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The application of models under the European Union's Air Quality Directive:

A technical reference guide

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Executive summary

This technical reference guide provides a general overview of the use of models with regard to the consolidated Directive 2008/50/EC on ambient air quality and cleaner air for Europe (the AQ Directive). This guide has three key aims:

- To provide common technical guidance for the use of air quality (AQ) modelling in relation to the EU's AQ Directive;
- To provide a central reference point for the development of a harmonised approach to modelling;
- To promote good practice in AQ modelling.

1.1 Why is this guide important?

Previous AQ directives based air quality assessment and reporting largely on monitored measurement data. However, the 2008 directive places more emphasis on the use of models combined with monitoring data for a range of applications, as specified below.

Europe has not routinely employed a unified approach to air quality modelling. This has resulted in a range of models being applied, at both national and local level, in various forms and with differing and often incomparable quality assurance methods. As the application of air quality models increases in Europe, so too does the demand for a harmonised approach to quality assurance for these models. Several kinds of models are required to address a variety of applications on different spatial and temporal scales. It is thus not envisioned that a single reference model will ever be in place within Europe. However, it is expected that **models be comparable, well documented, and validated for their required applications** in order to achieve reliable modelling results.

In order to facilitate this, the Forum for Air Quality Modelling in Europe (Fairmode, http://fairmode.ew.eea.europa.eu/) was established in 2008 as a joint action of the European Environment Agency (EEA) and the European Commission's Joint Research Centre (JRC). This technical reference guide is an output of that joint action.

1.2 Important considerations highlighted by this guide

This technical reference guide provides a general overview of the use of models in regard to the AQ Directive, reflecting the current state of modelling within Europe. It is important that the following are considered when developing **protocols for model evaluation**:

- the structure of the evaluation protocol is common to all (spatial and temporal) scales, but the details in the protocol should be scale specific, target/pollutant specific and application specific;
- the model evaluation protocol is built upon a broad consensus among the various interested parties relevant to its correctness and suitability, it should be open and easily accessible;
- the datasets needed for model evaluation differ for the different scales;
- model evaluation focuses not only on final concentration levels, but also on the different modules (emission, meteorology) relevant for simulation of concentrations;
- a sensitivity analysis, an uncertainty analysis and (results of) model intercomparisons are embedded in the model evaluation process.

Models applied for **assessing the existing AQ situation** aim at indicating exceedances of AQ Directive and national limit or target values, calculating population exposure and health impacts, and identifying air pollutant source contributions. Model applications can address a combination of those three aims. Air quality models are rarely used without any reference to measurement data. Many modelling applications will use monitoring data for validation purposes, i.e. will compare modelled and measured results (often reverting to statistical methods). Modelling results are particularly useful in assessments to provide supplementary information for the geographical area (on a certain spatial scale) not covered by measurement data. Modelling can be further applied to calculate population exposure at concentration levels above, for example, limit values. It is also possible to fuse interpolated measurement data and AQ modelling data into a single integrated map or to incorporate monitoring data directly into AQ model calculations during the modelling process (data assimilation).

1.3 Modelling, mitigation and planning

This guide underlines the connection between the design of effective mitigation strategies and knowledge of **air pollutant sources**. Here too, AQ modelling plays a central role. In a city, for example, there are sources over which local authorities have some form of control (e.g. traffic), but there are also sources outside the city, outside the country or even the continent over which they have no control (transboundary or long-range transport of air pollution). Meteorological conditions and their changes over time, addressed in many AQ models, have a decisive influence on the levels of certain air pollutants (e.g. ozone). For most model applications, contributions from anthropogenic sources are recorded by addressing sectors (e.g. traffic, industry) or sub-sectors (e.g. heavy-duty or light-duty vehicles). AQ models can also be coupled to measured concentrations to infer emission strengths (inverse modelling).

Examples of **natural air pollutant sources**, as defined in the AQ Directive, are wind-blown and Sahara dust, wild-land fires, 'sea spay' events and volcanic eruptions. Air pollutant measurements, including chemical analysis in the case of particulate matter, in combination with modelling methods, such as back trajectory modelling, can be used for source apportionment and pollutant quantification.

Though not directly written into the AQ Directive, source apportionment studies will generally be required to assess the causes of exceedances of air quality thresholds, the contribution from natural sources and neighbouring countries, and the contribution from re-suspended road sand and salt.

Current air quality legislation and management is based on the principle that Member States divide their territories into a number of AQ zones and agglomerations (e.g. cities). Monitoring of air pollutant source contributions everywhere in those areas would not be possible. This means that modelling, usually in combination with monitoring, is the methodology most likely to be used for this application. Some source emissions, e.g. fugitive dust and road sand and salt, may be so poorly known that monitoring must provide the basis for source apportionment. Source apportionment is relevant for the AQ Directive in a number of ways, but the major aspect is related to planning.

Air quality planning, as required in the AQ Directive, is a clear extension of AQ assessment and source allocation of air pollutants. Addressing longer-term developments, planning involves the identification of possible measures to reduce emissions, the development of emission reduction scenarios using modelling, and the iteration of the process to determine optimal mitigation scenarios (including the feasibility of the emission scenarios). Plans with other EU Member States address transboundary air pollution. Regional-scale AQ models are required by countries to assess source-receptor relationships. In relation to short-term AQ action plans, many national, regional (e.g. at county level) and local authorities have established AQ model forecasting and warning systems.

The AQ Directive does not require impact assessments or plans to be carried out prior to any changes in emissions (i.e. *ex ante* model predictions). Air quality plans are only required in relation to cases where exceedances of limit and target values have occurred. However, modelling is an important tool when drafting air quality plans. Fairmode's main focus is urban-scale modelling. However, local-scale model applications often rely on 'nested' modelling approaches using European-, regional-, local/urban- and street-level model applications, where each lower-scale model uses results of the higher-scale model as boundary conditions. Fairmode's aim is also to further explore interfaces, complementarily and relationships **with urban-scale and European-scale integrated modelling approaches**.

As modelling methods and data sources improve, it is expected that models will be increasingly applied within the AQ communities. This, and future guidance documents from Fairmode are intended to support this development by providing recommendations and clarifications and contributing to a harmonised understanding.

1 Introduction

1.1 Background

In May 2008, the European Parliament and the Council adopted a new consolidated European Union (EU) Directive on ambient air quality and cleaner air for Europe — Directive 2008/50/EC (EC, 2008). This Air Quality (AQ) Directive replaced earlier directives simplifying and streamlining existing provisions, and introducing new provisions, in particular new objectives concerning $PM_{2.5}$ and the possibility of postponing the attainment year of some limit values. Whilst previous directives have based assessment and reporting largely on measurement data, the new AQ Directive encourages the use of AQ models in combination with monitoring in a range of applications.

The Directive relating to arsenic, cadmium, mercury, nickel and polycyclic aromatic hydrocarbons in ambient air (heavy metals and PAH), Directive 2004/107/EC (EC, 2005), is also addressed by this technical reference guide, as this directive is also in force. A review of the directives is planned by 2013. In the reference document presented here, we refer to these two pieces of legislation collectively as the 'EU Air Quality Directive' or simply the 'AQ Directive'. If necessary, specific distinctions between the two will be made.

Modelling may be used as a tool to supplement monitoring data for assessment purposes when reporting exceedances of AQ standards. Depending on the level of concentrations (in relation to upper and lower threshold values), modelling may be applied as either supplementary information or as the exclusive source of assessment. In this regard, the AQ Directive allows for a reduction in the number of monitoring stations in any zone or agglomeration ([1]) when appropriate modelling is also carried out. Air quality models alone cannot be used for checking the exceedances of the air quality limit values where the concentrations are higher than the upper assessment threshold. Further, modelling cannot be applied alone in zones and agglomerations where the long-term objectives for ozone have been exceeded.

Modelling is an important complementary tool on which to base action plans, both short and long term. Applications for postponement of attainment years require such plans, as does reporting when limit values of the AQ Directive are exceeded. Source apportionment of air pollutants, including the assessment of transboundary and natural contributions, is an important application of models if sufficient knowledge is to be acquired for the effective implementation of such plans.

Modelling is also used extensively in air quality forecasts, providing next-day and near real-time information to the public and for the implementation of short-term action plans. This is required in the AQ Directive when concentrations exceed, or are expected to exceed, alert and information thresholds.

1.2 Why use models?

Historically, air quality assessment has been based on monitoring data, as this is considered to be as close to reality as is possible, as well as being the parameter on which health and ecosystem impacts have been studied. Even though modelling is often seen as being more uncertain than monitoring, there are three major reasons for using models in combination with monitoring for air quality assessments.

- The spatial coverage of monitoring is usually limited. Modelling can potentially provide complete spatial coverage of air quality.
- Modelling can be applied prognostically, i.e. it can be used to predict the air quality as a result of changes in emissions or changing meteorological conditions.

([1]) For definition, please see Table 2.1.

- Modelling provides an improved understanding of the sources, causes and processes that determine air quality.

In regard to the AQ Directive, there are clear advantages in using models for reporting, for example:

- models can provide assessment within zones in areas where monitoring is not carried out, and generally support the fulfilment of siting requirements for monitoring;
- the number of monitoring sites can potentially be reduced, saving costs;
- models can be used to develop and detail measures taken to reduce poor air quality.

Modelling, however, does not provide all the answers, and there are a number of limitations attached to models, as shown below:

- models require extensive input data that are not always reliable or easily acquired, particularly in relation to emissions and meteorology;
- models remain uncertain in their predictions; extensive validation, inter alia by using monitoring data, is required before models can be applied with confidence;
- the ability of models to represent the real world is limited as regards spatial resolution and process descriptions, for instance. Models remain a representation of reality;
- effective and quality controlled modelling requires expert users and interaction with model developers under most situations.

It is the aim of Fairmode (see Box 1.1) to promote the advantages and to address the disadvantages listed above. In particular, activities in Fairmode aimed at improving and harmonising the quality assurance of models will provide transparency and increased understanding of their applicability.

1.3 Aims of this guide

Modelling, like monitoring, requires expert implementation and interpretation. Models must also be verified and validated before they can be confidently used for air quality assessment or management. This document aims at providing reference and guidance for the use of models in relation to the AQ Directive. It provides an interpretation of the AQ Directive from a modelling perspective, outlining how models can be applied. It also refers to background information and guidance on good practices for achieving reliable modelling results through example case studies, references and links to other relevant documents. This information is available via the Fairmode website (Fairmode, 2011b). We will refer to this information in the guide as follows:

Technical guidance will be developed in parallel with other activities of Fairmode, with the intention of providing recommendations on good practices in modelling, and the assessment of model uncertainty. The most up-to-date version of the respective documents can be found on the Fairmode website (Fairmode, 2011a), where it is also possible to register to participate in Fairmode activities.

The general technical reference guide on modelling presented here is a product of the joint JRC/EEA initiative. The European Commission has produced a number of other official guidance documents, accessible through the European Commission website on air quality (EC, 2011a). These address a range of other issues relevant to the AQ Directive, but may also complement this document when modelling is involved (see also Chapter 8).

