage: 20% of the reference period of the directive's long-term limit value (1 year), by example five 2 weeks periods evenly distributed over the year, or two 5 week periods corresponding to the seasons with maximum and minimum pollution levels (typically during winter and summer periods).

- Minimum data capture: 90% of the time of the campaigns, allowing for a failure (leakage, theft, vandalism, presence of insects) of the diffusive samplers during 10% of the time.

3.4.3. Specific information on existing diffusive samplers

Diffusive samplers for ambient air measurements have been developed for various pollutants. The Palmes diffusion tube for the measurement of SO_2 and NO_2 is certainly the best known, but several other types are widely used today (Palmes, 1973; 1976). Figure 3 gives an example of currently available diffusive samplers. Other kinds of samplers are today available, covering almost all the gaseous pollutants foreseen by the Framework Directive (Brown,1993). A guide for the selection and the application of the diffusive sampling technique is currently being prepared by CEN - Technical Committee 264 - Working Group 11 (CEN,1996).

The following table gives a review of the existing diffusive samplers and of their analytical principles:

Pollutant	**Analytical principle**
SO_2	Chemical absorption + colorimetry / ion chromatography
NO_2	idem
NO_x	idem (same as for NO_2 + oxidation layer)
O_3	Chemical absorption + colorimetry
CO	Chemical absorption + colorimetry
BENZENE	Chromatographic adsorbent + GC analysis

It should be noted that the principle of molecular diffusion does not adapt to particulate matter, and that the diffuse sampling technique is therefore not applicable for PM10 or heavy metals (Plants have been used as passive samplers for some of these substances, but this is a surrogate for deposition rather than for concentration measurements).

In urban areas, the spatial variation for primary pollutants such as NO, CO, Pb, PAH’s and benzene is mainly determined by their emissions from automotive traffic. As a result of this, one single pollutant representative of the emissions from automotive traffic may be used as indicator for the other pollutants, when determining areas of maximum concentrations. This "indicator approach" is however valid only if large industrial sources with low level emission heights are not present in the area. Particularly for Pb, PAH or benzene, this cannot be taken for granted. Nor is this approach acceptable for secondary pollutants such as NO_2.

3.5. Use of a mobile laboratory in areas of maximum concentrations

3.5.1. General methodology

The methodology allows evaluation of the maximum concentration levels in a zone over a period that is representative of the reference period(s) of the limit value. It is used as a preliminary assessment method in order to verify whether a zone is in exceedance or near-exceedance of the limit values, and determine the ongoing assessment regime that will be required under Article 6 of the Framework Directive.

Mobile laboratories or transportable measurement stations used for stationary measurements at fixed sites, usually combine the advantages of automated measurement methods (continuous, time-resolved measurements) with mobility or flexibility. For pollutants for which automated measurement methods are not available, mobile laboratories may also be equipped to perform non-automated measurements (PM10, heavy metals, PAH’s). The duration, the periods and the frequency of the campaigns or measuring periods will have to be established so as to be representative of the reference period of the limit value (1 hour, 24 hours, 1 year).

The location of maximum concentration levels in a zone will be chosen taking into account the source distribution, local meteorological conditions and orography. The types of sources present in an area are very important when choosing a measuring site. Impact from elevated point sources is often difficult to measure at one point at ground level because both wind direction and wind speed, and their variation with height is important for the location of the maximum ground level impact. For monitoring the pollution from roads, the impact will decrease with the distance from the road, and the level of pollution will on average be proportional to the volume of traffic. Time-series of hourly concentrations should reflect the pattern of traffic intensity. The highest concentrations for 24-hour periods should be expected to be located in areas where the road runs parallel to the most frequent wind-directions, or where the curvature of the road allows impact from several wind-directions. For monitoring pollution mainly from area-sources the location should be chosen close to the centre of the area, and avoid direct impact from "super local" sources in the vicinity (example: small incinerators or petrol stations). In complex situations resulting in a high variability of the pollutant distribution (sources of different origins, complex terrain and meteorology), it is advisable to perform the measurements in different representative locations.

When applying this methodology the following steps are proposed:

1. Establish the location of expected maximum concentration from either existing measurements, from information from similar zones, emissions inventories or modelling studies. The diffusive sampling technique (see 3.4) used as a tool to determine the spatial distribution of pollutants, may constitute an alternative technique to assess the areas of maximum concentration levels.
2. From time series of existing measurements or from information from similar zones, determine the periods of maximum pollution levels.
3. Perform the measurements as specified in the data quality requirements.
4. Compare the obtained measurement results with the limit values of the Directive (see 3.7) and select the appropriate assessment regime.

3.5.2. Data quality requirements

When performing the measurements with a mobile laboratory, the following data quality requirements are proposed. These data quality objectives are only indicative, and may be strengthened where possible.

- Maximum uncertainty of the measurements: ±15% for gaseous pollutants and ± 30% for particulate matter measurements (for single measurements averaged over the reference period and at the level of the limit value, taking into account errors of sampling, calibration and instrument performances). The measurements should be supported by an adequate QA/QC programme during the period of the campaigns (periodic in-situ calibration and calibration check, proper maintenance of instrumentation), and the quality of the measurements should be fully documented.

- Minimum time coverage: For long-term limit values (typically 1 year), 20% of the reference period, by example five 2 weeks periods evenly distributed over the year, or two 5 week periods corresponding to the seasons with maximum and minimum pollution levels (typically during winter and summer periods). For short term limit values (24 hour and shorter), 3 months during the expected period of increased pollution levels.

- Minimum data capture: 90% of the time of the campaigns or measurement periods, allowing for a failure of the instrumentation during 10% of the time.

Better estimates of minimum time coverage can be calculated from stochastic sampling from an existing series of monitoring data in a similar situation. This exercise has been carried out in the EC Working Groups on particulates and on benzene (see position papers, to be published)

3.5.3. Specific information for some pollutants

The mobile laboratory would be equipped with one analyser for each of the pollutants under consideration. The selected measurement method shall comply with the reference method of the respective Directives as well as with the quality objectives. The following table gives an example of possible measurement methods to be used for the assessment.

Pollutant	**Measurement method**
Sulphur dioxide	UV fluorescence
Nitrogen dioxide	Chemiluminescence
PM10	Sampling on filter + gravimetry (manual method), beta attenuation, oscillating micro-balance
Lead	Sampling on filter + atomic absorption spectrometry, ICP, X-ray fluorescence (manual method)

A mobile laboratory can easily combine measurements of various pollutants, and may constitute a unique screening tool for pollutants for which cost effective measuring techniques are not available (PM10, heavy metals).

3.6. Use of a mobile laboratory for grid monitoring

3.6.1. General methodology

Further to the assessment of pollution levels in areas of maximum concentrations, a mobile laboratory can also be used to assess the pollutant spatial distribution over a larger area. Grid monitoring is performed by dividing the particular area of interest into a grid of squares, and by measuring the pollution levels in each grid cell. The measurements are made during short periods of time at each intersection of the grid lines, and repeated over the course of a year. The dates and hours for the measurements are chosen randomly but in such a way that they are evenly distributed over the months, the days of the weeks and the hours of the day. The measuring schedule is laid out so that no neighbouring intersections are measured on the same day. The single values measured at the four corners of each grid are used to calculate the mean concentration value for each grid cell and the pollutant concentrations isopleths over the area. Percentile values can be estimated statistically from the accumulated frequency distribution.

Note that the method is not suitable to characterise air quality hot spots, for which additional sampling should be carried out.

A typical example of this methodology is illustrated by a study made in Karlsruhe for NO_2, see fig. 4: Example of Karlsruhe - Grid monitoring of NO_2 levels (UMEG,1996). In this particular case, the area was divided into a grid with a density of 1 x 1 km, and half-hourly measurements were repeated 26 times over the year, resulting in 104 half-hourly measurements for each grid square. The measurements were performed between 6 a.m. and 10 p.m., resulting in an overestimation of the concentration levels, but measurements during the night may be considered when a higher accuracy is necessary.

The proposed methodology is of particular interest in cases where a limited number of measurements are required (small agglomerations), or when other kinds of screening techniques are not available (SPM).

When applying this methodology in the case of a preliminary assessment, the following steps are proposed:

1. Construct a grid over the area under investigation taking into account the density of the grid specified in the data quality requirements.
2. Prepare the measurement schedule, by choosing randomly over the year, the dates and hours for the measurements in such a way that they are evenly distributed over the months, the days of the weeks and the hours of the day, taking care that no neighbouring intersections are measured on the same day.
3. Perform the measurements with the mobile laboratory at the intersection of each grid.
4. Calculate the yearly average concentration for each grid cell from the single values measured at the grid intersections.
5. Make a graphical presentation of the pollutant distribution by means of iso-concentration plots over the area.
6. Estimate percentile values by comparison with extended and time resolved measurement series from similar measurement locations.
7. Compare the obtained measurement results with the limit values of the directive and select the appropriate assessment regime.

3.6.2. Data quality requirements

When performing the measurements, the following data quality requirements are proposed. These data quality objectives are only indicative, and may be strengthened where possible:

- Maximum uncertainty of the measurements: ±15% for gaseous pollutants and ± 30% for particulate matter measurements (for single measurements averaged over the reference period and at the level of the limit value, taking into account errors of sampling, calibration and instrument performances). The measurements should be supported by an adequate QA/QC programme during the period of the campaigns, and the quality of the measurements should be fully documented.

- Minimum time coverage: For long-term limit values (typically 1 year), 100% of the reference period, randomly spread over all the measurement sites.

- Minimum data capture: 90% of the time of the campaigns or measurement periods, allowing for a failure of the instrumentation during 10% of the time.

- Minimum grid density: In the case of agglomerations, it is proposed to apply a grid density of 15 times the initial number of measurement stations required for mandatory measurements (Ni). This would result in a number of 30 grid cells for agglomerations with a population of 250.000 inhabitants, of 60 grid cells for agglomerations with a population number of 1.000.000 inhabitants and of 150 grid cells for an agglomeration of 6.000.000 inhabitants (see Daughter Directive proposal for SO_2, PM10, NO_2 and Pb).

3.6.3. Specific information for 4 first pollutants

See 3.5.3

3.7. Data evaluation and uncertainty assessment

When the measurements have been carried out, the relevant statistical quantities (annual average, percentile values) for which limit values are defined, are to be estimated. This is particularly relevant for preliminary assessments. Particularly for higher percentiles, and for short measuring periods, this introduces major uncertainties. To our knowledge, no generally accepted methodology is available; we introduce here some important aspects only.

In principle, the problem may be approached by assuming a certain frequency distribution of the concentration, and determining the basic parameters for this distribution. An obvious choice is the log-normal distribution, which allows for estimation of the median and logarithmic standard deviation, from which all percentiles can be calculated. Clearly estimates of higher percentiles become progressively more uncertain in this procedure.

However when estimating these concentration statistics from the measurements, the following aspects should be considered:

3.7.1. Meteorological variability

The variability of the meteorological parameters (wind, temperature, atmospheric stability, precipitation, ...) constitute an important factor affecting the frequency distribution of the measured concentrations. When calculating the concentration statistics from the measurements, the meteorological conditions during the measurement period must be checked to be representative of the normal meteorological conditions, and, if not, the measurements should be corrected accordingly. The measurements are to be classified according to meteorological classes, and their weight/frequency adjusted in accordance with the frequency of occurrence of meteorological classes over a long (10-30 years) period. This method is recommended if the measurement period is at least one year.

An alternative possibility is:

- Take the same measurement period from a comparable station with long term continuous measurements
- Compare the statistics for the short term period and the long term period and calculate correction factors
- Apply these correction factors to the short term, indicative measurements

3.7.2. Empirical relations for various emission situations

From literature, (semi)-empirical relations may be found between one hour average concentrations and their longer-term averages (day, month, year), and relations between those averages and percentiles. However, temporal variations of concentrations depend a.o. on the source environment, and, consequently, these relations can be quite different for situations with pollutant emissions from different source categories (point, line, area). For continuous elevated point-sources, the impact at one point at ground level will be more dependent upon variability in dispersion conditions than for line or area sources. The peak-to-mean ratio for a point source is generally much higher than the ratios for line and area sources. A location where the pollution level is dominated by contributions from area-sources reflects the variation in area-source strength with time more than the variations in dispersion conditions.

Estimating concentration statistics from a limited number of measurements can therefore be a difficult task. The proposed methodology is best indicated in the case of area- and line-sources, i.e. in urban situations where the air pollution is diffuse and mainly dominated by automotive and domestic heating emissions. In the case of point sources, it is generally not possible to assess the relevant quantities from supplementary measurements. For assessment in these cases, the combination of emission data and model calculations should be preferred.

3.7.3. Correction for uncertainty of measurements

The impact of measurement uncertainty on concentration statistics is discussed by Van der Wiel *et al.* (1988) The variations related to measuring imprecision introduce upward shifts in the percentiles, which become increasingly important for higher percentiles. The reliability of this procedure is dependent on the size of the data base; also, in some cases with rarely occurring high concentrations, as for example around point sources, the correction may result in even larger errors.

3.7.4. Uncertainty of individual measurements

The uncertainty of measurements in field conditions depends on:

- the performances of the measurement system (sampling, calibration, analysis);
- the expertise of the laboratory responsible for the measurements or, in practice, the quality system implemented by the laboratory;
- the spatial representativeness of the selected measurement locations.

Standard testing procedures have been established to determine the uncertainty of the measurements by a given instrument in laboratory and field conditions, in particular for type approval of the instrumentation. It is however far more difficult to estimate the measurement uncertainty in routine field conditions. This estimation can only be performed experimentally by submitting the measurement system to quality control in field conditions over a longer period of time (typically 3 months).

Concerning the spatial representativeness of the measurement location, a wrong location will undoubtedly lead to an underestimation of the true concentration, as the measurement strategy is aimed at the measurement of the highest concentrations. In practice however, it will be impossible to estimate the extent of the associated uncertainty. It is therefore proposed not to consider this element in the uncertainty estimation, but to require a detailed report on the siting criteria.

On the basis of experience obtained from the QA/QC programmes organised by the Joint Research Centre for SO_2 and NO_2 measurements, an estimation of the uncertainty for measurements made by a mobile laboratory and by the diffusive sampling technique is given in the following table (De Saeger, 1996). In both cases, the assumption was made that the laboratory was implementing a recognised quality system (ISO 9000, EN 45001) and using up to date instrumentation.

	Estimated uncertainty SO_2 and NO_2 measurements (95% confidence interval)	
Source of errors	**Mobile laboratory (hourly mean value)**	**Diffusive samplers (2-week average)**
Sampling Sampling efficiency Losses in the sampling line	-5%	±15%
Calibration chain Primary calibration Transfer standard Calibration check in station	±10%	±5%
Instrument response Precision, stability, linearity Selectivity Environmental variables (T, P, RH %) Maintenance	±10%	±25%
Propagated uncertainty	±15%	±30%

The regular organisation of quality controls during the measurement period constitute therefore the only way to contain the uncertainty of the measurements within the established limits and to document the quality of the determinations.

3.8. References

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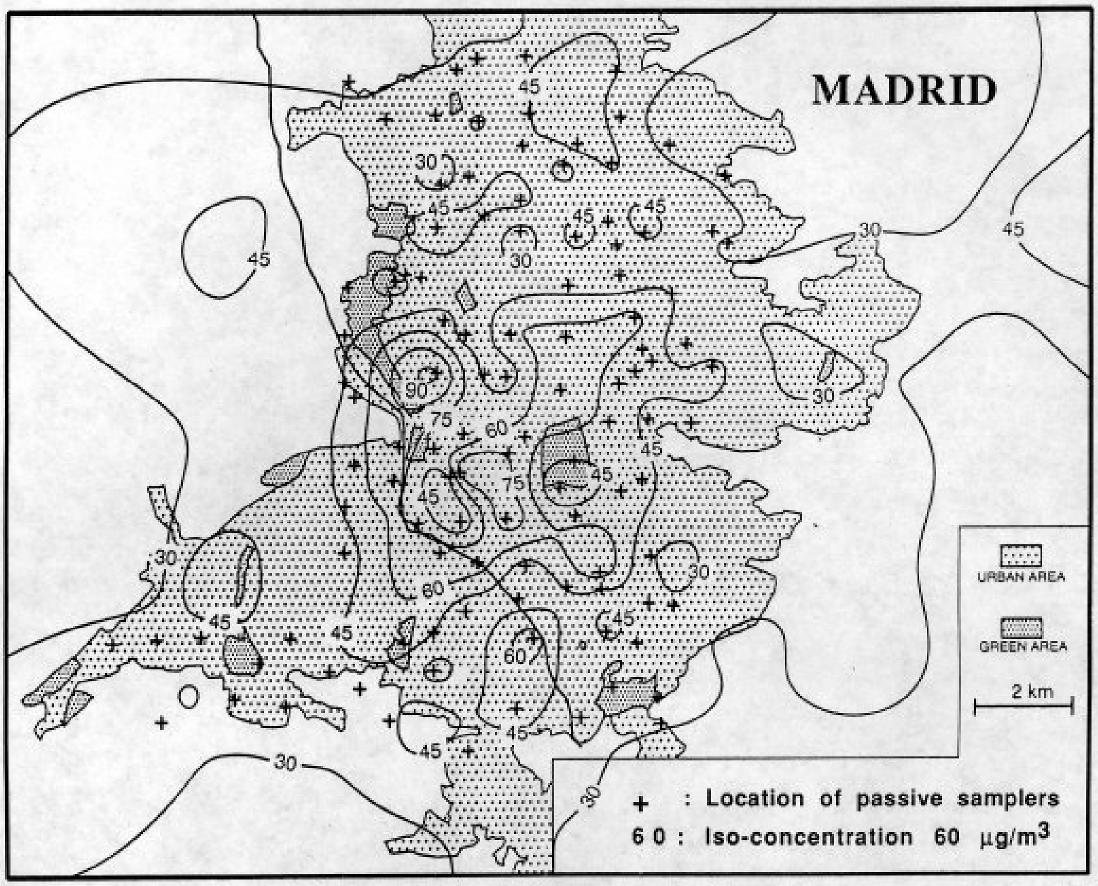
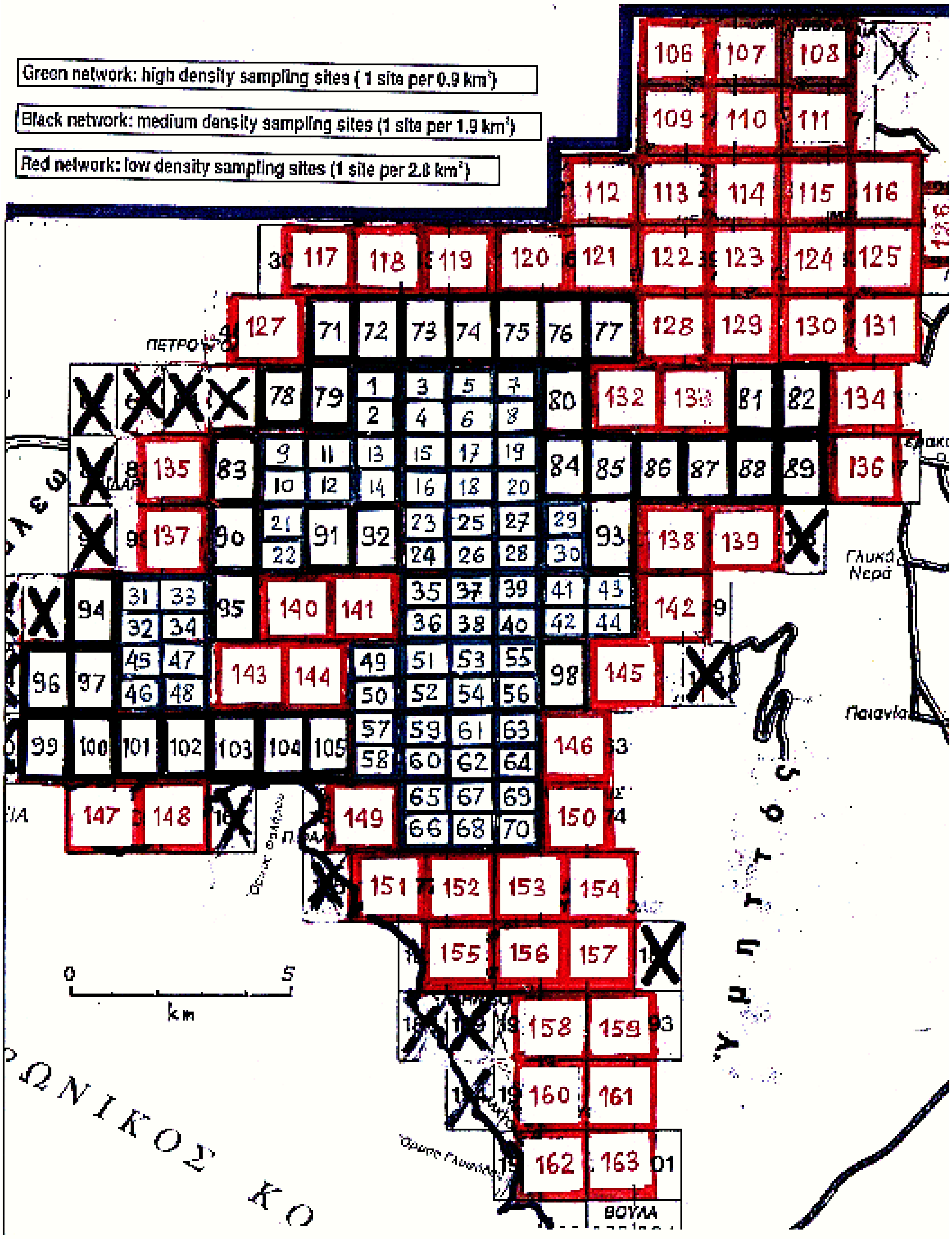
Figure 1.



Assessment of the NO2 spatial distribution by diffusive sampling measurements (example of Madrid)

Figure 2.

Indicative monitoring of NO2- SO2 in Athens by diffusive samplers



Grid construction for diffusive sampling measurements in an urban area (example of Athens)

Figure 3.