The major aims of this document are:

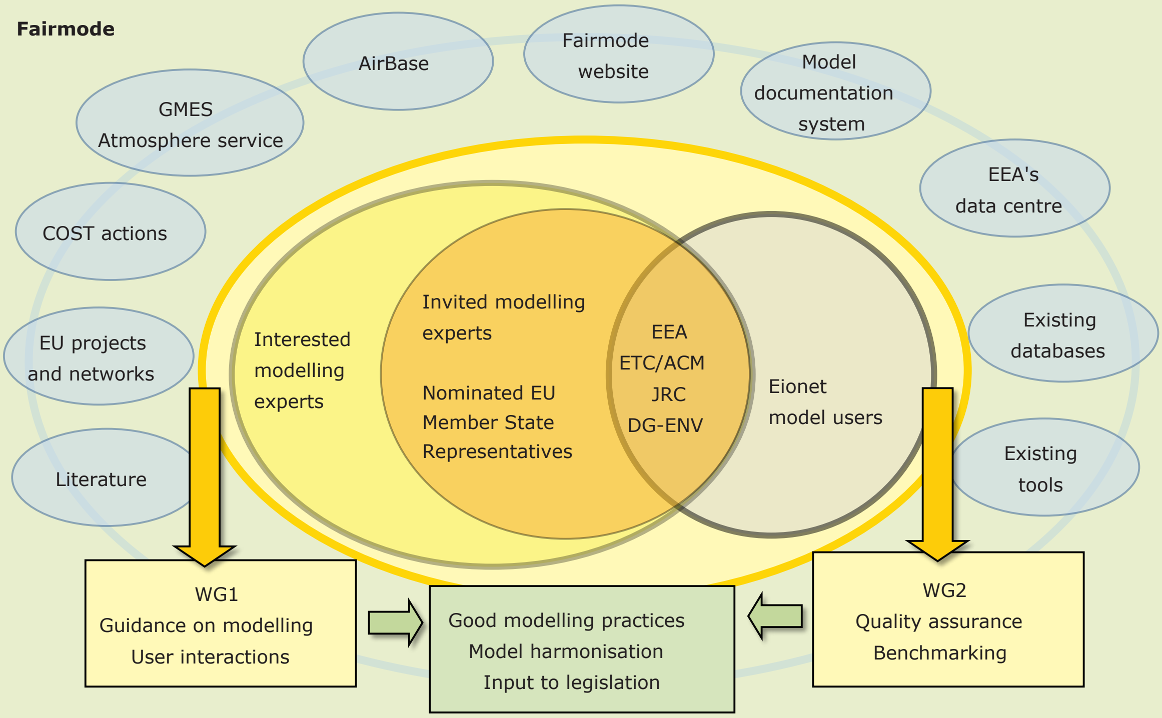
- to provide a technical reference guide for the user of air quality modelling in regard to the EU's AQ Directive (EC, 2008a) and the Directive on heavy metals and polycyclic aromatic hydrocarbons in ambient air (EC, 2005);
- to promote good practice in air quality modelling and assessment;
- to provide a central reference point and develop a harmonised understanding of model requirements in regard to the AQ Directive.

1.4 Scope and structure

This document deals with the application of air quality models. These models are mathematical tools used to quantify concentrations and deposition of air pollutants as a result of emissions into ambient air. These mathematical tools are chiefly based on physical and chemical processes but may also be derived based on statistical relationships.

The structure and form of this document is intended to facilitate model users and researchers in determining the requirements, possibilities and limitations when using models for applications in regard to the AQ Directive. The following chapters provide:

Box 1.1 Forum for Air Quality Modelling in Europe — Fairmode



Fairmode (http://fairmode.ew.eea.europa.eu/) has been set up in view of the possibility of increased modelling use in air quality assessment within the context of implementing EU air quality legislation. The main aim of Fairmode is to bring together AQ modellers and users in order to promote and support the harmonised use of modelling practices for the assessment of air quality by EU Member States as well as European Environment Information and Observation Network (Eionet) member and cooperating countries, particularly in the context of air quality legislation.

Fairmode is co-chaired by the JRC and the EEA. It is supported by a steering group currently comprising the EEA, the European Commission's JRC and Directorate-General for the Environment (Environment DG), representatives of Eionet, including the EEA's European Topic Centre on Air and Climate Change Mitigation (ETC/ACM), and some modelling experts invited by the JRC. Fairmode holds annual plenary meetings that are attended by country representatives and interested modelling experts. The Commission has asked the EU Member States to nominate national Fairmode experts.

Fairmode has two working groups (WGs): WG 1 is led by EEA, and WG 2 is led by the JRC. The chapter on model quality assurance and evaluation (Chapter 5) constitutes the main JRC input for the current report. The network aims to link to other existing European databases, networks and projects, such as AirBase, the Air Quality Reference Laboratories (Aquila), European Cooperation in Science and Technology (COST) actions and the Global Monitoring for Environment and Security (GMES) Atmosphere Core Service.

- a summary of the EU's AQ Directive;
- a technical understanding of the EU's AQ Directive in regard to the use of modelling;
- a summary on reporting requirements to the European Commission when modelling is used;
- a more detailed description of model quality assurance and evaluation methodologies;
- a description and sample applications for the use of modelling in reporting assessments;
- a description and sample applications for the use of modelling in regard to air quality planning;
- recommendations on a number of technical topics in regard to the AQ Directive when modelling is applied, including assessment of non-anthropogenic contributions to air quality and contributions to particulate matter (PM) from road sanding or salting;
- definitions of relevant concepts.

This report does not provide in-depth recommendations or practical solutions to all modelling requirements needed for assessment. However, a number of indicative examples have been compiled and are accessible through the Fairmode web portal (Fairmode, 2011a). Reference is also made to a number of articles and reports where more details may be found.

1.5 Audience

This document is intended for use by authorities, consultancies and research bodies involved in air quality assessment and mitigation planning that address the EU's AQ Directive in the EU Member States and the European Environment and Information Network (Eionet) air quality community. The main part of the document should provide the basic information for authorities to make decisions on the extent to which modelling can be employed in their assessment and management activities. The supporting website, annexes and references provide broad overviews as well as specific examples to help guide authorities and modellers in these activities.

2 Summary of the 2008 Air Quality Directive

This chapter summarises the AQ Directive in regard to thresholds, limit values, critical levels, reduction targets, target values, etc. The reader should refer to the AQ Directive for the definitive reference to the summary provided here. Most of this information is contained in Annex II, Annex VII, Annex XI, Annex XII, Annex XIII and Annex XIV of the AQ Directive.

2.1 Concepts and definitions

In this section, a number of terms and concepts necessary to understanding the AQ Directive are defined. Many of these are provided in the AQ Directive itself (Article 2); however, some terms are not defined and these are also explained here (from the model user's perspective). The list in Table 2.1 is intended to supplement those provided in the AQ Directive and are listed under topics. These descriptions are a guide to the reader, for an official interpretation of all terms the reader is referred to the AQ Directive itself.

2.2 Where does the AQ Directive apply?

The AQ Directive applies to all outdoor locations, excluding workplaces. It is applied within individual zones and these zones are defined by the Member States to cover their complete territory. The air quality requirements for health, such as limit and target values, apply everywhere within the zone, but are not to be assessed (Annex III.A.2 of the AQ Directive):

- at any locations situated within areas where members of the public do not have access and there is no fixed habitation;
- on factory premises or at industrial installations to which all relevant provisions concerning health and safety at work apply;
- on the carriageway of roads and on the central reservations of roads where there is normally no pedestrian access.

Note that these exceptions exclude exposure during road transport activities. This means, for example, that the AQ Directive does not cover the environment within a bus, but will cover the ambient environment when passengers step out of the bus. It also does not cover cyclists whilst on the road, but does cover cyclists on bicycle paths.

With regard to the protection of vegetation and ecosystems, the AQ Directive aims to protect areas distant from urban and industrial sources, leaving protection in these near-source regions to the Member States (Annex III.B.2 of the AQ Directive). Specifics concerning this, in regard to modelling, are discussed in Section 3.5 of this document.

2.3 Limits and target values for the protection of human health

The various health-related limits and levels for the legislated pollutants of Directive 2008/50/EC are provided in Table 2.2. This includes the limit values, target values, assessment threshold values, long-term objectives, and information and alert thresholds, as defined in Table 2.1. Some of these values are accompanied by specific conditions, so for definitive reference the reader is referred to the AQ Directive itself.

2.4 Limits and target values for the protection of vegetation

The various ecosystem-related target values and levels for the legislated pollutants of Directive 2008/50/EC, as stated in Table 2.1, are provided in Table 2.3. Some of these values are accompanied by specific conditions, so for definitive reference, the reader is referred to the AQ Directive itself.

Table 2.1 List of the terms and their definition contained in the AQ Directive

Concept	Meaning
	Pollutant levels and values
Limit value	A pollutant level not to be exceeded, in regard to human health. It is legally binding (Article 2.5).
Critical level	A pollutant level not to be exceeded, in regard to vegetation or ecosystem protection, for every year.
Margin of tolerance	Relates to the limit value and is given as a percentage. This provides, under specified conditions, a flexibility for compliance with the limit value (Article 22).
Target value	A pollutant level not to be exceeded. Generally applicable after a certain period (e.g. in 3 to 5 years) after a certain date. It is not legally binding (Article 2.9).
Alert threshold	A short-term pollutant level for which immediate steps must be taken.
Information threshold	A pollutant level for which immediate information to the public must be given.
Upper assessment threshold	A pollutant level, beneath the limit value, where a combination of modelling and monitoring (and/or indicative measurements) may be used for assessment.
Lower assessment threshold	A pollutant level, beneath the upper assessment threshold, where a modelling (or objective-estimation techniques) may be used for assessment.
Long-term objective	A pollutant level to be obtained in the long term.
	Exposure levels and values (related to $PM_{2.5}$)
Average exposure indicator (AEI)	This is the urban background pollutant level and has been introduced in relation to $PM_{2.5}$ (Annex XIV)
Exposure concentration obligation	A level applied to the AEI that should be obtained over a given (three-year) period.
National exposure reduction target	A percentage reduction in the AEI to be achieved over a given period.
	Measurement types
Fixed measurements	These are measurements with the most strict data quality objectives (Annex I), which are to be used when the pollutant is above the upper assessment threshold.
Indicative measurements	These are measurements with less strict data quality objectives than normal fixed measurements (Annex I). For some pollutants (particulate matter and lead), this has the same data quality objective as modelling.
Objective-estimation techniques	These are methods (not specified) with even less strict data quality objectives than the indicative measurements (Annex I). The relative uncertainty in these methods should be < 100 %.
	Other defined concepts
Zone	This is a part of the territory of a Member State which has been delimited by this country for the purpose of air quality assessment and management.
Agglomeration	This is normally an urban zone with more 250 000 inhabitants. For agglomerations established by a Member State with a population of 250 000 inhabitants or less, population density per km^2 has to be given.
Proportionate measures	These seem not to be defined explicitly but can possibly be interpreted to mean 'all necessary measures not entailing disproportionate costs'.
Contributions from natural sources	Contributions from emissions not caused directly by human activities: volcanic eruptions, seismic activities, geothermal activities, wild-land fires, high wind events, sea sprays, and the atmospheric re-suspension or transport of natural particles from dry regions.
	Undefined concepts
Combine	The AQ Directive often refers to a 'combination' of monitoring and modelling. This is not defined; see Section 3.3 of this document.
Supplementary	The AQ Directive often refers to 'supplementary' methods of assessment. This is no defined but it is understood to refer to all methods other than the use of fixed measurements. The best indicator of the term is given in Article 7.3a: 'the supplementary methods provide sufficient information for the assessment of air quality with regard to limit values or alert thresholds, as well as adequate information for the public.'