Example of currently available diffusive samplers

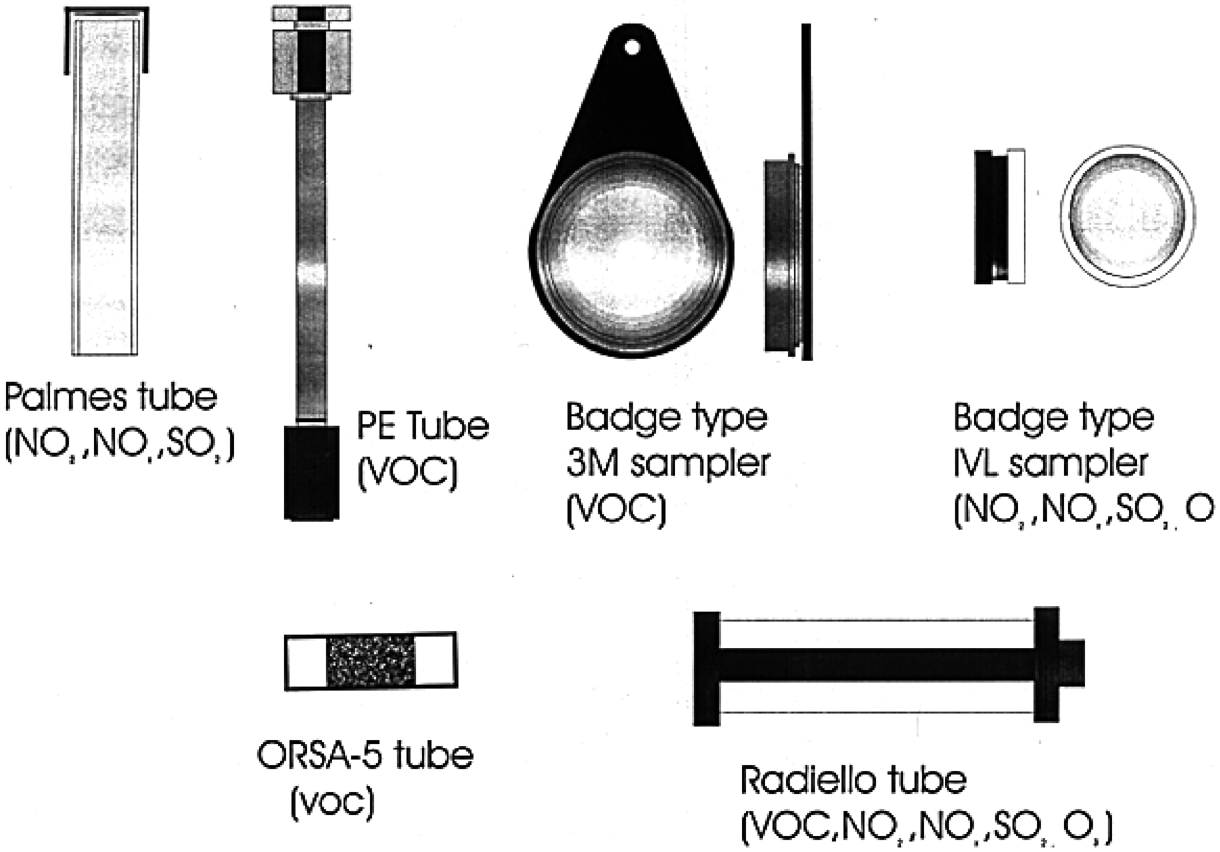
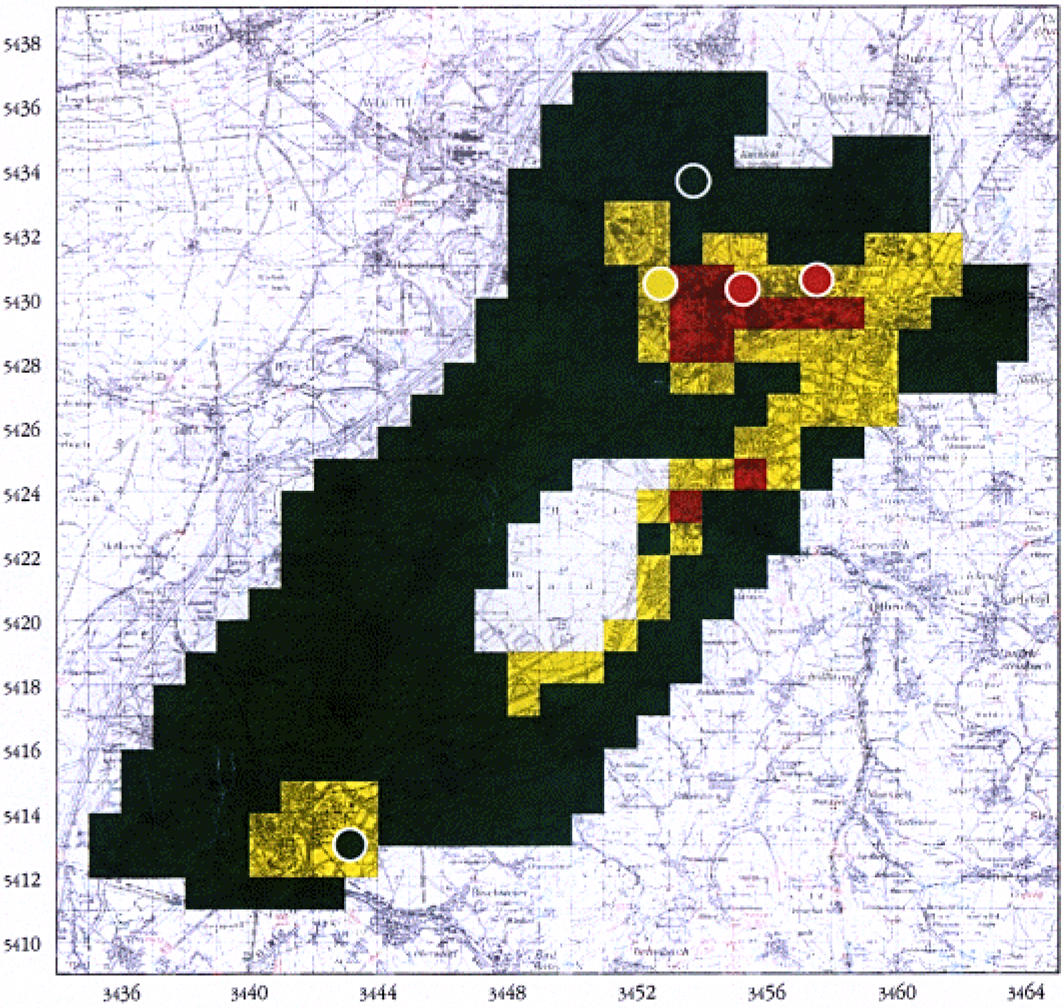


Figure 4.

Use of a mobile laboratory for grid monitoring (example of Karlsruhe)



MEẞGEBIET:	Großraum Karlsruhe Rastatt
MEẞZEITRAUM:	August 1994 - Juli 1995
EINHEIT:	$\mu g/m^3$

🟩
🟨 36 < K ≤ 44
🟥 44 < K

K: Konzentration

Räumliche Verteilung der Stickstoffdioxidkonzentrationen im Meßgebiet Karlsruhe/Rastatt

Berechnet aus den Mittelwerten der Beurteilungsflächen

UMEG

4. Human activity and emission inventories

This chapter provides guidance on compiling emission inventories as part of a supplementary assessment. The primary objective is to produce an emission map of the zone. This map provides basic information on the air pollution situation in the zone, and information needed to run simple models for calculation of the concentration of air pollutants, as described in chapter 5. In this case, the specifications of the emission inventory should be determined by the input requirements of the model and hence, indirectly, by the chemical, spatial and temporal resolutions of the air quality quantities (concentrations) as specified in the Directives.

In principle, calculation of peak concentrations (both in space and in time), requires emission inventories with very high space and time resolution; however, in a number of cases, these peak concentrations may be assessed on the basis of more aggregated emission information using statistical information on the time variation of the emissions, while the emission factor methodology allows to compile emission estimates for individual sources, streets and other areas where high concentrations are expected. For secondary pollutants, such as ozone, nitrogen dioxide, and sulphate or nitrate particulates, more complex models are needed requiring data on emissions of so-called precursors, from which the pollutant is formed by chemical conversion.

A standard methodology, harmonised at the European level, has been developed and applied in the CORINAIR project and documented in the EMEP/CORINAIR Atmospheric Emission Inventory Guidebook (EMEP/CORINAIR, 1996). Within this project a complete, consistent and transparent emissions database for all of the European territory for the base years 1990 and 1994 is available. Member States may have more detailed and up-to-date emission inventories for particular zones. If however, no specific emission inventory for the zone under study is available such an inventory can be derived from the most recent CORINAIR inventory available, using the methodology described in this chapter.

The CORINAIR database can be used directly to calculate background concentrations, resulting from emissions outside the region under study.

4.1. General methodology

An atmospheric emission inventory can be defined as a collection of data presenting an emission of a pollutant (to air) and related parameters including:

- chemical identity: characterises the chemical properties of the pollutant;
- activity or technology: characterises the cause of the emission and relates it to (human economic) activity;
- location: describes both the location on the map and the height of the release (stack height);
- time dependence: in general emission inventories store emissions as annual totals. The temporal patterns are in most cases modelled in the air quality assessment.

These parameters are presented in turn in relation to the use of the inventory for air quality assessment.

Chemical identity: the pollutants (or pollutant classes) considered in the inventory. Focusing on the air quality theme, some relevant pollutants (or pollutant classes) to be considered are: SO_2, NO_x, VOCs, (fine) Suspended Particulate Matter (SPM), such as PM10 and PM2.5, and CO. Among VOCs, some substances are relevant concerning their effects on health (for example benzene), others for their chemical reactivity related to ozone and other photochemical pollutants production. For the last mentioned phenomenon speciated VOC-emissions are required. Other relevant pollutants are heavy metals (HM), such as Pb, Hg, Cd, As, Ni, and persistent organic pollutants (POP) such as PAH (polycyclic aromatic hydrocarbons) and dioxins. For a number of these pollutants information is available in CORINAIR90, more will be available in CORINAIR94. In some cases however (benzene, speciated VOC's, SPM) additional information is needed, as no standardised methodology has been developed to date.

Activity or technology: an emission source nomenclature is needed that includes anthropogenic and natural activities. The SNAP97 (Selected Nomenclature for Air Pollution, version 1997) developed by the EEA (ETC/AE) and EMEP is the most complete and detailed list presently available. This nomenclature is used for the CORINAIR inventory by the 18 EEA member countries and others. SNAP97 will be presented in the 1998 revised version of the joint EMEP/CORINAIR "Atmospheric Emission Inventory Guidebook". Table 4.1 lists the main SNAP sectors and their relation to the economic sectors as defined in the EC Fifth Environmental Action Programme A more detailed list is provided in Annex 1. To fully define an emission source related to combustion, reference should be made to the fuel used.

SNAP is a three level hierarchical nomenclature:

SNAP level 1 -	11 main sectors
SNAP level 2 -	76 sub-sectors
SNAP level 3 -	375 activities

Table 4.1. Main sectors in CORINAIR 94 and their relation to economic sectors as defined in the Fifth Environmental Action Programme.

Main SNAP sector	Definition	Target Sector
1	Combustion in energy and transformation industries	Energy
2	Non-industrial combustion plants	Energy and Consumers
3	Combustion in manufacturing industry	Industry
4	Production processes	Industry
5	Extraction and distribution of fossil fuels / geothermal energy	Energy
6	Solvent and other product use	Several
7	Road transport	Transport
8	Other mobile sources and machinery	Transport
9	Waste treatment and disposal	Several
10	Agriculture *)	Agriculture
11	Other *)	

*) SNAP97 differs from SNAP94 by that the category forestry, land use and wood stock change has been moved from sector 10 to sector 11. Sector 11 was called "Nature" in SNAP94.

Emission type and location: in air quality assessment, point, line and area sources are usually considered. Line sources and area sources are statistical descriptions of a large number of relatively small point sources. Examples of line sources are roads, railways, and shipping routes. Urban areas can be seen as area sources. Whether or not a group of small sources can be described as line or area source, depends on the spatial resolution required. Hence, the classification of point, linear and area sources is not strict: it depends on the scope of the assessment and on cost-effective considerations. The spatial resolution of CORINAIR does not provide for allocation to line sources. Member States may have detailed local inventories which do include such sources. The Large Combustion Plant Directive reporting process yields data on point sources. These data can be and are incorporated into the CORINAIR structure. As from 2002 the IPCC Directive will call for emission reporting by individual companies, increasing the amount of data available on large point sources.

Time distribution of the emission: For microscale or local scale estimation, as well as for the simulation of air pollution episodes, high time resolution emission inventories are needed. To estimate background concentration of primary pollutants a lower temporal resolution is sufficient. Time resolution of the emissions in principle follows the time resolution of the activity rate. If required a time resolved emission pattern therefore should be derived from annual totals using statistical information on the time dependency of the activities. These can be, for example, traffic counts or seasonal and daily temperature variations. In some cases these temporal disaggregations are part of the models and in some cases the models require an hour by hour emission input. Generally, local assessments require more detail than is available from the CORINAIR database. As a screening estimate however the EMEP/CORINAIR emission factors can be used at higher spatial resolutions, provided that the activity data are available at that higher resolution.

High or low spatial resolution of emission data is one of the most important dimensions which characterises emission inventories. For microscale or local scale assessments, inventories with high spatial resolution are needed. To estimate background concentration, inventories with low spatial resolution are sufficient.

Recently, the ETC/AE produced a report describing the methodology to derive a more spatially detailed inventory from the CORINAIR inventory (Cirillo et al. 1996).

Point source emissions available in CORINAIR can be used directly. For area sources two approaches are available:

- The emission factors provided in the EMEP/CORINAIR Guidebook make no reference to spatial resolution; hence this methodology can be applied at any spatial scale. This approach needs activity data at the spatial resolution required in the assessment;
- A top-down approach uses proxy variables to estimate spatially resolved emission patterns at a higher spatial resolution than available in CORINAIR. These proxy variables are for instance population density, road length or area. In this approach a relatively small number of data has to be available at sufficient spatial resolution. Chapter 7 of the above Review Study gives details of this method.

This latter approach may be used if detailed local inventory information is lacking, or if information for different local areas is not sufficiently comparable. The uncertainties in such a method however are quite large for a particular location. The overall picture however might be quite informative.

4.2. Information on some pollutants and examples

Table 4.2 presents the (provisional) main source sector split of the emissions in Europe as stored in the CORINAIR94 emissions inventory for the components relevant for this document. It is clear that for SO_2 industrial activities are by far the most important source, whereas for CO, NO_x and NMVOC transportation is the most important contributing activity. Table 4.3 and 4.4 give some more detail for the transportation sector (main SNAP sectors 07 + 08). Important issues for compiling emission inventories for the relevant pollutants will be discussed in more detail below.

Table 4.2. Main sector split of European total emissions in 1994[1] (%, totals for EU member states).

Main SNAP sector	SO2	NOx	NMVOC	CO
Combustion in energy and transformation industries	51	19	1	1
Non-industrial combustion plants	7	4	3	12
Combustion in manufacturing industry	17	9	0	6
Production processes	3	2	6	5
Extraction and distribution of fossil fuels / geothermal energy	0	1	5	0
Solvent and other product use	0	0	23	0
Road transport	4	48	30	62
Other mobile sources and machinery	2	15	5	7
Waste treatment and disposal	0	1	1	5
Agriculture	0	0	18	1
Other	16	0	8	0
Totals	100	100	100	100

Table 4.3. Emissions from the target sector Transport (SNAP sectors 07 + 08) in 1990 (Gg)

	SO_2	NO_x	NMVOC	CO
Road Transport	718	7,846	6,766	38,919
Off road vehicles and machines	153	1,147	418	1,690
Railways	40	199	33	84
Shipping	351	785	155	275
Air traffic (LTO + taxing)	20	179	71	174
Total transport	**1,283**	**10,156**	**7,442**	**41,143**
Share in European total (%)	4.6	56.7	34.2	59.0

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[1] As available in April 1997

Table 4.4. Emission by road transport in Europe 1990 (Gg).

	SO_2	NO_x	NMVOC	CO
Western Europe	521	6,833	5,648	33,100
Eastern Europe	198	1,013	1,118	5,820
European road traffic	**718**	**7,846**	**6,766**	**38,919**
Share in European total (%)	2.6	43.8	31.1	55.8

4.2.1. Sulphur dioxide

As is shown in table 4.5 an assessment of ambient SO_2 concentrations should primarily take into account the emissions from stationary combustion in larger installations. About 85% of the emissions of SO_2 in Europe originate from these sources. Since these emissions are largely emitted from high stacks, the ground level concentrations are influenced by sources at larger distances. This might average out major short time fluctuations, so it is expected that annual total emissions are sufficient for the assessment of SO_2 air quality. In considering short term exceedance statistics, particularly around sources with lower emission heights, this will be no longer valid, and time variations in emission strength should be considered explicitly. Note, however, that the variability of meteorological conditions will at least be as important for ambient concentrations as the variability in emission. Such variability might be assessed by using models that estimate higher percentiles in the long term frequency distribution of hourly average concentrations, using average emissions as an input.

Table 4.5. Top SNAP level 3 activities, causing 90% of cumulative SO_2 emissions in 1990 (%).

	SNAP activity	cumulative percentage
1	public power and cogeneration - combustion plants ≥300 mw	49.1%
2	commercial, instit. and resid. - combustion plants < 50 mw	59.4%
3	industrial combustion - plants < 50 mw	67.7%
4	industrial combustion - plants ≥ 300 mw	74.1%
5	industrial combustion - plants ≥ 50 mw and < 300 mw	78.5%
6	nature - volcanoes	80.6%
7	public power and cogener. - combus Plants ≥ 50 and < 300 mw	81.9%
8	industrial combustion - refinery processes furnaces	83.3%
9	industrial combustion - sinter plant	84.6%
10	district heating - combustion plants ≥ 50 mw and < 300 mw	85.8%
11	district heating - combustion plants < 50 mw	86.7%
12	other mob. sources - marine activities: national sea traffic	87.6%
13	industrial combustion - cement	88.4%
14	production proc. - sulphuric acid	89.1%
15	road trans. - heavy duty vehic. and buses : rural driving	89.7%
16	commercial, instit. and resid. - combustion plants ≥ 50 mw	90.3%

4.2.2. Nitrogen dioxide

Table 4.6 presents the major contributors to NO_x emissions in Europe at the SNAP level 3 (activities). At this level, large power plants are the largest source activity for this pollutant. However, road transport and other mobile source activities come into play as the second through seventh and 9th highest activities emitting almost 40% of all NO_x. At SNAP level 1, road transport contributed more than 50 % in the EU-12 countries in 1990, and locally in cities this may be even higher. Since these sources are low level sources, emitting in many cases directly into the living areas of densely populated regions, assessment of air quality with respect to nitrogen oxides should in most cases concentrate on mobile sources and especially on road traffic.

An inventory for NO_2 should hence concentrate on urban scale and on road traffic. Detailed emission estimates, both in high temporal and spatial resolutions, can be obtained from traffic density data and emission factors as published in EMEP/CORINAIR Guidebook chapters on traffic emissions, and other literature. The methodology is available in the Copert II software system (Ahlvik et al, 1997), which in fact can be used at higher resolutions. A typical value for the percentage of NO_x directly emitted as NO_2 would be 5 %.

Software tools like the CAR model (Eerens et al, 1993), Mobile5 (USEPA, 1993), OSPM (Berkowicz et al, 1997) and CTB can be used to estimate emissions and concentrations from traffic densities, based upon either default emission factors or, when available, more specific emission factors for the region under study. These and other air pollution models for the calculation of concentrations are described in a COST 615 inventory.(Schatzmann et al., 1996)

Table 4.6 SNAP level 3 activities causing 90% of cumulative NO_x emissions in 1990 (%).

		cumulative percentage
1	public power and cogeneration - combustion plants ≥ 300 mw	18.5%
2	road transport - passenger cars : rural driving	28.0%
3	road trans. - heavy duty vehicles and buses : rural driving	35.6%
4	road transport - passenger cars : urban driving	42.3%
5	road transport - passenger cars : highway driving	47.9%
6	road trans. - heavy duty vehicles and buses : highway driving	53.5%
7	other mob. sources - off road vehic. and machines: agriculture	57.6%
8	commercial, instit. and resid. - combustion plants < 50 mw	61.6%
9	road trans. - heavy duty vehicles and buses : urban driving	65.3%
10	industrial combustion - plants < 50 mw	68.5%
11	other mob. sources - marine activities: national sea traffic	71.1%
12	industrial combustion - plants ≥ 300 mw	73.5%
13	industrial combustion - cement	75.8%
14	industrial combustion - plants ≥ 50 mw and < 300 mw	77.4%
15	other mob. sources - off road vehicles and machines: industry	78.8%
16	road transport - light duty vehicles < 3.5 t : urban driving	80.2%
17	road transport - light duty vehicles < 3.5 t : rural driving	81.3%
18	other mob. sources - railways	82.4%
19	other mob. sources - airports (lto cycles and ground act.)	83.4%
20	industrial combustion - sinter plant	84.4%
21	road transport - heavy duty vehicles > 3.5 t and buses	85.3%
22	public power and cogener. - combus. plants ≥ 50 and < 300 mw	86.2%
23	road transport - passenger cars	87.1%
24	w.t.d. - open burning of agricultural wastes (except 10.03)	88.0%
25	other mobile sources - marine activities: national fishing	88.8%
26	production processes - nitric acid	89.4%
27	other mobile sources - off road vehicles and machines	89.9%
28	road transport - light duty vehicles < 3.5 t : highway driving	90.5%

4.2.3. Lead

Emission data on lead are incomplete at the European and the EU level within CORINAIR. It is expected however that road traffic will also in the case of lead be a major contributor to emissions. These emissions depend on the legislation on lead content in gasolines and the availability and use of unleaded gasolines. Most exceedances of the air quality limits, however, are expected around metal industries, because of emissions from stock piles and from stacks. Member States may have specific emission inventories for these sources.

Contrary to the case of NO_2, the environmental effects of lead are long term exposure effects. Hence long term average air pollutant concentrations are relevant to the assessment of air quality with respect to Pb. This means that also long term average emissions are sufficient and hence less detailed traffic density information is needed as compared to the case of NO_2.

Table 4.7. gives some values for emission factors and the assumptions underlying them. These factors should be modified if the assumptions do not hold for the region under study. At small scales and for low speeds, the COPERT methodology can be applied. As many countries decrease the amount of lead in gasolines, the problem will be decreased too.

Table 4.7. Examples of Pb emission factors for road traffic For different assumptions the emission factors should be adapted accordingly; for instance, fuel lead content is different in the Member States.

Assumptions		
Lead content of gasoline	140	mg/litre
Percentage of leaded gasoline sales (national average)	25	%
Percentage of vehicle km's using gasoline as a fuel	65	%
Percentage emitted to the atmosphere	75	%
Average speed	Emission factor	Unit
13 km/h	0.00190	gram/km/vehicle
19 km/h	0.00155	gram/km/vehicle
44 km/h	0.00114	gram/km/vehicle
100 km/h	0.00122	gram/km/vehicle

4.2.4. Particulates

Even less information is available for the emissions of particulate matter on a Community-wide scale.(PM10). In a recent study (Berdowski et al., 1996) particulate emissions in Europe have been estimated. The most important sources are stationary combustion of solid fuels, road transport and production processes. Table 4.8 presents the European (EU15) totals for 1990 as derived from this study. Major uncertainties may still exist in these estimates.

A number of Member States have developed more recent estimates.

Table 4.8. PM_{10} emissions (EU15, 1990) per source category as estimated by TNO.

SNAP sectors	Source sector	emission (kton/year)
1, 2, 3	Total stationary combustion	1,350
7, 8	Total transport	670
10	Agriculture	310
9	Waste processing plants	100
4, 5	Total process emissions	460
	Total	2,900

4.3. Uncertainty assessment

In the joint EMEP/CORINAIR Atmospheric Emission Inventory Guidebook and particularly in the chapter on "Verification concepts" suggestions are provided in detail for procedures and techniques that can be used to assess the validity of the emission data included in inventories. The text box in chapter 2 (from the EMEP/CORINAIR Guidebook) defines relevant concepts in this respect.

The available data is not always sufficient to develop quantitative statistical measures of the data accuracy; in these cases subjective rating schemes and evaluations are used to describe the relative confidence associated with specific estimates.

Uncertainty analysis: uncertainty estimates for emissions data are important for assessing both the inherent uncertainty of the emissions estimates for individual facilities and the range of emissions magnitude represented by all sources in a study area; to proceed in these analyses, information on the distribution of parameter values, or at least on their range, is needed. The aim is to evaluate the variability, and hence the uncertainty, related to the emission estimation. The chapter “Verification concepts” of the EMEP/CORINAIR Guidebook provides a methodology for representing the overall quality of the databases. A data quality rating procedure is recommended. Each emission factor is assigned a data quality rating according to the following definitions. This table includes a rough indication of the error range associated with each quality rating.