Table 2.2 Summary of air-quality directive limit values, target values, assessment thresholds, long-term objectives, information thresholds and alert threshold values for the protection of human health

Human health	Limit or target (#) value				Time extension (c)	Long-term objective		Information (b) and alert thresholds	
Pollutant	Averaging period	Value	Maximum number of allowed occurrences	Date applic-able	New date applicable	Value	Date	Period	Threshold value
SO_2	Hour	350 µg/m³	24	2005				3 hours	500 µg/m³
	Day	125 µg/m³	3	2005					
NO_2	Hour	200 µg/m³	18	2010	2015			3 hours	400 µg/m³
	Year	40 µg/m³	0	2010					
Benzene (C_6H_6)	Year	5 µg/m³	0	2010	2015				
CO	Maximum daily 8-hour mean	10 mg/m³	0	2005					
PM_{10}	Day	50 µg/m³	35	2005	2011				
	Year	40 µg/m³	0	2005 (a)	2011				
$PM_{2.5}$	Year	25 µg/m³ (#)	0	2010 (d)		8.5 to 18 µg/m³	2020		
		20 µg/m³ (ECO)		2015					
Pb	Year	0.5 µg/m³ (#)	0	2005					
As	Year	6 ng/m³ (#)	0	2013					
Cd	Year	5 ng/m³ (#)	0	2013					
Ni	Year	20 ng/m³ (#)	0	2013					
BaP	Year	1 ng/m³ (#)	0	2013					
O_3	Maximum daily 8-hour mean averaged over 3 years	120 µg/m³ (#)	25	2010		120 µg/m³	Not defined	1 hour	180 µg/m³ (b)
								3 hours	240 µg/m³

Note: The majority of EU Member States (MS) have not attained the PM_{10} limit values required by the Air Quality Directive by 2005 (EC, 2008a). In most urban environments, exceedance of the daily mean PM_{10} limit is the biggest PM compliance problem. 2010 is the attainment year for NO_2 and C_6H_6 limit values. A further important issue in European urban areas is also exceedance of the annual NO_2 limit value, particularly at urban traffic stations.

ECO: The exposure concentration obligation for $PM_{2.5}$, to be attained by 2015, is fixed on the basis of the average exposure indicator (see main text), with the aim of reducing harmful effects on human health. The range for the long-term objective (between 8.5 and 18) indicates that the value is depending on the initial concentrations in the various Member States.

(#) Signifies that this is a target value and not a legally binding limit value; see EC, 2008a for definition of legal terms (Article 2).
(a) Exceptions are Bulgaria and Romania, where the date applicable was 2007.
(b) Signifies that this is an information threshold and not an alert threshold; see EC, 2008a for definition of legal terms (Article 2).
(c) For countries that sought and qualified for time extension.

(d) The PM2.5 from target value (25 µg/m³) will become a limit value in 2015.

Source: EC, 1999a; EC, 2000; EC, 2002a; EC 2004; EC, 2008a.

Table 2.3 Summary of air quality directive critical levels, target values and long-term objectives for the protection of vegetation

Vegetation	Critical level or target value ([a])			Time extension	Long-term objective	
Pollutant	**Averaging period**	**Value**	**Date applicable**	**New date applicable**	**Value**	**Date**
SO_2	Calendar year and winter (October to March)	20 µg/m³				
NO_X	Calendar year	30 µg/m³				
O_3	May to July	AOT40 18 000 (µg/m³).hours averaged over 5 years	2010		AOT40 6 000 (µg/m³).hours	Not defined

Note: AOT40 is an accumulated ozone exposure, expressed in (µg/m³).hours. The metric is the sum of the amounts by which hourly mean ozone concentrations (in µg/m³) exceed 80 µg/m³ from 08.00 to 20.00 Central European Time each day, accumulated over a given period (usually three summer months). The target value given in the air quality legislation is 18 000 (µg/m³).hours and the long-term objective is 6 000 (µg/m³).hours.

([a]) See EC, 2008a for definition of legal terms (Article 2).

Source: EC, 1999a; EC, 2002a; EC, 2008a.

3 Understanding of the AQ Directive in regard to modelling

3.1 Model applications in the AQ Directive

Models may be applied to a range of applications relevant to the AQ Directive. Modelling is explicitly named in regard to the application of assessment. In this document, we will consider the wider range of applications, which typically involve the following types.

1. **Assessment of the existing air quality**
   (a) Models can be used to supplement or even replace monitoring data under specified conditions. These conditions are related to the various categories of pollutant levels and are described in Section 3.2 of this document.
   (b) Given adequate quality and resolution, a model can be used to reduce the number of measurements by up to 50 % (not including ozone, see Annex IX), unconditional on the pollutant levels (Articles 7.3, 10.3 and 14.2).
   (c) Given adequate quality and resolution of a model, it can be used to reduce the number of measurements of ozone by one third (Annex IX).

This topic will be described in more detail and illustrated with examples in Chapter 6.

2. **Management: mitigation and planning for future air quality**
   When preparing air quality plans and abatement measures, models will need to be used for a thorough analysis of the impact of these measures on the air quality. The use of models is not stated explicitly in the AQ Directive for this management activity. It is nevertheless not possible to perform this analysis properly without the appropriate models. Such analysis includes short-term air quality modelling of hours to days (air quality forecasting) as well as long-term planning of several decades (emission scenarios and abatement measures). This topic will be described in more detail, and illustrated with examples, in Chapter 7.

3. **Source apportionment**
   Though not directly written into the AQ Directive, source apportionment studies will generally be required to assess the causes of exceedances of air quality thresholds, the contribution from natural sources and neighbouring countries, and the contribution from re-suspended road sand and salt. Monitoring of these source contributions everywhere in a zone or agglomeration would not be possible. This means that modelling, usually in combination with monitoring, is the most likely methodology to be used for this application. Some source emissions, e.g. fugitive dust and road sand and salt, may be so poorly known that monitoring must provide the basis for source apportionment. Though source apportionment constitutes part of any air quality assessment, this topic is of particular importance and will be described separately in more detail, and illustrated with examples, in Chapter 8.

3.2 When can models be used for the assessment of existing air quality?

The AQ Directive defines a range of situations where models can be applied for assessment instead of, or in combination with, fixed measurements. According to the present air quality legislation, modelling results cannot replace measurements for compliance checking when limit values are exceeded. However, in principle, modelling can be used anywhere; unlike monitoring, there is no minimum requirement regarding the use of models, i.e. there is no requirement that modelling be used at all for the assessment of existing air quality. The AQ Directive defines the following situations where models can be applied.

1. Models can always be used to supplement fixed measurement data regardless of the pollutant levels. The advantage of this is that the number of monitoring stations may be reduced (Articles 7.3, 10.3 and 14.2).
2. Article 6 of the AQ Directive stipulates when, and in what way, modelling may be used for air

quality assessment, not including ozone, based on the level of pollutants. Modelling can be used:
(a) to supplement monitoring, when a zone is in exceedance of the upper assessment threshold;
(b) in combination with monitoring, when a zone is in exceedance of the lower assessment threshold;
(c) to replace monitoring, when a zone is below the lower assessment threshold.

3. Article 9.2 and Annex II.B go on to state that when monitoring data are available for fewer than five years, the period for which the threshold levels are to be assessed, then short-term measurement campaigns combined with modelling may be used to determine both upper and lower exceedance thresholds.

3.3 Combined use of measurements and models for assessment

In Articles 6 and 9 of the AQ Directive, the combined use of measurements and modelling is encouraged and allowed for in reporting when exceedances are below the upper assessment threshold. There are no specifics provided as to the level of combination or how the combination can be made. There are clearly a multitude of methods available for combining monitoring and modelling, ranging from advanced data assimilation methods to simple validation of models. A further discussion on combining monitoring and modelling is provided in Section 6.3 of this document. In addition, future activities in Fairmode will address the question of good practices for combining models and monitoring (link to the Aquila network; Aquila, 2011).

3.4 What types of models can be used?

The AQ Directive does not specify prerequisites for the actual models to be used. As long as the model complies with the quality objectives (Annex I), then it may be applied. However, according to the technical guidance given in this document, the following general 'fit-for-purpose' criteria should apply:

- the model has the appropriate spatial and temporal resolution for the intended application;
- the model is adequately validated for the particular application, and is well documented;
- the model contains the relevant physical and chemical processes suitable for the type of application, the scale and the pollutant for which it is applied;
- the relevant emission sources for the application are adequately represented;
- suitable meteorological data are available.

In Table 3.1, a list of the application scales, the pollutants, and the typical types of models, or required processes, is provided. A comprehensive listing of air quality models used in Europe can be found at the EEA, 2011b; Model Documentation System (MDS). In addition, European Cooperation in Science and Technology Action 728 (COST 728, 2011) has developed a model inventory that provides information on a large number of mesoscale air quality and meteorological models.

Table 3.1 is to be considered as indicative; for every modelling application, a more thorough assessment of the required model types should be made. There are several reports available to support the choice of model and good modelling practices. The SATURN project Studying Atmospheric Pollution in Urban Areas (SATURN; Moussiopoulos, 2003) provided a review of air quality models for use in urban applications. The EU Sixth Framework Programme (FP6) project ' Air quality assessment for Europe' (Air4EU) (Air4EU, 2007) provided a number of reports recommending good practice for the use of models in air quality assessments.

In addition to the meteorological, dispersion and chemical modules that are the major elements of most air quality models, there are also a number of emissions sources that require process modelling. These may include sea salt, road dust, traffic and industrial emissions, biogenic emissions, home heating emissions and wind-blown dust. The methods used for such emission models will differ according to both compound and scale. Some emission models require detailed information on activities and meteorological conditions, whilst others may be based on aggregated emission data and require only simple modelling. Information on emission modelling can be found in a variety of sources, e.g. the *EMEP/EEA air pollutant emission inventory guidebook* (EEA, 2009).

3.5 The spatial and temporal resolution of the models

The required resolution, both temporal and spatial, varies depending on the pollutant and on the type and scale of the assessment. This section discusses these points and relates model resolution to the AQ Directive requirements for temporal and spatial representativeness.

Table 3.1 List of typical model characteristics, formulations and processes, for the various scales and pollutants needed for air quality assessment

	Area of assessment		
Description	**Local/hotspot (1–1 000 m)**	**Urban/agglomerate (1–300 km)**	**Regional (25–10 000 km)**
Model type	Gaussian and non-Gaussian parameterised models Statistical models Obstacle-resolving fluid dynamical models Lagrangian particle models	Gaussian and non-Gaussian parameterised models Eulerian chemical transport models Lagrangian particle models	Eulerian chemical transport models Lagrangian chemical models
Meteorology	Local meteorological measurements Obstacle-resolving fluid dynamical models Diagnostic wind field models	Mesoscale meteorological models Localised meteorological measurements Diagnostic wind field models	Synoptic/mesoscale meteorological models
Chemistry	Parameterised or none	Ranging from none to comprehensive, depending on application	Comprehensive
Emission modelling	Bottom-up traffic emissions Source-specific emissions	Bottom-up and/or top-down emission modelling Emission process models	Top-down emission modelling Emission process models
Compound	**Local/hotspot**	**Urban/agglomerate**	**Regional/continental**
PM_{10}	No chemical processes	Deposition Secondary inorganic particle formation	Deposition Primary (combustion) particles Secondary inorganic and organic particle formation Suspended dust Sea salt
$PM_{2.5}$	No chemical processes	Deposition Secondary inorganic particle formation	Deposition Secondary inorganic and organic particle formation
NO_2	Simple photo-oxidant chemistry Statistical/empirical relations	Limited photo-oxidant chemistry Photo-stationary scheme Statistical/empirical relations Deposition	Deposition Full photo-oxidant chemistry
NO_X	No chemical processes	No chemical processes Full photo-oxidant chemistry for larger scales	Full photo-oxidant chemistry
O_3	As in NO_2	As in NO_2	As in NO_2
SO_2	No chemical processes	Deposition Secondary inorganic particle formation	Deposition Secondary inorganic particle formation Full photo-oxidant chemistry
Pb	No chemical processes	Deposition No chemical processes	Deposition Specialised chemical schemes
Benzene	No chemical processes	n/a	Deposition Full photo-oxidant chemistry
CO	No chemical processes	No chemical processes	Full photo-oxidant chemistry
Heavy metals and B(a)P	No chemical processes	Deposition Specialised chemical schemes	Deposition Specialised chemical schemes

3.5.1 *Spatial resolution of the models*

The AQ Directive specifies the placement of measurement sites (Annex III.B.1) related to health protection, and notes that if modelling is used then the same type of criteria should apply (Annex III.A.1). From a modelling perspective, the following points concerning resolution should be made:

- Assessment should occur at sites where the concentrations are highest, e.g. the kerbside or close to strong sources, as well as in areas representative of the exposure of the general public, i.e. the urban background. However, in regard to the positioning of traffic sites (Annex III.C of the AQ Directive), the AQ Directive states that these 'shall be at least 25 m from the edge of major junctions and no more than 10 m from the kerbside'.
- For industrial areas, concentrations should be representative of a 250 x 250 m^2 area; for traffic emissions, the assessment should be representative for a 100-m street segment (Annex III.B.1.b of the AQ Directive).
- Urban background concentrations should be representative of several square kilometres (Annex III.B.1.c of the AQ Directive).