The EMEP/CORINAIR Guidebook presents a default table for quality ratings for each relevant pollutant at the level of the 11 main SNAP sectors in CORINAIR.

rating	definition	typical error ranges
A	an estimate based on a large number of measurements made at a large number of facilities that fully represent the sector;	± 10 to 30 %
B	an estimate based on a large number of measurements made at a large number of facilities that represent a large part of the sector;	± 20 to 60 %
C	an estimate based on a number of measurements made at a small number of representative facilities, or an engineering judgement based on a number of relevant facts;	± 50 to 150 %
D	an estimate based on a single measurements, or an engineering calculation derived from a number of relevant facts and some assumptions;	± 100 to 300 %
E	an estimate based on an engineering calculation derived from assumptions only.	± order of magnitude

The quality of a regional emission inventory compiled according to this guidance also depends on the quality of the additional data used in the procedure. Error propagation theory might be applied to estimate the uncertainties of the resulting inventory, using the error estimates of the table above. It is expected that the use of the proxy variables in the top down approach will not add dramatically to the uncertainties, provided that a proper choice is made as to which proxy variable is used for each activity.

In UK emission inventories estimated uncertainties are: (Ken Stevenson, AEA Technology, private communication)

SO2	± 10%
NOx	± 30%
NMVOC	± 50%
CO	± 40%
PM10	± 50%

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5. Modelling

5.1. Introduction

Air pollution modelling may be seen as a method for providing information on air quality on the basis of what we know of the emissions, and of the atmospheric processes that lead to pollutant dispersion, transport, chemical conversion and removal from the atmosphere by deposition.

Models have become a primary tool for analysis in most air quality assessments mainly for the following reasons:

- A picture of the air quality in a zone may be obtained - in contrast to the limitations in the spatial coverage of air quality measurements.
- The relation between air concentrations and the emissions causing these can be made explicitly and quantitatively by modelling, which is most important for supporting air quality management.
- Models are the only available tool if the impact on air quality of possible future sources or of alternative future emission scenarios is to be investigated.

Air pollution models can be used in a complementary manner to air quality measurements, with due regard for the strengths and weaknesses of both analysis techniques. Modelled information is necessarily uncertain due to deficiencies in our knowledge of emissions and atmospheric processes; this disadvantage may be largely offset by validation of models with the help of measurements, or by assessing air quality by combination of information from modelling and measurements. In fact, if a concentration map is to be made on the basis of measurements, model results provide essential information for interpolation. The use of interpolation in assessments of air quality measurements alone is to be recommended only if emission information cannot be made available or if acceptable models cannot be found, and if monitoring data with sufficient spatial and temporal coverage are available.

5.2. Selection and application of models

For air quality assessment by modelling, a wide variety of models have been developed, some of which have been made readily accessible and easy to use by combination with user-friendly software. Others can only be operated by specialists, or even exclusively by the developers. Information on the state of the art of modelling and on models and model applications is available in various EEA publications prepared by the European Topic Centre on Air Quality (Moussiopoulos *et al.*, 1996; de Leeuw *et al.*, 1996, Tønnesen et al., 1997) and others (Olesen and Mikkelsen, 1992; Kretzschmar *et al.*,1994, 1996; NATO-CCMS, 1992, 1994, 1996; COST 615, 1996)

The European Topic Centre on Air Quality has prepared a pilot model documentation centre accessible via the Internet (ETC-AQ home page: http://*www.etcaq.rivm.nl*; model documentation centre: http://aix.meng.auth.gr/lhtee/database.html). Here, descriptions of the models, their application areas and their status with respect to evaluation and validation are to be provided.

Models and model applications can be distinguished on the basis of many criteria, such as the underlying physical concepts, the temporal and spatial scale, type of source, type of component and type of application. For assessments under the EC Air Quality Directives almost the whole range of the above criteria is involved.

In particular for assessing air quality in an urban environment, where often the highest concentrations are found, one should be aware of the following aspects:

- Spatial scale. The local-to-regional scale models (see Moussiopoulos *et al.,* 1996) are broadly speaking related to the mesoscale. It has been recognized that, particularly in southern Europe, urban scale problems (local circulation systems, as sea and land breezes) can only be treated successfully by the aid of mesoscale air pollution models in a sufficiently large model domain.
- Temporal scale. Both short term models (maximum hourly concentrations) and long-term models (yearly mean concentrations) are needed. Meteorological statistics are needed for calculation of percentiles and/or exceedance frequencies.
- Underlying physical concept. There is a variety of models that can be considered. For example, in case of uniform terrain, representative meteorological data and appropriate emission data, the Gaussian models provide reliable results for long term average values of relative inert pollutants such as SO_2, NO_X and lead. In complex meteorological and topographical conditions however, the transport processes may be conveniently simulated by the aid of models which solve numerically the atmospheric diffusion equation (Eulerian approach) or describe fluid elements that follow the instantaneous flow (Lagrangian approach). Both approaches are usually embedded in prognostic meteorological models.
- Type of application. This report is mainly concerned with regulatory applications. The relevant models are able to provide spatial distribution of high episodic concentrations and of long-term averaged concentrations for comparison with air quality limit values or thresholds.
- Type of source. Usually, in a city, all the source categories are involved (e.g. line, point and area sources). For studying the urban air quality, most of the small sources are combined into larger area sources, while the largest point sources are often considered individually in the calculation.
- Type of component. In case of reactive pollutants, chemical modules should be included in the model. The complexity of these modules varies from those including a simple reaction (e.g. transformation of SO_2 into sulphates) to those describing photochemical reactions as in the cases of ozone and NO_X.

Although atmospheric models are a basic tool in air quality assessment studies their limitations should always be taken into account. Thus, before attempting to select or apply a model one should have in mind that uncertainties in model results may be large, introduced either by the model concept and/or by the input parameters. In particular:

- There is no one model capable of properly addressing all conceivable situations even for a broad category such as point sources.

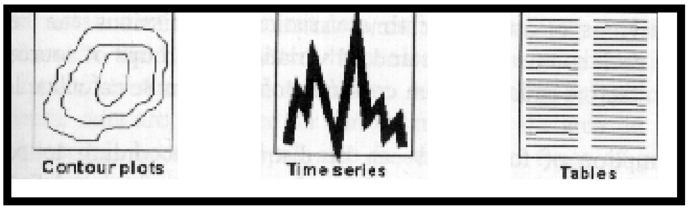
- Meteorological as well as topographical complexities of the area, which are usually associated with potential exceedance of air quality standards, are rarely responsive to a single mathematical treatment; case-by-case analysis and judgement are frequently required.
- Consistency in the selection and application of models, input data and air quality data is very important. It is useless to calculate an air quality field with a spatial resolution that is much higher than that of the emission field.
- It is necessary to get balance in the detail and accuracy of the data involved: emissions inventory, meteorological data, and air quality data. Availability of appropriate data should be investigated before applying any model. A model that requires detailed, precise input data should not be used when such data are not available.
- The representativeness of model results may be limited; in most models a spatial and temporal averaging is introduced which may complicate a direct comparison with measurements at a given location and time.
- The involvement of specialists is necessary whenever the more sophisticated models are used or the area of interest has complicated meteorological or topographic features.

Particularly for first screening purposes, or in case of limited input information, the use of simple models may be appropriate. A description of such simple air pollution models for calculating the concentrations from different sources in an urban environment is provided in Annex 2. If initial screening leads to the conclusion that levels may be of the order of the limit values, more sophisticated models should be selected.

In short, the procedure for modelling involves the following steps:

1. Define the pollutant, and the output quantity to be modelled (concentration fields, or (spatial maximum) concentrations in streets or near point sources, usually for concentration statistics, for instance annual average, 98 percentile of hourly values ...)
2. Define the time resolution needed (the averaging time for the concentration)
3. Define the "model output area" for which the model calculations should be made (usually a zone or agglomeration) and the spatial resolution needed.
4. Define the accuracy in the output quantity that is required
5. Determine the model area (this may extend considerably beyond the output area, particularly in case of pollutants with long range transport!)
6. Investigate the availability of emission data (in the model area)
7. Investigate the availability meteorological and topographical data (in the model area)
8. Investigate available air quality data (in the model output area)
9. Check available computer resources
10. Select models that are suitable for the pollutant (taking into account its chemistry and deposition), for the relevant output quantity, with the appropriate resolution in space and time, within the required accuracy, and for the area under consideration (taking into account its topography and meteorological characteristics)

11. Consider the computer requirements of the model(s); if these surpass available computer resources, reconsider model choice.
12. Reconsider the requirements on emission and meteorological data of the model(s) selected and, if necessary, collect more detailed input data (or reconsider the model choice)
13. Prepare input data
14. Run the model
15. Compare results to available air quality data and critically evaluate. If necessary, rerun model (This will involve specialists guidance). Annex 3 lists model evaluation parameters (Grønskei *et al.*, 1997) that are recommended for comparing model results and air quality data.
16. Map output; here various forms of output can be made, for example:

    Contour plots appropriate for presenting the concentration fields and the spatial maxima

    Time series appropriate for calculating the exceedances, annual average, 99.7 percentiles.

    Tables appropriate for presenting the concentration statistics.
17. Assess uncertainty.

5.3. Application to four pollutants

In the following tables, some aspects are considered of model studies for the four pollutants for which a Daughter Directive is currently under discussion. The models listed do not form a complete list of suitable models, and are not indicative for any preference, but merely serve as examples. These models generally calculate the contribution of particular sources to the concentration; a background concentration, either obtained from wider scale modelling, or from measurements, is then added.

	Quantities to be calculated	Source characteristics	Examples of models used
Sulphur dioxide	**24 h average concentration** exceedances < 3 times a year (approximately a 99 percentile) **1h average concentration** exceedances < 24 times a year (approximately a 99.7 percentile) **annual average concentration** example: (Borrego et al. 1996)	mainly from elevated point sources for power or heat generation Long-range transport (over distances of 1000 km and more) is very important Locally, small point sources, residential heating and traffic may be contributing to exceedances. These local sources may be taken into account as area or line sources.	**Microscale (urban roadways)** ADMS-Urban (Carruthers et al., 1995), UDM-FMI (Kukkonen et al., 1996),CAR (Eerens et al., 1993) CAR-FMI (Harkonen et al., 1995), MISCAM (Eichhorn et al., 1996),OSPM (Berkowicz et al,1997) ABC (Röckle, 1990), CPBM (Yamartino and Wiegand, 1986), MUKLIMO (Sievers, 1986) **sub-mesoscale (area sources)** UDM-FMI (Kukkonen et al., 1996),TREND (van Jaarsveld, 1995), PAL (Petersen and Rumsey, 1987) **Elevated point sources** STACKS (Erbrink, 1995), IFDM (Cosemans et al., 1992), UDM-FMI (Kukkonen et al., 1996), HPDM (Hanna and Chang, 1993), TREND (van Jaarsveld, 1995), OML (Olesen et al., 1992), ADMS (Carruthers et al., 1995), ISC (EPA, 1987), CTDMPLUS (Perry et al., 1989), POLARIS (Borrego et al., 1996)
Particulate matter	**24 h average PM10 conc.** **annual average PM10 conc.**	point stationary combustion sources area sources for residential heating area or line sources for road traffic for secondary fraction of PM10, sources of SO_2, NOx and NH_3 in a large area to be taken into account.	Models should be capable to calculate secondary sulphate, nitrate and ammonium aerosol, next to calculating dispersion and transport of PM10. As removal by deposition is strongly dependent on particle size, the size distribution of the particles should be taken into account in non-local applications.