These statements concerning representativeness place limits on the modelling to be carried out. The following examples help to illustrate this.

- It is sufficient to calculate the kerbside concentration at 100-m intervals along a road, including the most affected side of the road, when the road segment is longer than 100 m.
- If Gaussian type models are used for traffic emission modelling, then receptor points (the point at which the concentration is calculated) need to be closer than 10 m to the kerbside, but 25 m from the edge of major junctions. In fact, most models will provide concentrations at some predefined distance from the kerb, e.g. 5 m or 10 m, to ascertain the local traffic contribution. Though there may be good reasons from a modelling perspective to define a minimum distance (e.g. due to increased uncertainty in the model close to the source), the AQ Directive does require that the limit values be applied everywhere. As a result, model receptor points should be placed directly at the kerbside or some allowance made for the distance of the receptor point from the kerbside.
- In regard to the positioning of the receptor points in the model, the AQ Directive also states that the pollutants should be monitored at the height of between 1.5 m and 4 m, the breathing zone for people (Annex III.C). Modellers should also conform to this when positioning receptor points in their models.
- If hotspots occur at road junctions of less than 100-m extent, then it is not sufficient to calculate the concentrations at just one point, e.g. one receptor point using a Gaussian model; several points representing a 100-m-long segment would be required instead.
- When assessing industrial sites using Gaussian or non-Gaussian plume-type models, then the concentrations should be calculated at a resolution not greater than 250 m, and preferably less in order to establish spatial averages at 250 x 250 m^2 resolution.

In regard to the protection of vegetation and natural ecosystems, the AQ Directive is intended to cover regional background levels of air pollutants within any zone in areas where ecosystems are dominant, i.e. not in urban areas. For measurements, this is expressed in terms of the distances that monitoring stations should be placed away from major sources (Annex III.B.2). From a modelling perspective, when gridded models are used, this can be interpreted in terms of model resolution and proximity to urban areas, as follows.

- Assessment should be performed more than 20 km away from an agglomeration (Article 2.17) and more than 5 km away from built-up areas or other sources of pollution, e.g. roads with a traffic volume of > 50 000 vehicles per day (Annex III.B.2).
- The area for which the calculated concentrations are valid is 1 000 km^2, roughly a 30 x 30 km^2 grid (Annex III.B.2).
- There are exceptions where terrain is complex or where small-scale ecosystems are found. It is then possible to redefine the representative area as smaller, with a subsequent increase in model resolution (Annex III.B.2).

From a modelling perspective, this implies that grid resolutions of between 20 x 20 km^2 and 30 x 30 km^2, or less, are suitable for assessment responding to ecosystem protection needs. A problem may occur in relation to mixed grids, where emissions from major sources, such as major roads or industrial districts in rural areas, are included in a grid that is considered to be rural in nature. Under such conditions, Eulerian models of 20 x 20 km^2 to 30 x 30 km^2 resolution will not deal with these sources effectively. It may then be necessary to employ some type of sub-grid modelling or 'plume-in-grid' model to address the impact of local sources, if a

Table 3.2 Relation between the AQ Directive temporal averaging period and application region to the model temporal and spatial resolution

	AQ Directive		Model	
Compound	**Temporal averaging**	**Spatial region**	**Temporal resolution**	**Spatial resolution**
PM_{10}	Annual mean Daily mean	Hotspot Urban Rural	Hourly	Individual hotspot 1–5 km 10–50 km
$PM_{2.5}$	Annual mean	Urban Rural	Annual	1–5 km 10–50 km
Speciated PM	–	Rural	Hourly — Daily	10–50 km
NO_2	Annual mean Hourly	Hotspot Urban	Hourly	Individual hotspot 1–5 km
NO_X	Annual mean	Rural	Hourly	10–50 km
O_3	8-hour mean	Suburban Rural	Hourly	5–50 km
SO_2	Hourly mean Daily mean Annual mean Winter mean	All	Hourly	All
Pb	Annual mean	Hotspot Urban	Annual	Individual hotspot 1–5 km
Benzene	Annual mean	Hotspot Urban	Annual	Individual hotspot 1–5 km
CO	8-hour mea$_n$	Hotspot Urban	Hourly	Individual hotspot
Heavy metals and B(a)P	Annual mean	Hotspot Urban	Annual	Individual hotspot 1–5 km

representative assessment down to a resolution of 5 km is to be made.

It should be noted that the AQ Directive does not imply that ecosystems smaller than 1 000 km^2 or less than 5 km from major sources should be ignored. Rather, it is up to the Member States to address the ecosystem protection of these areas.

3.5.2 Temporal resolution of the models

The required temporal resolution of the models is related first and foremost to the limit values and critical levels of the pollutant being considered. In cases such as nitrogen dioxide (NO_2), where hourly exceedances are addressed, in principle a model will need to provide hourly mean concentrations of that pollutant. The same is true for particulate matter (PM_{10}), ozone (O_3), sulphur dioxide (SO_2) and carbon monoxide (CO), pollutants that require hourly or daily mean concentrations to calculate the necessary percentiles. Having said this, it is also possible to develop a statistical model that relates annual mean NO_2 levels to hourly exceedances, for instance, and then apply this to derive the NO_2 exceedances. In such a case, hourly monitoring data would be used to develop the relationship.

Table 3.2 summarises the relevant spatial and temporal resolutions needed for the models, for the different compounds. In this regard, it is important to be aware of the areas where the AQ Directive is to be applied, i.e. in regard to population and ecosystems, as discussed in Section 2.2.

3.6 Model quality objectives as described in the AQ Directive

The modelling quality objectives are described in Annex I of the AQ Directive along with the monitoring quality objectives. The former are represented in Table 3.3. The quality objectives are given as a relative uncertainty (%). Uncertainty is then further defined in the AQ Directive to mean the following:

> 'The uncertainty for modelling is defined as the maximum deviation of the measured and calculated concentration levels for 90 % of individual monitoring points, over the period considered, by the limit value (or target value in the case of ozone), without taking into account the timing of the events. The uncertainty for modelling shall be interpreted as being applicable in the region of the appropriate limit value (or target value in the case of ozone). The fixed measurements that have to be selected for comparison with modelling results shall be representative of the scale covered by the model.'

Note that the definition of uncertainty for modelling is slightly different to that for monitoring. In Annex IV of the Directive on heavy metals and PAH (EC, 2005), the data quality objectives are provided; they are listed as relative uncertainties, and a single value of 60 % is indicated for all compounds (see Table 3.3). For modelling, the uncertainty is defined in a similar manner to the AQ Directive:

> 'The uncertainty for modelling is defined as the maximum deviation of the measured and calculated concentration levels, over a full year, without taking into account the timing of the events.'

It does not state to what precisely the uncertainty will be compared for modelling. However, for the measurement uncertainty, it is noted that:

> 'The uncertainty of the measurements should be interpreted as being applicable in the region of the appropriate target value.'

As a result, the method for defining uncertainty in the Directive on heavy metals and PAH (2004/107/EC) is best assumed to be the same as for the AQ Directive (2008/50/EC).

It is important to note that these model quality objectives apply only to assessment of the current air quality when reporting exceedances. There are no model quality objectives for other applications in the AQ Directive, such as planning or forecasting. However, there is clearly an expectation when using models for these other applications that they been verified and validated in an appropriate, albeit unspecified, way.

3.6.1 *Mathematical formulation of the AQ Directive quality objectives*

As in the previous directives, the wording of this text needs further clarification in order to become operational. Since values are to be calculated, a mathematical formula is required. As such, the term 'model uncertainty' remains open to interpretation. Notwithstanding this, we suggest the following application, termed the relative directive error (RDE) and defined mathematically at a single station as follows:

$$RDE = \frac{|O_{LV} - M_{LV}|}{LV}$$

where O_{LV} is the closest observed concentration to the limit value concentration (*LV*), and M_{LV} is the correspondingly ranked modelled concentration. The maximum of this value found at 90 % of the available stations is then the maximum relative directive error (MRDE).

This formulation is similar to that recommended by Stern and Flemming (2004), called the relative percentile error (RPE), which is defined at a single station as:

$$RPE = \frac{|O_P - M_P|}{O_P}$$

where O_p and Mp are the observed and modelled concentrations at the percentile (*p*), used to define the exceedance percentile. There are two major differences between the formulations: first, in the choice of using the closest value to the limit value or using the defined percentile; and second, in the choice of using the limit value or the observed concentration of the percentile in the denominator for the calculation. When the observed percentile concentration is the same as the limit value, then these two formulations are equivalent. When dealing with annual means, the concept is the same, but only one value is available for the calculation, i.e. $O_{p,LV}$ and $M_{p,LV}$ are replaced by the observed and modelled annual means.

There are arguments both for and against the RDE interpretation. For instance, if observed annual mean concentrations are well above the limit value, then the use of the limit value concentration in the denominator, rather than the observed concentration as in RPE, can lead to large relative errors, e.g. RPE may be satisfied, but not RDE. However, the opposite is true when the observed and modelled concentrations are well below the limit value. In such cases, the use of RPE can lead to high and unacceptable relative errors that would otherwise have been acceptable using the RDE interpretation.

3.6.2 *Example of an uncertainty estimate*

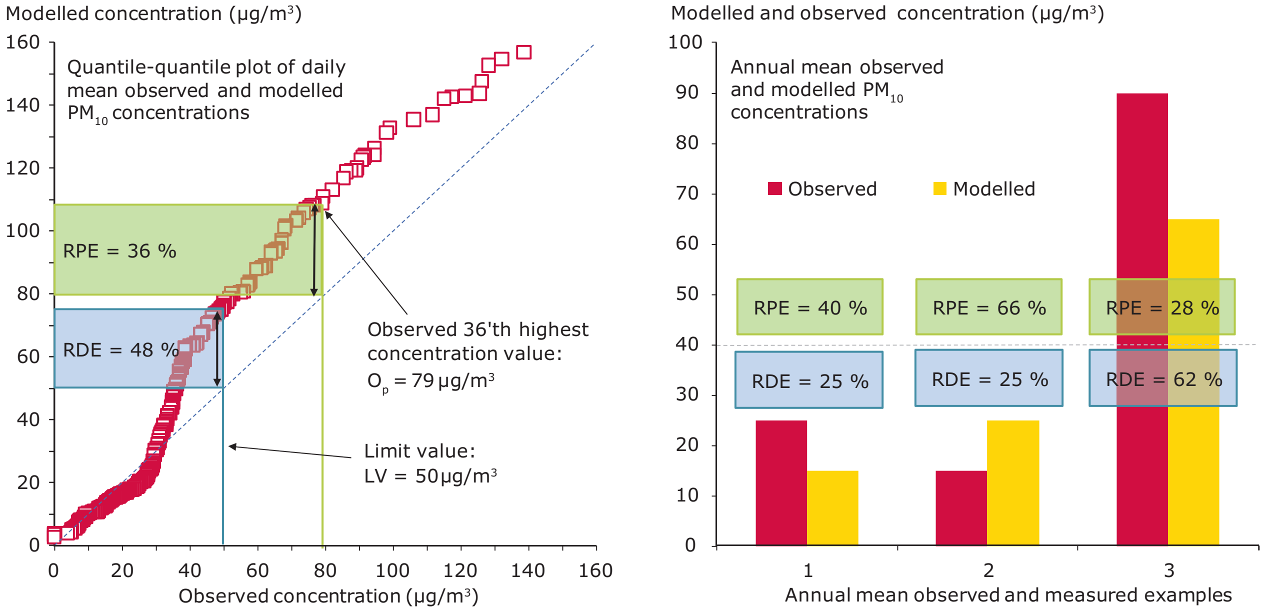
The above formulation is best demonstrated by an example showing the calculation of RDE and RPE for both daily and annual mean PM_{10} concentrations (Figure 3.1). In this example, modelled and observed daily mean concentrations of PM_{10} are ranked from highest to lowest, and the ranked values are plotted against one another in a quantile-quantile plot. In this case, the observations show that the number of observed days in exceedance of the limit value (50 µg/m³ — see Table 2.2) is 63. The correspondingly ranked model concentration at the observed limit value is 75 µg/m³. The resultant RDE will then be RDE = |50 — 75|/50 = 48 %. To determine the RPE, we see that the 36th highest observed daily mean concentration is 79 µg/m³, 29 µg/m³ above the limit value. The corresponding model 36th percentile is 108 µg/m³. From this, the RPE = |79 to 108|/79 = 36 %.

In this example, the results do not differ by a large amount, and indeed this will likely be the case when the percentile value is in the vicinity of the limit value. For extreme cases, where there are no exceedances or where there are many exceedances, these two error estimators can diverge significantly (Figure 3.1, right), but this will depend on the model characteristics. Note that in the example shown above, PM_{10} daily mean data have been used. However, there are currently no quality objectives in the AQ Directive for daily mean PM_{10} concentrations.

Also included in Figure 3.1 (right) are three fictional annual mean PM_{10} concentrations, both modelled and observed. RPE and RDE are calculated for these three cases using equations 1 and 2. In this case, the outcomes can be significantly different.

Despite these large differences, there is no clear and accepted quantitative method for calculating model uncertainty for the quality objectives stated in the AQ Directive. The intention, as also stated in the AQ Directive, is that it is most important to assess uncertainty around the limit (or target) value, as it is this uncertainty that is the most important. Any assessment of uncertainty should be interpretable as an uncertainty around the limit value, i.e. even if there are no data close to the limit value, the expected uncertainty at the limit value should be provided. Unfortunately, determining this may also be subjective.

Figure 3.1 Relative directive error (RDE) and relative percentile error (RPE) for both daily and annual mean PM_{10} concentrations



Note: Left graph: Quantile-quantile plot demonstrating how to calculate the RDE and RPE for daily mean PM_{10} as described in the text for percentiles. The example is from a traffic station in Oslo, 2003.
Right graph: Bar chart demonstrating how to calculate the RDE and RPE for fictitious annual mean PM_{10} concentrations.

Table 3.3 Summary of the modelling quality objectives, called 'uncertainty', as stated in Annex I of the AQ Directive and Annex IV of the Directive on heavy metals and PAH

Modelling uncertainty	SO_2, NO_2, NO_X and CO	Benzene	PM_{10}, $PM_{2.5}$ and Pb	Ozone and related NO and NO_2	Benzo(a) pyrene, arsenic, cadmium, nickel, total gaseous mercury
Hourly	50 %	—	—	50 %	—
8-hour averages	50 %	—	—	50 %	—
Daily averages	50 %	—	Not yet defined	—	—
Annual averages	30 %	50 %	50 %	—	60 %

3.6.3 Understanding of the '90 % of stations' requirement

The AQ Directive states that the uncertainty will be determined from the maximum of 90 % of the available monitoring stations. This is interpreted as a clause that allows a number of outliers, i.e. 10 % of the stations, to be excluded from the uncertainty calculation. It is perhaps not intended to be taken literally, as this would mean that any model domain with less than 10 stations will not have the luxury of excluding any outliers; however, it is not open to any other understanding. Unfortunately, there are many urban areas with less than 10 stations, especially ones representing the same scale as the model. Consequently, the AQ Directive should be interpreted to state that all the stations must be used in the calculations when the number of suitable stations is less than 10. It is worth noting for clarity (see Section 3.6.4) that only stations representative of the same spatial scales as the model are to be applied in the uncertainty assessment.

3.6.4 Representative scale of models and observations

The AQ Directive quite rightly appreciates that models have a defined spatial scale for which they are representative (e.g. a 2 x 2 km^2 grid), and as such, cannot be expected to provide adequate results on smaller scales, e.g. near roads or industrial sources. Although the question of how large an area is represented by a monitoring station can be open to discussion, expert judgment can be used based on knowledge of the local environment surrounding the monitoring station. If this is not available, then station classifications, e.g. traffic, and industrial and urban background, can be used to match the model's resolution. This is one of the subjects of Fairmode activities.

4 Reporting and public information when using models

This chapter deals with the various reporting and communication needs as set out in the AQ Directive (Articles 26 and 27), with emphasis on assessment and plans. Many of these reporting needs are equally applicable whether models are used or not. In this regard, the relevant reporting needs related to modelling are highlighted, whilst the general aspects of reporting are also covered.

4.1 Requirements for current reporting to the European Commission when using models for assessment of existing air quality

The overall requirements for the reporting of air quality assessment are provided in Article 27 and Annex I, Section B of the AQ Directive. To aid in such reporting, the European Commission has provided a questionnaire (EC, 2011b); they have also provided a guidance document to assist in completing the questionnaire (EC, 2011c). This questionnaire is based on the earlier daughter directives, up to and including the fourth daughter directive on heavy metals and PAH (EC, 2005). Assessment reports should be provided within nine months of the completion of the reporting period. This means that such reports are due by 30 September every year. The results are summarised annually in the so-called Questionnaire Report, compiled by the EEA with support of the ETC/ACM (Jimmink et al., 2010). Following the introduction of the new AQ Directive, new implementing provisions regarding reporting are being developed. These will introduce a new reporting mechanism (e-Reporting) that will consider consolidated requirements for reporting and exchange of modelled information.

Most air quality assessments already reported can be found at EEA (2011a) within the individual country folders, under the heading 'European Union (EU), obligations'.

4.1.1 The questionnaire on air quality assessment

Most of the questionnaire is dedicated to monitoring data, zone specification and reporting of exceedances. Sheets 8 through 10 show that the exceedance status in relation to limit and other threshold values must be indicated. If this status is based solely on modelling, then this must be indicated with the letter 'm'.

From sheets 19a to 19k of the questionnaire, results of any supplementary methods used for determining exceedances are required. This includes spatial information on the exceedance in relation to surface area, road length and population exposed. These results are preferably reported as concentration maps, submitted in annexes.

Methods used will be indicated as a reference to sheet 20. On sheet 20 direct references to the supplementary methods applied are required. These will most likely be national reports that are also publicly available. When modelling is used as a supplementary method, this must be indicated and appropriate referencing has to be included. It is not requested that detailed information be given in the questionnaire itself.

Sheets 21 to 24 refer to information concerning the exceedance of SO_2 and PM_{10} limit values due to natural events and winter sanding. Within these sheets of the questionnaire, reference must be made to the methods used to assess the natural contribution to these exceedances. If models have been used, these must be referred to and documentation made available. Sheets 21 to 24 will need to be updated for the 2008 AQ Directive, as the range of natural sources has been expanded since the previous Directive (EC, 1999).

Sheet 25 of the questionnaire refers to the contribution of transboundary pollution to air quality. Currently this sheet refers only to consultation with the other EU Member States rather than to any justification or assessment of the contribution from other countries. However, in any

Table 4.1 EU-27 share of zones where modelling was also used to report exceedances, 2004–2007

Exceedance also based on modelling	2004	2005	2006	2007
O_3-vegetation	2.2	3.6	2.9	6.1
O_3-health	2.1	3.3	2.0	7.1
PM_{10} daily	10.0	9.3	7.2	8.1
NO_2 annual	12.0	10.6	4.4	10.8
PM_{10} annual	9.0	8.0	6.0	7.1
NO_X	19.0	2.8	6.9	7.0
NO_2 hourly	10.0	10.3	8.5	6.1
SO_2 daily	8.0	8.8	7.7	9.7
SO_2 hourly	13.0	12.1	10.6	10.3
SO_2 annual	21.0	14.4	7.2	6.9
Lead	15.0	19.3	17.9	30.3
Benzene	13.0	12.5	31.1	21.7
CO	14.0	9.6	11.9	17.9
SO_2 winter	19.0	19.4	5.4	7.1

Note: According to the current air quality legislation, **compliance checking** can only be based on measurements. The numbers above are only indicative. The percentages of zones are not the best indicator for a 'trend' but more an overview for the current year. This is because zone delimitation can change from year to year within a country, for every single pollutant and for each health or ecosystem protection endpoint. An in-depth update of information indicated in this table will be available by the end of 2011. Note that there are approximately 1 000 zones in total (every year).

Source: Taken from Vixseboxse and de Leeuw, 2009.

consultation process, clearly justified arguments are required and modelling will be invaluable for this.

4.1.2 Information required concerning models used for assessment

Annex I, Section B of the AQ Directive describes the information required concerning any modelling activities that are used for reporting assessment. It is cited here for clarity.

> 'The following information shall be compiled for zones or agglomerations within which sources other than measurement are employed to supplement information from measurement or as
> — the sole means of air quality assessment;
> — a description of assessment activities carried out;
> — the specific methods used, with references to descriptions of the method;
> — the sources of data and information;
> — a description of results, including uncertainties and, in particular, the extent of any area or, if relevant, the length of road within the zone or agglomeration over which concentrations exceed any limit value, target value or long term objective plus margin of tolerance, if applicable, and of any area within which concentrations exceed the upper assessment threshold or the lower assessment threshold;
> — the population potentially exposed to levels in excess of any limit value for protection of human health.'

Some of this information is to be provided directly in the questionnaire (e.g. reference to methods, extent of road, and population exposed). The remaining information (e.g. uncertainty analysis, and description of the methods and results) is too extensive to be included in the questionnaire and is not required by the European Commission. This information should, however, be available in case the need arises to substantiate the assessment results more extensively.

4.1.3 Current status of reporting that includes the use of models for assessment

An analysis of the questionnaires returned by the Member States from 2004 to 2007 (Vixseboxse and de Leeuw, 2008) shows that some form of modelling was used by 13 of the 27 Member States to determine the exceedance status in their zones. Such modelling activities were not evenly distributed over the different legislated pollutants: lead (Pb) (30.3 %), benzene (21.7 %) and CO (17.9 %) were the pollutants most frequently reported using modelling (Table 4.1). The use of modelling for these pollutants has been seen to be increasing. In comparison, the use of modelling for the pollutants SO_2, NO_2, nitrogen oxides (NO_X) and PM_{10} between 2004 and 2007 is significantly less, at 7 % to 10 %. There is no strong trend in the use of modelling. Further to these, a number of more extensive examples presenting 'good practice' in model assessment are provided in Chapter 6 and via the Fairmode website (Fairmode, 2011b).

4.2 Reporting air quality plans when using models

All Member States in exceedance of any limit or target values after their attainment date (Article 23), or requesting a postponement of attainment deadlines of limit values (Article 22), are required to submit air quality plans for meeting the requirements as laid out in the AQ Directive, though this is not explicitly requested in regard to the heavy metal and PAH Directive. Since many of these plans are made with the use of models, their reporting will generally involve information concerning the predicted outcomes of any measures planned to be taken. Such plans should be reported no later than two years after the end of the year when the first exceedance was observed.

An overview of reports and plans submitted to the European Commission in 2005 can be found in Nagl et al. (2006) and Van den Hout (2007).

4.2.1 Reporting air quality plans

The obligations of the Member States with regard to air quality plans is provided in Article 23 of the AQ Directive. Further to this, the AQ Directive provides extensive information on the reporting of air quality plans. These are contained in Annex XV and Article 28 of the AQ Directive as well as in the Commission Decision 2004/224/EC (EC, 2004) that lays down arrangements for the reporting of information on plans and programmes (renamed 'air quality plans' in the 2008 AQ Directive: EC, 2008a) for the previous AQ Directive 96/62/EC. A specific 2004/224/EC form, provided as an Excel spreadsheet, is available for this purpose (EC, 2011d).