Nitrogen dioxide and nitrogen oxides	1h average concentration exceedances < 8 hours a year (equivalent to 99.9 percentile) example: (Valkonen et al., 1996) annual average NO_2 conc. annual average NO_x ($NO+NO_2$)	area or line sources for road traffic elevated sources for power generation Exceedances may be primarily expected in streets or in districts with heavy traffic, or close to industrial sources of NO_x.	Microscale (urban roadways) The models may be the same with the ones for SO_2 with the addition of a simple atmospheric chemistry scheme for NO_2 transformation sub-mesoscale (area sources) UDM-FMI (Kukkonen et al., 1996), ADMS-Urban (Carruthers et al., 1995), OZIPM4/EKMA (Jeffries and Sexton, 1987) Elevated point sources In mesoscale, the models may be the same with the ones for SO_2, with the addition of a simple atmospheric chemistry scheme for NO_2 transformation and deposition: UDM-FMI (Kukkonen et al., 1996), or more comprehensive photochemical models: UAM (Chico and Lester, 1992),, CALGRID (Yamertino et al, 1992), CIT (Russel et al., 1988, EZM (Moussiopoulos, 1995)
Lead	annual average conc. of Pb	road traffic, (diminishing source due to penetration of lead-free gasoline). Possible exceedances to be expected in streets with busy traffic in countries where leaded gasoline is still in use. point sources of metal industries where exceedances are expected due to major emissions both from chimneys and from ore heaps.	Microscale (urban roadways) As for SO_2 sub-mesoscale (area sources) As for SO_2 Elevated point sources Stock piles

Key measurements - necessary data for different source types

line sources microscale - street canyons	area sources microscale small point sources	elevated point sources
source data location of road, road width, height and configuration of buildings along road, vehicle type, vehicle count, vehicle average speed, monthly/hourly variation emission	source data source dimensions, height, location and orientation, monthly/hourly variation emission	source data location, source height, diameter, efflux velocity, efflux temperature, pollutant emission rate, monthly/hourly variation emission
meteorological data (on hourly basis) date, time cloud cover, temperature, wind speed and direction at roof level	meteorological data (on hourly basis) date, time cloud cover, temperature, wind speed and direction	meteorological data (on hourly basis) date, time, cloud cover, temperature, net radiation, wind speed and direction. Atmospheric boundary layer parameters as mixing height and wind profile. For mesoscale/ long range transport where the surface wind climatology is not uniform, the field of many atmospheric parameters may be necessary
		receptor data terrain height at receptor location. For long range transport the terrain description is necessary
background concentrations	background concentrations	background concentrations

chemical data: If chemistry is involved data for spatial and temporal emission inventory are necessary. Also indicated background concentrations at the examined area.

5.4. Uncertainty of model results

Uncertainty assessment gives a measure of how a model can simulate real world conditions. Whereas in assessing model validity the emphasis is placed on the segments that comprise the model, in assessing model accuracy-uncertainty the emphasis shifts to the model accuracy as a complete unit.

There are at least four fundamental difficulties in comparing air quality observations to model predictions:

- On the scale of the model, the observations are points in space, whereas the predictions generally represent volume averages.
- The observations contain measurement errors or uncertainties
- The model may not represent properly the atmospheric processes involved
- Errors in the model input parameters (emission and meteorological data) may affect model results. Even if a model is an ideal formulation of the process, the predictions will be in error if the inputs are in error.

Annex 4 provides information on model uncertainty related to meteorology.

From the information presented in this Annex, an accuracy of ±10% may be envisaged for ensemble averages in the most ideal combinations of circumstances, or perhaps 10-20% for certain long-term averages in less ideal circumstances (excluding the special cases of stagnant or confined airflow), but in many circumstances of practical interest the uncertainties may at best be several tens per cent statistically for the whole zone and factors of two or more for individual points within the zone.

Concerning the accuracy of urban photochemical models, (having in mind that the measurement errors are on the order of at least 10%) we should generally expect:

- the models have difficulty predicting the maxima at the right time and place, although the predicted peaks are in the correct general areas and the offsets in time are random within 2h limits. Thus it is rather difficult to predict the peaks in the same location as a monitoring network.
- the outputs between different models vary only in the location of the peaks, rather than everywhere on the grid.
- underprediction of the estimated concentrations. An evaluation study showed that several photochemical models underpredicted the daily maximum (from anywhere in the region), with biases ranging from 10-30% and correlation coefficients above 0.8. For the case of daily maximum constrained to the monitoring sites, the estimated biases ranged from 31 to 42%.
- less variance in the predictions than the variance in the observations

Some methods for assessing the accuracy of a specific air quality model by comparing modelled results to measured concentrations are:

Bias evaluation	Ratio of the difference between the mean predicted concentration and the mean observed concentration to the mean observed concentration
Error analysis	The root mean square of the difference between predicted and observed concentrations
Time correlation	Correlation between observed and predicted concentration with time at a given station
Space correlation	Correlation between observed and predicted concentration distributions across a monitoring network at a given time
Peak analysis	Comparisons of magnitudes and locations of peak observed and predicted concentrations
Distribution functions	Observed and predicted cumulative distribution functions are compared to see if they are significantly different

Annex 2 provides formulae for some of these methods.

Time and space correlations are useful, but it should be realised that the correlation coefficients can mask many strange variations in the data. For this reason, a combination of evaluation methods is best, including a subjective judgement by an experienced modeller.

In general, most urban diffusion models yield correlations between hourly values of observed and predicted concentrations at a given station of about 0.6 to 0.8. According to Hanna *et. al* (1982) this result seems to be independent of the number of statements in the computer model. Good results appear to depend mainly on good knowledge of emissions and wind velocities.

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6. Recommendations for specifications of preliminary assessment

In this chapter, recommendations are provided for preliminary assessment as defined in the introduction to this report.

Two different types of recommendations are covered:

- assessment techniques to be used (measurements, emissions, modelling or combinations)
- requirements of accuracy and spatial resolution

6.1. Preliminary assessments

According to the FWD Article 5, Member States, who do not have representative measurements of the level of pollutants for all zones and agglomerations, shall undertake series of representative measurements, surveys or assessments, in order to have data available in time for implementation of the Daughter Directives.

The purpose of the preliminary assessment is to identify all areas of exceedance of the limit value, and of the upper and lower assessment thresholds where assessment in compliance with the Directives is necessary. Here, the upper and lower assessment thresholds, commonly referred to as x% and y% of the limit values, are the levels referred to in article 6.3 and 6.4 of the FWD which set out the framework for different assessment regimes, depending on the maximum pollution levels which occur in an agglomeration or other zone. For the four pollutants for which a Daughter Directive has been proposed in 1997, these levels have been calculated to provide a safety margin below the limit value to take into account interannual variability of the levels; in fact, (100-x)% is two times the standard deviation of interannual variation of the quantity or statistic under consideration.

Recommended assessment specifications are:

either: (for zones in agglomerations):

- indicative measurements on fixed positions with high resolution (see 3.4)

or: (for all zones, including agglomerations) combination of:

- emissions (minimum 50 x 50 km resolution , 5x 5 km in agglomerations, and including the largest sources (streets, point sources, or other) on an individual basis)
- modelling (background, contribution of largest sources)
- indicative measurements (see 3.3 - 3.6)

As indicated in Article 5, existing monitoring information can be used whenever appropriate.

It is strongly recommended to report the estimated total relative uncertainty of the estimated concentrations. If this uncertainty exceeds (100-x)%, while the pollution level is above y% of the limit value, it is recommended to repeat the assessment with more precise assessment tools (measurement techniques, emission inventory techniques, air pollution models). If this is not possible by available methods, this should be reported to the Commission, since in that case development of better methodology would appear to be necessary.

6.2. Criteria for judging existing assessments

Member States may have existing data on air quality for some or all zones and agglomerations. This document should provide criteria for Member States and the Commission to judge whether such existing information is sufficient for a preliminary assessment (FWD, Article 5), or whether additional work should be carried out.

In essence, the recommended assessment specification is equivalent to the case described in 6.1. It is recommended to map all areas of (potential) exceedance in the zone, with a documented total relative uncertainty of less than (100-x)% in these exceedance areas, where x% is the upper assessment threshold referred to in article 6.3 of the FWD.

7. Documenting the assessment; update procedure

The FWD requires only that Member States report the methods used to carry out preliminary assessments to the Commission. Member States will need however to retain clear documentation on methods and results for their use in implementing the FWD and daughter legislation, and they may wish to share and exchange this information with other Member States.

It is recommended that the results are documented taking into account minimum quality assurance criteria: the report is dated, the authors and the competent institutions and bodies (art. 3 of FWD) and their addresses are named, and the report is explicitly authorized by the competent authorities.

7.1. Mapping of results

Results are recommended to be primarily produced in the form of maps. Such maps may be produced for each of the quantities/statistics as referred to in limit values and threshold or target values for the pollutant(s) under consideration.

A useful map has a scale such that it clearly shows the limits of the zone, in relation to national and sub-national boundaries. A practical suggestion is to use a normal map as background .
In the zone, areas of exceedance resulting from the preliminary assessment are indicated, either by isolines for the limit value, and for x% and y% of the limit value, or by grid grey scales with a scale enabling to read x%, y% and 100% of the limit value. Here, x% and y% are the upper and lower assessment thresholds levels referred to in article 6.3 and 6.4 of the FWD,

If limit values are expected to be exceeded, it is recommended to indicate the extent of exceedance by the measured or calculated maximum concentration, and/or by isolines indicating suitable multiples of the limit value. Areas of exceedance should be presented on maps with sufficient resolution to see the location of maximum concentrations, in relation to relevant sources and proposed measuring sites. It is recommended to describe and discuss the results as mapped, including uncertainties (see below). Note that different assessment techniques may be used alone or in combination for different parts of the map.

7.2. Documenting of procedures followed

It is recommended to describe and document the work that has led to the map(s). More specifically, the documentation should:

- describe assessment activities carried out;
- report specific methods used, with references to descriptions of the method;
- report sources of data and information.

7.3. Documenting uncertainties

It is desirable to report the most likely total uncertainty in the concentration, either in absolute concentration units, or in relative terms. Uncertainties in, and resulting from emissions, measurements and model results may be presented and discussed separately, and the uncertainties in the mapped quantities (isolines, grid grey scales) may also be estimated. Methodology for this is to be further developed on the basis of expertise and experience in the Member States.

7.4. Updating procedure

It is recommended to update each assessment at the latest 5 years after the date of the initial assessment carried out under the requirements of the FWD, or earlier, if the air quality situation changes appreciably or, in case of revision of the limit or target values.

Appreciable changes to be considered are:

- changes in the zone of more than (30) % in human activities relevant to emission of the pollutant(s) (traffic volume, industrial production, population number, energy consumption, tourist visits, etc.) or changes smaller than this if they are likely to lead to an exceedance of a limit value or of an upper or lower assessment threshold.
- major changes in the distribution of emission sources (redesign of road or highway network, closing or establishing of major industrial plants, etc).

Annex 1. SNAP 97 subsector definitions (SNAP level 2)

SNAP	definition
0101	public power
0102	district heating plants
0103	petroleum refining plants
0104	solid fuel transformation plants
0105	coal mining, oil and gas extraction / distribution plants
0201	commercial and institutional plants
0202	residential plants
0203	plants in agriculture, forestry and aquaculture
0301	industry - comb. in boilers, gas turbines & station. engines
0302	industry - process furnaces without contact
0303	industry - processes with contact
0401	processes in petroleum industries
0402	processes in iron and steel industries and collieries
0403	processes in non ferrous metal industries
0404	processes in inorganic chemical industries
0405	processes in organic chemical industries (bulk production)
0406	processes in wood, paper pulp, food and drink industry & other industry
0408	production of halocarbons and SF6
0501	extraction and 1st treatment of solid fossil fuels
0502	extraction, 1st treat. and loading of liquid fossil fuels
0503	extraction, 1st treat. and loading of gaseous fossil fuels
0504	liquid fuel distribution (except gasoline distribution in 0505)
0505	gasoline distribution
0506	gas distribution networks
0601	paint application
0602	degreasing, dry cleaning and electronics
0603	chemicals products manufacturing or processing
0604	other use of solvents and related activities
0605	use of N2O, HFC, NH3, PFC or SF6
0701	passenger cars
0702	light duty vehicles < 3.5 t
0703	heavy duty vehicles > 3.5 t and buses
0704	mopeds and motorcycles < 50 cm^3
0705	motorcycles > 50 cm^3
0706	gasoline evaporation from vehicles
0707	automobile tyre and brake wear
0801	other mobile & machinery - military (if not included elsewhere)
0802	other mobile & machinery - railways
0803	other mobile & machinery - inland waterways
0804	other mobile & machinery - maritime activities
0805	other mobile & machinery - air traffic
0806	other mobile & machinery - agriculture
0807	other mobile & machinery - forestry
0808	other mobile & machinery - industry
0809	other mobile & machinery - household and gardening

0810	other mobile & machinery - other
0902	waste incineration
0907	open burning of agricultural wastes (except on field 100300)
0909	cremation
0910	other waste treatment
1001	cultures with fertilisers except animal manure
1002	cultures without fertilisers
1003	on field burning of stubble, straw, ...
1004	enteric fermentation
1005	manure management
1006	use of pesticides and limestone
1009	manure management regarding nitrogen compounds
1101	non managed broad-leafed forests
1102	non managed coniferous forests
1103	forest and other vegetation fires
1104	natural grassland and other vegetation
1105	wetlands (marshes-swamps)
1106	waters
1107	animals
1108	volcanoes
1109	gas seeps
1110	lightning
1111	managed broad-leafed forests
1112	managed coniferous forests
1121	changes in forest and other woody biomass stock
1122	forest and grassland conversion
1123	abandonment of managed lands
1124	CO2 emissions from/or removal into soils
1125	other

Annex 2. Urban dispersion models

This annex documents simple models for first estimation or screening.

An urban area contains thousands, or even millions, of individual sources. The application of a diffusion model to each source is impractical. Consequently most of the small sources are combined into larger area sources of strength $\mathbf{Q}_a$ (mass per unit time per unit area), and it is assumed that the emissions from the ground surface are uniform over that particular area.
Diffusion from the largest point sources can be calculated individually and the resulting concentrations at a receptor point can be added to the contribution from the area sources.

A. Area source model

In order to estimate by hand calculations the 1hr average air concentration at an arbitrary receptor point (**o**) due to area source emissions, a modified expression of the ATDL urban diffusion model (Hanna, 1972; Gifford and Hanna, 1973) may be used:

$$\mathbf{C} = \frac{(2/\pi)^{1/2}}{\mathbf{uc}(1-\mathbf{d})}\left\{(\Delta\mathbf{x}/2)^{1-\mathbf{d}}\mathbf{Q}_{\mathbf{ao}} + \sum_{\mathbf{i=1}}^{\mathbf{n}}\mathbf{Q}_{\mathbf{ai}}(\Delta\mathbf{x}/2)^{\mathbf{1-d}}\left[(2\mathbf{i}+1)^{1-\mathbf{d}} - (2\mathbf{i}-1)^{1-\mathbf{d}}\right]\right\} \qquad (A.1)$$

where

C, the concentration (micrograms m^{-3})

o, denotes the location of the receptor point

n, is the number of grid blocks (of size $\Delta\mathbf{x}$), necessary to reach the upwind edge of the urban area, starting from the receptor point.

$\mathbf{Q}_{\mathbf{ai}}$, for **i=o,1,2,...,n**, are source strengths (microgram sec^{-1} m^{-2}), constant over a distance $\Delta\mathbf{x}$.

u, is the wind speed, assumed constant within the mixing layer.

c,d are the Brookhaven National Laboratory parameter values, (Smith, 1968), as listed in Table 1.

Table A.1. Brookhaven National Laboratory parameter values a, b, c and d in equation (A.1) and in the formulas for the dispersion parameters , $\sigma_y = ax^b$ and $\sigma_z = cx^d$

atmospheric conditions	insolation	wind speed	a	b	c	d
very unstable	strong-moderate	< 2	0.40	0.91	0.40	0.91
unstable	strong-moderate	2-3	0.36	0.86	0.33	0.86
neutral	moderate-slight	3-4	0.32	0.80	0.22	0.80
estimated Pasquill D	moderate-slight or night	> 4	0.32	0.75	0.15	0.75
stable	night	2-4	0.31	0.71	0.06	0.71

Note that these values represent one choice; alternative datasets exist. Note also the dependence of the dispersion parameters on averaging time (see end of this annex).

Basic assumptions

- The pollutants are assumed to be uniformly mixed in a layer, whose height is proportional to the vertical dispersion parameter $\sigma_z(\mathbf{x})$, where $\mathbf{x}$ is the total distance from the urban area.

Simpler approach

When the distribution of emissions is quite smooth, as it is often the case in residential urban areas, the calculated concentration (C) at any receptor point is usually proportional to the emissions Q_{ao} in the grid square in which the receptor is located. In this case it is sufficient to use the following simpler relation:

$$\begin{aligned}\mathbf{C} &= \mathbf{A}\frac{\mathbf{Q_{ao}}}{\mathbf{u}} \\ &= (2/\pi)^{1/2}\frac{[\Delta\mathbf{x}(2\mathbf{N}+1)/2]^{1-\mathbf{d}}}{\mathbf{c}(1-\mathbf{d})}\frac{\mathbf{Q_{ao}}}{\mathbf{u}}\end{aligned} \qquad \text{(A.2)}$$

the expression $\Delta\mathbf{x}(2\mathbf{N}+1)/2$ denotes the distance to the edge of city.
The following values for the dimensionless factor A are suggested:

atmospheric conditions	**A**
neutral or average	200
stable	600
unstable	50

Note, however, that A is slightly dependent on $\Delta\mathbf{x}$.

Additional contribution from other sources

The urban area source model can give the average concentration over a broad area. In a street canyon or adjacent to a highway in an urban area, there is an additional contribution to the concentration from local sources. In this case the total concentration $\mathbf{C_t}$ is the sum of the spatial average **C** (calculated from equation (A.1)) and the local $\mathbf{C_l}$ component. Finally, the concentrations resulting at a receptor point from large point sources, $\mathbf{C_p}$, can also be added to the spatial average concentration **C**.

B. Elevated point sources

In order to estimate the contribution from an elevated point source $\mathbf{C_p}$, (Fig. 1) of strength Q, the following Gaussian relation can be used:

$$\mathbf{C} = \frac{\mathbf{Q}}{2\pi\sigma_y\sigma_z\mathbf{u}}\mathbf{e}^{-y^2/2\sigma_y^2}\left[\mathbf{e}^{-(\mathbf{z}-\mathbf{h})^2/2\sigma_z^2} + \mathbf{e}^{-(\mathbf{z}+\mathbf{h})^2/2\sigma_z^2}\right] \qquad \text{(A.3)}$$

where

C	is the concentration (micrograms m^{-3});
Q	is the source strength (micrograms sec^{-1});

u	is the wind speed at the plume height;
y	refers to the horizontal direction at right angles to the plume axis with y equal to zero on the axis;
z	is the height above the ground;
σ_y, σ_z	are standard deviations of the concentration distribution **C**, in the y and z direction and are calculated from table A.1;
h	is the effective plume height (stack height plus plume rise). The plume rise can be calculated by using the appropriate formulas, summarised in table A.2.

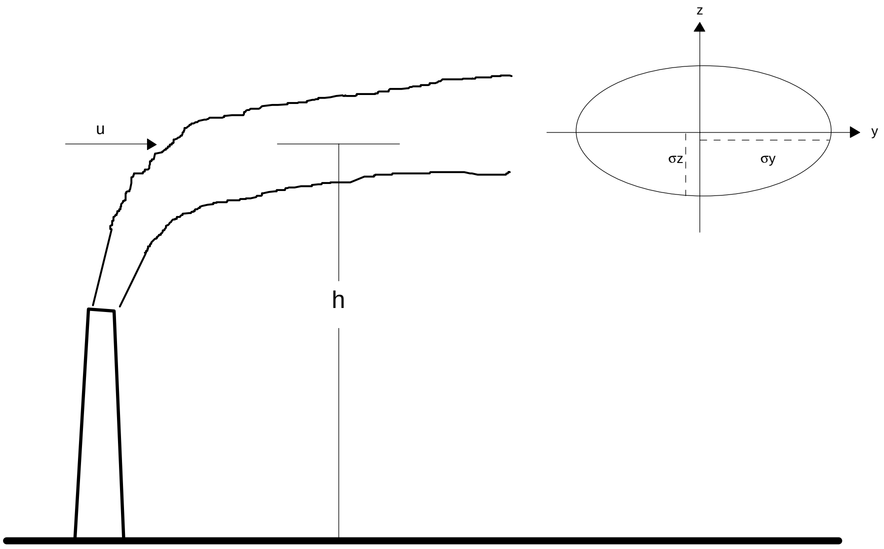

Figure B.1. Diagram of plume, illustrating concepts important in the Gaussian plume formula.

Table B.1. Plume rise formulas according to the plume characteristics and atmospheric conditions

plume type		atmospheric conditions	formulas
bent-over	buoyant	strong wind stable	$h = 2.6\left(\frac{F_o}{us}\right)^{1/3}$
		strong wind neutral, unstable	$h = 16F_o^{1/3}u^{-1}x^{2/3}$
	jet	strong wind neutral	$h = 3D\left(\frac{w_o}{u} - 1\right)$
vertical	jet	low wind stable	$h = 2.44\left(\frac{M}{s}\right)^{1/4}$
	buoyant	low wind stable	$h = 5.3F_o^{1/4}s^{-3/8}$

where

F_o	is the buoyancy flux , $F = \frac{g}{T_p}(T_p - T_e)V$;
M	is the momentum flux, **M=wV;**
s	is the atmospheric stability, $s = \frac{g}{T_e}\left(\frac{\delta T_e}{\delta z} + 0.01^\circ C/m\right)$;
V	is the plume volume flux ($V=wR^2$ for vertical plume and $V=uR^2$ for bent over plume);
w	is the plume vertical speed;
x	is distance from the stack;
D	is the stack diameter;
T	is the temperature.

Subscripts **p** and **e** denote plume and environment.

Note that alternative formulations for the plume rise exist.

Limitations

Although the Gaussian plume formula in general is appropriate to calculate the dispersion of elevated continuous major point sources, it has been demonstrated that it can lead to misleading results in special cases, such as in inhomogeneous terrain. For other simple models which could be used, see for instance Kretzschmar et al.,1994; Kretzschmar and Cosemans, 1996.

Longer averaging times

The diffusion parameters σ_y and σ_z are directly related to the standard deviations of the turbulent velocity fluctuations. Thus, as averaging time increases, the turbulent velocity fluctuations increase and hence σ_y and σ_z increase. Gifford suggests accounting for the effects of sampling time trough the empirical formula:

$$\frac{\sigma_{yd}}{\sigma_{ye}} = \left(\frac{T_{sd}}{T_{se}}\right)^{q} \qquad (A.4)$$

where,
d and e represent two different averaging times, and q is in the range 0.25 to 0.3 for $1hr<T_{sd}<100hr$ and equals approximately 0.2 for $3min<T_{sd}<1hr$.

The standard dispersion parameters given in table A.1, represent a sampling time T_{se} of about 10 min.

Extension to longer averaging times is made by solving the above equations for a variety of wind directions and then weighting each result by the frequency with which the wind blows from that direction.

C. Street canyon submodel

Consider the street canyon in figure A.2, where the important variables are defined. Depending on the wind direction, at roof level, the following relations can be used.

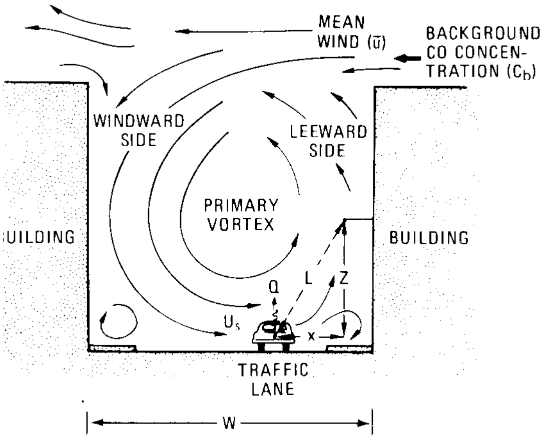

Figure C.1. Schematic of cross-street air circulation in a street canyon. (From Johnson et al, 1977)

Wind direction normal to the street axis
If the wind direction is nearly normal to the street, the equations for the concentration $\mathbf{C_l}$ in the street canyon are:

- **lee side,**

$$\mathbf{C_l} = \frac{\mathbf{KNq}/3.6}{(\mathbf{u}+0.5)\left[\left(\mathbf{x}^2+\mathbf{z}^2\right)^{1/2}+2\right]} \qquad (A.5)$$

- **windward side,** $C_l = \frac{KNq/3.6}{W(u+0.5)}$ (A.6)

where,

C_l	is the concentration (μg/m^3);
N	is the traffic flow (vehicles/hr);
q	is the emission factor (g/km);
u	is the wind speed at roof level (m/sec);
W	is the street width(m);
x and z	are horizontal distance and height (both in m) of the receptor point relative to the traffic lane;
K	is a dimensionless "best fit" constant ($K \approx 7$ is suggested).