Within this Excel spreadsheet, there are a number of sheets (seven in total) that must be filled in. To help Member States report plans within this form, the European Commission has provided a guidance document entitled 'Recommendations on plans or programmes to be drafted under the Air Quality Framework Directive 96/62/EC' (EC, 2003). A more recent guidance document entitled 'Guidance on reporting air quality plans to the European Commission under Decision 2004/224/EC' will soon be available. These documents can be found on the European Commission Environmental website (EC, 2011f).

There are a number of points in the guidance document mentioned above that are relevant for modelling. The reader is referred directly to that document for more information on reporting plans and programmes in general.

Two other documents, 'Assessment of plans and programmes reported under 1996/62/EC — Final report' (Nagl et al., 2006) and 'Overview of reports on plans and programmes for reducing air pollution submitted under Decision 2004/224/EC' (van den Hout, 2007), also provide information on the types and numbers of plans submitted to the European Commission by December 2005.

A number of examples of plans and programmes reported to the European Commission, and also some not yet reported, can be found in Chapter 7 of this document and via the Fairmode website (Fairmode, 2011b).

4.2.2 Reporting for the postponement of attainment deadlines and exemptions

Reporting of 'postponement of attainment deadlines and exemptions from the obligation to apply certain limit values' (Article 22) also requires an assessment of the current air quality and a report of air quality plans, similar to that described above. The European Commission provides guidance on this (EC, 2011g) and in particular provides a document to aid reporting (EC, 2008b), including an Excel-based spreadsheet developed from 2004/224/EC. For PM_{10}, several factors are considered to be relevant in applying for postponement or exemptions, including transboundary contributions, adverse climatic conditions and site-specific dispersion characteristics. These elements, as well as the required plans, need to be assessed and described when applying for postponement.

4.2.3 Reporting of short-term action plans

There are similar obligations for the reporting of short-term action plans (Article 24) as there are for air quality plans. Short-term action plans are intended to reduce the risk or duration of an exceedance of an alert threshold. The European Commission also requires that such plans be

Table 4.2 Updating frequency and averaging period required for the various pollutants for regular reporting to the public

Pollutant	Required frequency of updates	Preferred frequency of updates	Averaging period to be reported (excluding threshold reporting)	Public information or alert threshold averaging periods
SO_2	Daily	Hourly	Hour	3 hours
NO_2	Daily	Hourly	Hour	3 hours
Benzene	3 monthly	Monthly	Year	
CO	Daily	Hourly	Maximum daily 8-hour mean	
PM_{10}	Daily	Hourly	Day	
$PM_{2.5}$	-	-	Year	
Pb	3 monthly	Monthly	Year	
O_3	Daily	Hourly	Maximum daily 8-hour mean	1, 3 and 8 hours

drawn up, when appropriate or necessary, and made available to the public and the appropriate organisations (Article 24). In Article 24, Section 4, the AQ Directive goes on to state that by June 2010, the European Commission will publish a number of best practices of such plans, and that a project addressing this issue is currently being prepared.

4.2.4 *Reporting in regard to activities to reduce transboundary air pollution*

Article 25 of the AQ Directive deals with the question of transboundary air pollution. In this article, Member States are encouraged to cooperate to reduce the effects of transboundary air pollution; the European Commission should be present at and assist in discussions concerning this. There are no formal reporting requirements concerning these activities. This is highlighted in the questionnaire on air quality assessment and planning, which provides two sheets giving summary information on any cooperative activities between Member States (sheets 25a and 25b).

4.3 Communicating to the public when using models

Communicating air quality information occurs at two different levels. The first is the annual reporting activities of the Member States (Article 26) and the second is the regularly updated transfer of information (Annex XVI) concerning air quality monitoring and short-term forecasts. The most relevant application of models is in their use for forecasting. However, models may be used in all reporting activities following similar lines to those set out in Sections 4.1 and 4.2 above.

4.3.1 *Annual information for the public*

Article 26 of the AQ Directive lays out the requirements of the Member States in regard to the annual reporting of the air quality assessment and plans to the public. It is thereby intended that the relevant information on air quality be available in an accessible way to:

> '…the public, as well as appropriate organisations such as environmental organisations, consumer organisations, organisations representing the interests of sensitive populations, other relevant health-care bodies and the relevant industrial federations.'

There are no special requirements in regard to models or reporting of modelling results. It is up to the Member States to define how the information is communicated to the public, but it should be in line with that which is reported directly to the European Commission and to the EEA.

4.3.2 *Alert and information threshold to inform the public*

On a daily basis, Member States are obliged to inform the public first and foremost of any exceedances of the information and alert thresholds (Annex XII and Table 2.2 of the AQ Directive). These exceedances will generally be based on monitoring. The AQ Directive explicitly lays out the type of information that should be available when communicating information to the public in Annex XVI, Article 4. This includes:

- information on observed exceedance(s);
- information on the forecast for the following afternoon/day(s), including the geographical area of expected exceedances and the expected trends in the air pollution;
- information on the type of population concerned, possible health effects and recommended behaviour;
- information on preventive action to reduce pollution and/or exposure.

In the list above, the most relevant points for modelling are the forecasting of air quality for the following day(s) and the assessment of effective short-term mitigation strategies.

In the Directive on heavy metals and PAH, there are no obligations for alert reporting, though there are obligations for providing information to the public and authorities in Article 7.1 (see Section 4.3.3).

4.3.3 *Regular information for the public*

Also in Annex XVI (Articles 2 and 3), the AQ Directive indicates the general information on pollutant concentrations that should be made available on a regular basis. Table 4.2 shows the minimum frequency at which the information available for the various pollutants should be updated. The information should be available for the averaging period specified in the AQ Directive (Annex VII, XI and XIV; see summary in Table 2.2). This means, for example, that daily rather than hourly mean values of PM_{10} should be communicated. In addition to the regularly updated information, background information concerning the AQ Directive air quality objectives and the effect of air quality on health and vegetation is also required.

In the Directive on heavy metals and PAH, obligations for reporting to the public are contained in Article 7.1. Unlike the AQ Directive, it does not specify the required frequency of such information but indicates that updated information should routinely be made available to the public.

In general, regular reporting to the public occurs through the use of monitoring (see Table 4.3). However, there is no reason why spatially distributed air quality data (i.e. through modelling) should not also be made available to the public. Post-processing of either forecast results in combination with monitoring is a natural application of modelling for providing updated information on near real-time air quality. However, there are few such near real-time model updates currently available in Europe. The initiative 'Air Quality forecasts and observations in France and Europe' currently provides such analysed maps of France for ozone twice daily (PREVAIR, 2011). A similar task on a European scale is one of the focus points of the Global Monitoring for Environment and Security (GMES) Atmosphere Service project MACC (MACC, 2011) that intends to provide such information to the public.

4.3.4 *Air quality web portals in Europe*

Most Member States now have their own web portals for communicating their air quality to the public; Table 4.3 lists a number of them by country. Most of these web portals provide updated information on monitoring activities within the country, and some provide forecasts using models. All provide background information and links to reports.

Table 4.3 Examples of links to public information web sites for European countries

Country code	Country	Air quality public information site link	Monitoring information	Modelling information
BE	Belgium	http://www.irceline.be/	Hourly graphs Hourly maps	3-day forecasts for Belgium
BG	Bulgaria	http://www.icsr.bas.bg/icsrwebsite/departments/rdts/htdocs/index_EN.html	Daily average	
CZ	Czech Republic	http://portal.chmi.cz/portal/dt?action=content&provider=JSPTabContainer&menu=JSPTabContainer/P1_0_Home&nc=1&portal_lang=en#PP_TabbedWeather	Hourly average Hourly graphs	
DK	Denmark	http://www2.dmu.dk/atmosphericenvironment/byer/forside.htm	Hourly graphs	3-day forecasts for Denmark
DE	Germany	http://www.env-it.de/umweltbundesamt/luftdaten/index.html	Hourly graphs	3-day ozone forecasts for Germany
EE	Estonia	http://mail.klab.ee/seire/airviro/		
IE	Ireland	http://www.epa.ie/whatwedo/monitoring/air/	Hourly graphs	
EL	Greece	http://www.minenv.gr/1/12/122/12204/e1220400.html http://lap.phys.auth.gr/gems.asp http://lap.physics.auth.gr/forecasting/airquality.htm	Daily average	General forecasting for Athens 3-day forecasts for Athens Daily forecasts
ES	Spain	http://www.marm.es/es/calidad-y-evaluacion-ambiental/temas/atmosfera-y-calidad-del-aire/calidad-del-aire/mediciones/ http://verde.lma.fi.upm.es/wrfchem_eu/ http://www.troposfera.org/ http://pagina.jccm.es/ficheroscomunes/error404.htm http://www.bsc.es/caliope http://www.gencat.cat/mediamb/qaire/pronostic/pronostic_aire.htm http://gestiona.madrid.org/aireinternet/html/web/ModeloPredictivoAccion.icm?rangoModelo=24&ESTADO_MENU=4_1 http://www.ingurumena.ejgv.euskadi.net/r49-n82/es/vima_ai_vigilancia/prevision48.apl http://mca-retemca.ciemat.es/	General regional portals for AQ data	3-day forecasts for Europe 3 day forecasts of ozone for Spain 2-day forecasts for Europe and Spain Regional forecast for Castilla la Mancha Regional forecast for Cataluña Regional forecast for Madrid Regional forecast for País Vasco General web portal on atmospheric pollution modelling in Spain
FR	France	http://www.prevair.org	Hourly Twice daily maps	1-day French and European forecasts Near real-time analysis maps
IT	Italy	http://ita.arpalombardia.it/ITA/qaria/Home.asp http://www.aria-net.eu/QualeAria	Daily maps Daily graphs	Air quality forecasting for Lombardy region 48-hour forecasts of air quality for Italy
CY	Cyprus	http://www.airquality.gov.cy	Hourly graphs	
LV	Latvia			
LT	Lithuania	http://stoteles.gamta.lt/	Hourly average Hourly graphs	
LU	Luxembourg	http://www.environnement.public.lu/air_bruit/index.html	Hourly average Hourly graphs	

Table 4.3 Examples of links to public information web sites for European countries (cont.)

Country code	Country	Air quality public information site link	Monitoring information	Modelling information
HU	Hungary	http://www.met.hu/levegokornyezet/legszennyezettseg_elorejelzes/index.php?prod=terkep	Daily map	2-day forecasts for Budapest
MT	Malta	http://www.mepa.org.mt/airquality	Hourly average	
NL	Netherlands	http://www.lml.rivm.nl/	Hourly maps Hourly graphs	2-day forecasts for Netherlands
AT	Austria	http://www.umweltbundesamt.at/en/umweltschutz/luft/luftguete_aktuell/	Daily average	
PL	Poland	http://armaag.gda.pl/en/results.htm	Hourly maps Hourly graphs	
PT	Portugal	http://www.qualar.org/?page=7&subpage=1&PHPSESSID=c43ac9502aa658b258c016b399430608	Daily graphs Daily average	3-day forecasts for Portugal
RO	Romania	http://www.calitateaer.ro/	Hourly average Hourly graphs	
SI	Slovenia	http://nfp-si.eionet.europa.eu/Dokumenti/GIS/zrak	Hourly graphs Hourly maps	
SK	Slovakia			
FI	Finland	http://www.airquality.fi http://silam.fmi.fi/AQ_forecasts/v4/index.html	Hourly graphs	6-hour forecast for Finland
SE	Sweden	http://www.slb.mf.stockholm.se/e/ http://gems.ecmwf.int/d/products/raq/)		2-day forecasts
UK	United Kingdom	http://www.airquality.co.uk http://www.airqualityni.co.uk/ http://gems.ecmwf.int/d/products/raq/	Hourly graphs	1-day forecasts for the UK 1-day forecasts for Northern Ireland
	former Yugoslav Republic of Macedonia, theMacedonia FYR			
AL	Albania			
BA	Bosnia and Herzegovina			
CH	Switzerland	http://www.bafu.admin.ch/luft/luftbelastung/aktuell/index.html?lang=en	Hourly average Daily graphs Daily maps	
HR	Croatia			
IS	Iceland	http://www.reykjavik.is/desktopdefault.aspx/tabid-1007	Hourly average Hourly graphs	
ME	Montenegro			
NO	Norway	http://www.luftkvalitet.info	Hourly graphs	Winter forecasts for several cities in Norway
RS	Serbia			
SM	San Marino			

Note: Updates of this table will be made available via the Fairmode website (Fairmode, 2011b).