Wind direction parallel to the street axis
If the wind direction is nearly parallel to the street axis, the equations for the concentration C_l in the street canyon are:

$$C_l = \frac{1}{2}\left[C_l(\text{winward}) + C_l(\text{lee})\right] \qquad \text{(A.7)}$$

Limitation: The model as such is not suitable for calculation of NO_2 concentrations, which are mainly determined by chemical reaction of NO with ozone.

D. Highway submodel

The excess concentration C_l contributed by a major highway in an urban area is important for a distance less than 300m downwind of the highway. Consider the highway in figure A.3, the concentration at some distance **x** from the highway can be estimated from the relation:

$$C_l = \frac{Q.F(\varphi)}{u[h + \sigma_z(x)]} \qquad \text{(A.8)}$$

where

C	is the concentration (μg/m^3);
Q	is the line source strength (μg/s/m);
h	is the effective height of emissions due to initial dispersion (2-3m);
φ	is the angle between the wind direction and the highway;
σ_z	is the vertical dispersion parameter.
$F(\varphi)$	Function of φ ; for φ around $\pi/2$, $F(\varphi)$ is close to 1.

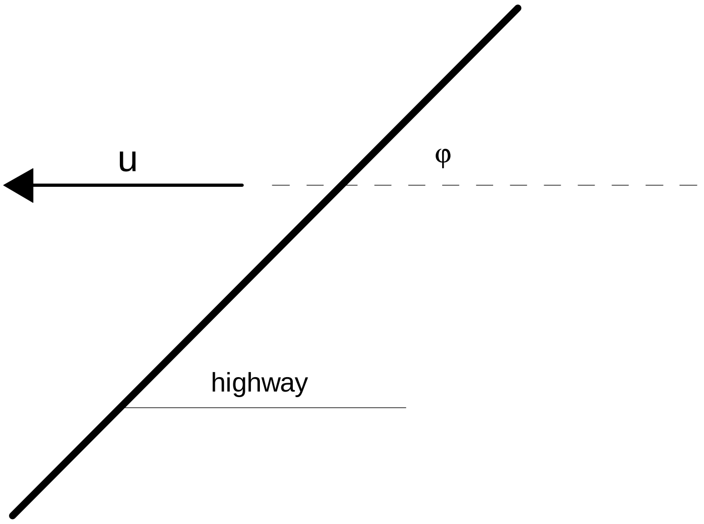

Figure D.1. Infinite line source pattern.

Limitation: This formula cannot be used to calculate concentrations on the highway, or in case the wind blows in the direction of the highway .

Meteorological data and emissions

All the models in this annex are best suitable for estimation of long term average concentrations. They should not be used for short term high percentile values, which are highly dependent on critical meteorological conditions.

For long term average concentrations, calculations can be made with average meteorological conditions. For wind speed, the annual average can be used. For wind direction, the most frequent direction can be taken. For point sources, neutral atmospheric conditions should be selected.

Appropriate choices must also be made for emission estimates, to make sure that they reflect typical conditions.

References

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Annex 3. Model evaluation parameters

Introduction

US EPA has given guidelines on procedures to be followed in evaluating air quality models (EPA, 1981, 1984), and a list of recommended model evaluation performance parameters. In this study statistical parameters have been selected in accordance with these recommendations (Fox, 1981, 1984). Selecting the parameters, results of Willmott (1982, 1985) were also taken into consideration.

Description of model evaluation performance parameters

Let T denote the number of data, and let O_t and P_t denote the observed and calculated (predicted) values at time t, t = 1,...,T. For each station the following model evaluation parameters are defined:

$\overline{O}$: Mean value of observations
$\overline{P}$: Mean value of predictions
σ_0 : Standard deviation of observations
σ_p : Standard deviation of predictions
NMD : Normalised mean difference
RMSE : Root mean square error
$RMSE_s$: Systematic RMSE
$RMSE_u$: Unsystematic RMSE
a, b : Intercept and slope of regression line
Corr : Correlation coefficient
IA : Index of agreement

The parameters are defined through the following set of equations:

Mean values:

$$\overline{\mathbf{O}} = \frac{1}{\mathbf{T}} \sum_{\mathbf{t}=1}^{\mathbf{T}} \mathbf{O}_\mathbf{t} \tag{B.1}$$

$$\overline{\mathbf{P}} = \frac{1}{\mathbf{T}} \sum_{\mathbf{t}=1}^{\mathbf{T}} \mathbf{P}_\mathbf{t} \tag{B.2}$$

These denote the usual arithmetical average values of the time series O_t and P_t.

Standard deviations:

$$\sigma_0 = \left(\frac{1}{\mathbf{T}-1} \sum_{\mathbf{t}=1}^{\mathbf{T}} \left(\mathbf{O_t} - \bar{\mathbf{O}} \right)^2 \right)^{0.5} \tag{B.3}$$

$$\sigma_{\mathbf{P}} = \left(\frac{1}{\mathbf{T}-1} \sum_{\mathbf{t}=1}^{\mathbf{T}} \left(\mathbf{P_t} - \bar{\mathbf{P}} \right)^2 \right)^{0.5} \tag{B.4}$$

These denote the usual standard deviations of the time series O_t and P_t.

Normalised mean difference:

$$\mathbf{NMD} = \left(\bar{\mathbf{O}} - \bar{\mathbf{P}} \right) / \bar{\mathbf{O}} \tag{B.5}$$

This dimensionless parameter is a measure of the bias of P versus O. Ideally it should be zero, or close to zero.

Root mean square error:

$$\mathbf{RMSE} = \left(\frac{1}{\mathbf{T}} \sum_{\mathbf{t}=1}^{\mathbf{T}} \left(\mathbf{O_t} - \mathbf{P_t} \right)^2 \right)^{0.5} \tag{B.6}$$

The RMSE is another measure of the size of the error produced by the model.

Systematic and unsystematic RMSE:

$$\mathbf{RMSE_s} = \left(\frac{1}{\mathbf{T}} \sum_{\mathbf{t}=1}^{\mathbf{T}} \left(\mathbf{O_t} - \hat{\mathbf{P}} \right)^2 \right)^{0.5} \tag{B.7}$$

$$\mathbf{RMSE_u} = \left(\frac{1}{\mathbf{T}} \sum_{\mathbf{t}=1}^{\mathbf{T}} (\hat{\mathbf{P}} - \mathbf{P_t})^2 \right)^{0.5} \tag{B.8}$$

where

$$\hat{\mathbf{P}}_{\mathbf{t}} = \mathbf{a} + \mathbf{b}\mathbf{O_t} \tag{B.9}$$

with a and b being the **intercep***t* and **slope of the regression line:**

$$\mathbf{a} = \bar{\mathbf{P}} - \mathbf{b}\bar{\mathbf{O}} \tag{B.10}$$

$$\mathbf{b} = \left[\sum_{\mathbf{t}=1}^{\mathbf{T}} \left(\mathbf{O_t} - \bar{\mathbf{O}} \right) \left(\mathbf{P_t} - \bar{\mathbf{P}} \right) \right] / \left[\sum_{\mathbf{t}=1}^{\mathbf{T}} \left(\mathbf{O_t} - \bar{\mathbf{O}} \right)^2 \right] \tag{B.11}$$

Here RMSE^2 = RMSE$_S^2$ + RMSE$_U^2$.

Willmott (1982) argues that systematic and unsystematic root mean square error gives valuable information on the possibility of model improvement.

For a good model the unsystematic portion of the RMSE is much larger that the systematic, while a large systematic RMSE indicates a poor model. For a more thorough discussion, see Willmott (1982).

Correlation coefficient:

$$\mathbf{Corr} = \frac{1}{\mathbf{T}} \sum_{\mathbf{t}=1}^{\mathbf{T}} \left(\mathbf{O}_{\mathbf{t}} - \overline{\mathbf{O}}\right) \left(\mathbf{P}_{\mathbf{t}} - \overline{\mathbf{P}}\right) / \left(\sigma_0 \cdot \sigma_{\mathbf{P}}\right) \tag{B.12}$$

This is the ordinary product-moment correlation coefficient.

Index of agreement:

$$\mathbf{IA} = 1 - \sum_{\mathbf{t}=1}^{\mathbf{T}} (\mathbf{P'}_{\mathbf{t}} - \mathbf{O'}_{\mathbf{t}})^2) / \sum_{\mathbf{t}=1}^{\mathbf{T}} (|\mathbf{P'}_{\mathbf{t}}| + |\mathbf{O'}_{\mathbf{t}}|)^2 \tag{B.13}$$

where

$$\mathbf{P'}_{\mathbf{t}} = \mathbf{P}_{\mathbf{t}} - \overline{\mathbf{O}} \quad \mathbf{and} \quad \mathbf{O'}_{\mathbf{t}} = \mathbf{O}_{\mathbf{t}} - \overline{\mathbf{O}} \tag{B.14}$$

The index of agreement has been recommended by Willmott (1982), as a better parameter to describe the “agreement” between the two time series O_t and P_t.

The index IA is a number between 0 and 1, with 0 indicating worst agreement, and 1 indicating best agreement.

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Annex 4. Limitations and uncertainties in meteorological estimates using dispersion models

Limitations and uncertainties of model prediction, related to the meteorological data are mainly due to:

- The special nature of those meteorological conditions and circumstances which occasionally lead to the worst pollution episodes;

- The availability in required resolution of the essential meteorological information;

- The basic inaccuracy and unrepresentativeness of the calculations of dispersion, even in the circumstances for which the dispersive action of the atmosphere is best understood.

Pasquill (1977) having in mind all the difficulties for collecting all the necessary meteorological information or the limitation of the dispersion relations only to idealised situations of air flow, constructed a very useful table with the best levels of accuracy which may be expected even in relatively simple circumstances. The values presented in this table (displayed on the next page) were based on comparison between measurements and simple dispersion formulas.

From this table an accuracy of ± 10% may be envisaged for ensemble averages in the most ideal combinations of circumstances, or perhaps 10-20% for certain long-term averages in less ideal circumstances (excluding the special cases of stagnant or confined airflow), but in many circumstances of practical interest the uncertainties may at best be several tens per cent statistically and factors of two or more individually.

Reference

Pasquill F. (1977), Atmospheric Diffusion. The dispersion of windborne material from industrial and other sources. 2nd edition John Wiley & sons

Uncertainty in pollution estimates (for a passive gas) derived from Pasquill (1977).

Nature of source and terrain	Conditions	Distance of travel (km)	Property estimated	Uncertainty
Ground level source on flat terrain	Overcast steady wind	0.1-1	Peak of time-mean (few minutes) crosswind distribution	a <0.1 b 0.1
	Generally unstable	<3		b 0.2
Moderately elevated plume (50-100m) over flat terrain	Generally unstable	1	Distance of maximum. Magnitude of maximum	b 0.3 b 0.35
Bouyant elevated plume over irregular terrain	Unstable or windy		Distance of maximum hourly average.	a 0.3 b 0.45
	Any except stagnation	10	Maximum hourly average.	a 0.35 b 0.5
			Long term average maximum	c 0.1
Plume in mixing layer	Unstable with inversion, definite wind field	100	Peak of time-mean (~1 hr) crosswind distribution	d 2.
Multiple sources in urban industrial complex	Any except stagnation	10	Long-term spatial mean	c 0.2
			Individual site, value averaged over few hours	b 1.0
			Extreme (1% of occasions) of few-hour average at individual site	d 2.0
As in 5, but source inventory not specified	Any except stagnation	10	Daily mean averaged over 100 sites at 1 site	b 0.25 b 0.35

The figures are fractional deviations, from the mean or actual values, of:
(a) ensemble average estimates in particular conditions (e.g. of wind speed or stability).
(b) individual values (r.m.s.) of cases forming the ensemble averages.
(c) long-term average estimates.
(d) extreme ratios 'estimate/actual'