5 Model quality assurance and evaluation

Though the AQ Directive outlines criteria for acceptable model **uncertainties** or quality objectives (Annex I and Section 3.6 of this document), it is generally understood that these alone are not sufficient to build confidence in the use of models for air quality applications. Models and their application in support of the AQ Directive should be reliable and trustworthy. Thus, model quality assurance is a crucial element that needs to be tailored to match the policy application. In this chapter, a brief overview of procedures for model **quality assurance**, model **evaluation** and model **validation** is presented, based on a synthesis of literature and experience from both Europe and North America.

The subject of model quality assurance is one of the major activities within Fairmode, and this chapter will be developed in parallel with these activities. Methods already practised and described in various projects, papers and reports are summarised and presented, and preliminary recommendations are provided based on these. Some concrete examples of model quality assurance and evaluation protocols are provided via the Fairmode website (Fairmode, 2011b). More detailed information resulting from relevant activities of Fairmode, such as further recommendations, examples, specific model evaluation criteria and validation documentation, and datasets, will be updated and become available via the Fairmode website (Fairmode, 2011a).

In general, the quality of models is understood in terms of their 'fitness for purpose' (Britter, 1994). The modelling experience indicates that there are no 'good' or 'bad' models. Evidence is rather based on the question of whether a model is suitable for the intended application and specified objectives. As such, the quality of a model is always relative and is measured against the **quality objectives** for any particular model application. Given the diverse literature and the range of definitions used to describe different aspects of model quality assurance, a glossary is provided in Table 5.1, defining the terms used in this document. As a starting point, we can explore the concepts of quality assurance and model evaluation, generally described as follows.

Quality assurance (QA) is an integrated system of management activities involving planning, documentation, implementation and assessment, established to ensure that the process, item, or service is of the type and quality needed and expected by the user (EUROTRAC 2, 2011a: see Table 5.1).

Model evaluation is the sum of processes that need to be followed in order to determine and quantify the model's performance capabilities, weaknesses and advantages in relation to the range of applications for which it has been designed (Following the terminology accepted by COST 732, 2011).

The relationship between model QA and model evaluation was highlighted by the work of the SATURN-EUROTRAC project (Borrego et al., 2003a):

> 'Model Evaluation is related to measuring model quality, while quality assurance is a process to guarantee the expected quality for decision making.'

5.1 Review of activities addressing quality assurance and model evaluation

Fundamentals of model quality assurance and evaluation of air pollution models can be found in a number of published documents: Chang and Hanna (2004), Borrego et al. (2003a; 2003b; 2008), Moussiopoulos et al. (2001), Moussiopoulos and Isaksen (2007), Canepa and Irwin (2005) and Steyn and Galmarini (2008). There are also a number of European and US projects and actions that provide extensive discussions on model quality assurance of varying kinds. In this section, we review these activities.

Table 5.1 Glossary of terms used in quality assurance and model evaluation

Concept	Meaning
Benchmarking	A standardised method for collecting and reporting model outputs in a way that enables relevant comparisons, with a view to establishing good practice, diagnosing problems in performance, and identifying areas of strength. A self-improvement tool (quality assurance tool) allowing modellers to compare some aspects of model performance, with a view to finding ways to improve current performance. Benchmarking provides modellers with an external reference and practices on which to base evaluation of the results and future developments. It can be seen as a diagnostic instrument, an aid to judgments on quality. Adapted from Vlãsceanu et al. (2004).
Model evaluation	The sum of processes that need to be followed in order to determine and quantify the model's performance capabilities, weaknesses and advantages in relation to the range of applications for which it has been designed.
Model intercomparison	The process of model assessment by the simultaneous comparison of modelling results provided by different models for the chosen situation.
Model Quality Indicators (statistical metrics)	Parameters that give information about the ability of the model to predict the tendency of observed values, errors on the simulation of average and peak observed concentrations, and type of errors (systematic or unsystematic) (Borrego et al., 2008).
Model quality objectives	A measure of the allowable deviation of model results from observations, e.g. as used in the AQ Directive, indicative of the model result acceptability. Provides an objective measure of model performance, usually in a simple metric (indicator).
Model validation	Comparison of model predictions with experimental observations, using a range of model quality indicators.
Model corroboration	Term preferred by the United States Environmental Protection Agency (US EPA) (2009) for the quantitative and qualitative methods used to assess the degree to which a model corresponds to reality (model validation). The agency prefers the term over 'validation', because 'it implies a claim of usefulness and not truth'.
Parameters	Predefined coefficients used in the model for process parameterisations. These have a degree of uncertainty to them and can be changed for conducting sensitivity analysis or to achieve calibration goals.
Quality assurance and control (QA/QC)	An integrated system of management activities involving planning, documentation, implementation and assessment, established to ensure that the model in use is of the type and quality needed and expected by the user.
Sensitivity analysis	A process to understand how a given model responds to changes in various model parameters, process descriptions and input data. Often used to infer a degree of model uncertainty based on the uncertainty of these parameters.
Uncertainty	A term used to describe a lack of knowledge about models, parameters, constants, data and concepts.
Uncertainty analysis	The process for characterising the model uncertainty.
Verification	The process of checking the computer code (algorithms and numerical techniques) to ensure that it is a true representation of the conceptual model upon which it is based.
Model calibration	The process of adjusting model parameters within physically defensible ranges until the resulting predictions give the best possible fit to the observed data, used in US EPA (2002) as an element in quality assurance planning for model development.
Operational evaluation	Statistical and graphical analyses aimed at determining whether the estimated values of the modelled variables are comparable to measurements in an overall sense (terminology used by US EPA).
Operational user evaluation	Part of model evaluation procedures, completed by model users. Refers in general to user-oriented documentation, user interface, assistance in inputting of data, clarity, flexibility and storage of output results.
Error	The measurable difference between two known quantities, i.e. model and observations.
Dynamic evaluation	This refers to the model's ability to react to changes in important input parameters, such as emissions or meteorology, in a satisfactory way.

5.1.1 *EU activities*

Model evaluation has been supported at EU level through both projects and networks of excellence. The following activities have included aspects of model QA and model evaluation.

- The European Commission's Model Evaluation Group (1994), Britter (1994) and Vergison (1996) developed recommendations on quality assurance protocols for models used in industrial hazardous gas release.
- The Initiative on *Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes* launched in 1991(HARMO, 2011), which has for the past decades promoted and encouraged a harmonised approach to model quality assurance.
- EUROTRAC-2 — SATURN, dealing with urban-scale models (EUROTRAC-2, 2011b).
- The Review of the Unified EMEP model hosted a model intercomparison study (van Loon, 2004).
- The modelling intercomparison exercises EuroDelta (2011) and CityDelta (Cuvelier et al., 2007) carried out by the European Commission Joint Research Centre, Institute for Environment and Sustainability (JRC-IES) in support of the modelling activities (urban to regional scales) within the CAFE ([2]) and NECPI ([3]) programme.
- ACCENT (2011), aimed at defining protocols and benchmark tests suitable for air quality assessment on regional and global scale.
- COST Action 728 (COST 728, 2011a), working on standardised model evaluation protocol for mesoscale meteorological models.
- COST Action 732 (COST 732, 2011), on quality assurance of microscale (obstacles-resolving) meteorological models.
- The Air4EU project (Air4EU, 2011) devoted special attention to validation strategy and uncertainty analysis for models for PM, NO_2 and O_3 assessment, covering a broad scale, from hotspot to regional.
- EUROTRAC-GLOREAM (GLOREAM, 2011) also focused on model performance and evaluation for global and regional atmospheric models where model quality objectives have been defined and tested for some target parameters.
- The web-based model evaluation platform ENSEMBLE (Galmarini et al., 2004a, 2004b and 2004c), originally developed for support to emergency response, has recently proved useful as a test bench for air quality models within the context of the COST 728 activity where it was used for a variety of case studies.

The main products of all these activities, related to model evaluation, can be briefly outlined as:

- model evaluation guidance and protocol document for microscale meteorological models (Britter and Schatzmann, 2007);
- model evaluation guidance for mesoscale models (Schluenzen and Sokhi, 2008);
- uncertainty analysis — methodologies and recommendations by Air4EU for models from hot spot through urban to regional scales (Borrego et al., 2006);
- models meta-database: ACCENT (2011), COST732 and COST 728 (COST 728/732, 2011), and the MDS of the EEA assisted by the ETC/ACM (EEA, 2011b).

5.1.2 *US experience*

The US EPA uses a wide range of models of differing complexity for regulatory decision-making. The EPA Quality system, defined in 2000, covers also environmental data produced from models (US EPA, 2000). Guidance on how to document quality assurance planning for modelling (e.g. model development, model application, as well as large projects with a modelling component) was published in 2002 (US EPA, 2002). In March 2009, the 'Guidance on the Development, Evaluation, and Application of Environmental models' was also published (US EPA, 2011). It presents recommendations and provides an overview of practices for ensuring and evaluating the quality of environmental models.

5.1.3 *A joint EU–North American initiative*

The EU–North American (NA) Air Quality Model Evaluation International Initiative (AQMEII), was recently established (2008), having recognised the

([2]) In 2005, the Commission launched the Thematic Strategy on Air Pollution and the Clean Air For Europe (CAFE) Programme, the first of seven Thematic Strategies in the EU's Sixth Environment Action Programme (EAP), 'Environment 2010: Our future, Our choice'.

([3]) The working group on the revision of National Emissions Ceilings & Policy Instruments (NECPI) was established under the CAFE Programme. Its main role was to provide technical assistance and expert advice to the Commission services in relation to the revision of the National Emissions Ceilings Directive (NECD).

necessity for exploring advanced methodologies for model evaluation, as well as the necessity to categorise the existing methods, including the identification of their limits. The main aims of this initiative are to bring together NA and EU regional-scale modelling communities, for an effective and efficient exchange of views and experiences through common activities, and to promote exploratory research in the field. The latter is achieved through thematic workshops that try to focus research activities and to identify research priorities. AQMEII (2011) is organised around the model evaluation frameworks of operational, diagnostic, dynamic and probabilistic evaluation (Dennis et al., 2009) that include the following.

- Operational evaluation: evaluation based on routine observation for both meteorology and air quality. The comparison focuses mainly on a one-to-one pairing of model output with monitoring data.
- Diagnostic evaluation: investigates the way in which specific physiochemical model processes can influence model results.
- Dynamic evaluation: deals with the model's ability to predict changes in air quality concentrations in response to changes in either source emissions or meteorological conditions. This also includes an assessment of the uncertainties in these inputs and their influence on the air quality predictions.
- Probabilistic evaluation: characterising the uncertainty of air quality model predictions; used to provide a credible range of predicted values rather than a single 'best estimate'.

Activities are being organised around and across these four themes that will involve the EU and NA modelling communities in a common modelling effort featuring both NA and the EU in air quality modelling case studies.

5.2 Review of protocols for model evaluation

From the activities outlined in Section 5.1, there are a variety of descriptions available on how both meteorological and air quality models can be evaluated. They cover common areas but are often grouped in categories that differ slightly. This section provides an overview of the key elements of model evaluation based on these works (see also the definitions in Table 5.1).

5.2.1 US EPA: description of model evaluation

The key elements of **QA**, according to US EPA (2002), are described below.

- **Planning:** problem definition, stating the specific problem to be solved, the outcome to be achieved or the decision to be made, definition of quality indicators and acceptance criteria.
- **Documentation:** model description, datasets, reporting requirements, documents update, etc.;
- **Implementation:** model application, model calibration and data requirements, but also user training;
- **Assessment:** scientific assessment, model performance evaluation, uncertainty analysis, sensitivity analysis, input data analysis and user oriented assessment.

Model evaluation is therefore inherently interwoven into the various components of model QA. The main elements of model evaluation refer to scientific evaluation, code verification, sensitivity analysis, uncertainty analysis, model validation, model intercomparison and model validation datasets (see Section 5.4).

The objective of **model evaluation** is to determine whether a model is of sufficient quality to inform a regulatory decision. Following an updated Guidance from the US EPA (2011), the process of model evaluation addresses four main elements:

- soundness of the science underlying a model;
- quality and quantity of available data supporting the choice of model;
- model corroboration (qualitative and/or quantitative methods for evaluating the degree to which a model corresponds to reality);
- appropriateness of a model for a given application.

These elements are viewed as an integral and ongoing part of the life cycle of a model — from development through application.

5.2.2 EU Model Evaluation Group: description of model evaluation

Within the EU, the Model Evaluation Group (1994), which was chiefly concerned with industrial-related accidental hazardous gas releases, proposed six steps to be followed in a model evaluation procedure:

- **model description** (brief description of the characteristics of the model, intended application range, theoretical background, parameterisations, data used, etc.);
- **database description** (complete description of the database to be used for the evaluation of the model, including data uncertainty estimation);
- **scientific evaluation** (description of the equations employed to describe the physical and chemical processes that the model has been designed to include);
- **code verification** (to analyse whether the conceptual model is correctly implemented in a computerised model, estimation of numerical error);
- **model validatio**n (comparison with experimental data, including statistical analysis);
- **user-oriented assessment** (includes documentation of the code and good practice guidelines).

The above steps of model evaluation have been further elaborated for the purposes of quality assurance of microscale meteorological models and for the purposes of evaluation of meteorological and air pollution mesoscale models.

5.2.3 EU COST 732: description of model evaluation

The Model Evaluation Guidance and Protocol Document (Britter and Schatzmann, 2007), related to microscale meteorological models, adopts five distinct elements. These are:

- scientific evaluation
- verification
- validation datasets
- model validation
- an operational user evaluation that reflects the needs and responsibilities of the model user.

The document provides step-by-step guidance for model evaluation, addressing both computational fluid dynamics (CFD) and non-CFD models (flow and/or dispersion) in a uniform manner whenever possible. The protocol highlights the importance of the model validation procedures and validation datasets. Following the recommendations, model evaluation exercises have been carried out as a basis for more detailed guidance on model evaluation approaches. The results are published on the COST 732 page (COST 732, 2011).

5.2.4 EU COST 728: description of model evaluation

The proposed model evaluation protocol for mesoscale meteorological models comprises three groups that summarise the key elements (Schluenzen and Sokhi, 2008). These are:

- general evaluation (includes model description and user oriented assessment);
- scientific evaluation (also includes database description);
- benchmark test (includes code verification and code validation).

These three elements are oriented towards the model developer, and the results should be summarised in a formalised evaluation protocol. A second part of the evaluation is the process of **operational user evaluation**. It is to be applied by model users and also includes checks for plausibility of model results, and when possible, quantitative comparison with results from other models and/or measurements. The results should be summarised in a good practice guideline.

5.2.5 GLOREAM: description of model evaluation

The model evaluation for regional scales adopted in the framework of the 'Global and regional atmospheric modelling' (GLOREAM) project (Builtjes et al., 2003) includes three different elements:

- a strategy protocol;
- a core activity of model runs;
- decision criteria for the success or failure of the model (defined prior to the model runs).

The strategy protocol is based on agreement with respect to target parameters (meteorological quantities or pollutant concentrations). It includes model quality objectives (MQOs), selected statistical indices, model documentation and other details of the performance tests.

5.2.6 Other aspects of model evaluation

Three other aspects are often considered relevant or necessary for model evaluation. These are uncertainty analysis, sensitivity analysis and model intercomparisons.

- **Uncertainty analysis** is the process for characterising the model uncertainty. According to Builtjes et al. (2007), uncertainty analysis should and will play a key role in presenting

model results. Special attention should be paid also to the process of communicating uncertainties, especially for decision-making. Uncertainty analysis covers a range of activities, including model intercomparison and sensitivity analysis. More details are given in Section 5.3.
- **Sensitivity analysis** is a process for understanding how a given model depends upon the information fed into it. Sensitivity testing can be performed with respect to models' chemistry/physics parameters or with respect to input data (emission, meteorology). The aim of sensitivity analysis is twofold. It can be used to propagate uncertainty in input parameters for uncertainty assessment and to assess the dynamic response of the model to changes in input data for which evaluation may also be necessary. Methods for sensitivity analysis are explained in Saltelli et al. (2005), for example.
- **Model intercomparison** is the process for assessing a model performance by simultaneous comparison of modelling results provided by different models for the chosen situation. The differences in model results can reveal the strengths and weaknesses of particular modules or parameterisation schemes, and can help to characterise conceptual uncertainties arising from the choice and implementation of the physical models applied.

5.3 The concept of model uncertainty

Models are simplifications of reality, and therefore always have some uncertainty associated with their application. The term uncertainty refers to a lack of knowledge or information on the models, parameters, constants, input data and beliefs/concepts (US EPA, 2009).

The **total model** uncertainty may be defined by the sum of three components (e.g. Borrego, 2003a and 2008; Chang and Hanna, 2004), shown below.

- **Model uncertainty:** associated with model formulation. May be due to erroneous or incomplete representation of the atmospheric dynamics and chemistry, numerical solutions, choice of modelling domain and grid structure.
- **Input data uncertainty:** related to emissions, observational data (accuracy and representativeness), meteorology, chemistry and model resolution.
- **Inherent variability:** due to random turbulence. This refers to stochastic and anthropogenic processes that by nature are not known. Applicable to short time scales (e.g. 1 hour).

It may be possible to reduce the first component (model uncertainty) by introducing more physically realistic and computationally efficient algorithms. The effect of input data errors may also be reduced to some extent by using more accurate measurements at representative locations, or improving the quality of emission inventories. However, the stochastic fluctuations are inherent for atmospheric processes and cannot be eliminated. Because of the effects of uncertainty and its inherent randomness, it is not possible for an air quality model to ever be 'perfect'. Thus, information on the total model uncertainty, for models supporting decision-making, is essential and it is as important as the modelling results themselves (Borrego et al., 2008).

Methods for assessing model uncertainty are varied and include some of the normal model evaluation methods where statistical parameters are assessed by comparison with observations. However, there are also other methods available for assessing model uncertainty. Over the past two decades, such methods have been developed to access uncertainty in meteorology, emissions, Gaussian regulatory models, photochemical air quality models and more complex chemical transport models (e.g. Irwin et al., 1987; Lumbreras et al., 2009; Sax and Isakov, 2003; Hanna et al., 2001). A comprehensive review of uncertainty and sensitivity methods as they are applied to atmospheric transport and dispersion models is given by Hanna (2007).

One approach to estimating uncertainty is based on Monte Carlo techniques; however, other statistical methods can be also applied: the maximum likelihood estimation technique (Koračin et al., 2007); the Taylor series approach (Yegnan et al., 2002); or ensemble modelling (Galmarini et al., 2004b, c; Vautard et al., 2008). The contribution of the different components to the total model uncertainty can be investigated through sensitivity analysis (input data), sensitivity analysis and/or model intercomparison (model uncertainty) and spectral analysis (stochastic variations). Some of the main methods available for assessing model uncertainty are summarised in Box 5.1.

A state-of-the-art review on uncertainty methodologies and on the impact of meteorological and air quality data input on modelled concentrations was presented by Miranda et al. (2008b). It also includes the uncertainty estimation of various input parameters (measured and modelled) as provided by some experts.

Recommendations for model uncertainty estimation were given in the Framework of the Air4EU project

(Builtjes et al., 2006; Borrego et al., 2008, Air4EU, 2006). It was recommended in that project to present a qualitative (e.g. graphical representation of time series and scatter plots), as well as quantitative (e.g. statistical) analysis of model results against measured values from the air quality network. Depending on the purpose of the model application, three levels of different complexity for estimating the total model uncertainty have been proposed by Borrego et al. (2008).

- The first level includes simple graphical analysis.
- The second level is based on statistical parameters.
- The third one is more comprehensive, detailing the total model uncertainty and the contribution of different components.

Box 5.1 Main methods available for assessing model uncertainty

1. **Monte Carlo analysis** is a commonly used method to determine model uncertainty based on uncertainties in model input variables (input data or model parameters). In this approach, a given model is run many times, using random simultaneous variations in a set of input variables. The model outputs, often presented in terms of probability distribution functions (PDFs) are then subjected to statistical analysis. There are a number of variations of the method. In its simplest form, the uncertainty in the input parameters is propagated through the model to determine the resulting model uncertainty based on these input parameters. When combined with observations, e.g. with the use of Monte Carlo Markov Chain methods, it can be used to provide estimates of the uncertainty in the input parameters themselves. The approach is computationally extensive, especially for complex modelling applications, and the number of ensembles used is generally very low (< 100). More efficient methods for sampling other than random selection are necessary for implementing the method.
2. **Sensitivity analysis** is used to estimate the variations in a model output caused by slight variations in a model input. It is most useful for modelling systems that are linear and that do not have complicated inter-correlations between various inputs (Borrego et al., 2008; Napelenok et al., 2008). In the case of near-linear sensitivities, this can be combined with Taylor series approaches to provide model uncertainty estimates based on uncertainties in the model input parameters. A particular form of sensitivity analysis is process-oriented sensitivity analysis, where a specific chemical or physical process is studied rather than a specific input variable.
3. **An ensemble of models** can be used to indicate uncertainty, not just in input parameters, as in the Monte Carlo approach, but also in the model formulation. The ensemble of different model outputs commprise different models (multi-model ensemble), different initial and boundary conditions, and/or different model physics modules. Although, in principle, an ensemble of models could be included in any Monte Carlo analysis, for practical reasons model ensembles are generally limited to the collection and statistical analysis of model output from a limited set of different models. The median and other percentiles of the distribution of the predictions of different models is then compared in relation to observations. The approach is rapidly growing in popularity among air quality modellers, (Galmarini et al., 2004b, c; Vautard et al., 2008; Rouïl, 2011).
4. **Model intercomparisons** and model ensembles are generally similar in the sense that they require output from multiple models. Model intercomparisons, however, are intended to assess not just the uncertainty, but also the reasons for the variability between models.
5. **Statistical analysis using observations** is the most common method for determining model uncertainty. Model output is compared directly to observations, statistically assessed using a number of metrics, and statements concerning the quality of the model are provided. In many ways, this follows the methodologies linked to validation but the aim of the assessment is intended to provide information on how uncertain a model is in regard to the observations. For this reason, particular metrics are preferred, such as BIAS, RMSE and SD (see Section 5.4.1) that reflect the PDFs of the model results. This method will then include not just model uncertainties but also monitoring, representativeness and stochastic uncertainties. The total model uncertainty is generally assessed in this way, but methods can be applied (e.g. Koračin et al., 2007) that attempt to distinguish between the different model uncertainties.

5.4 Model quality indicators (MQIs)

5.4.1 Quantitative indicators (statistical metrics)

When applying statistical analysis to evaluate model performance, different parameters are used to quantify how well the model fits the observations. These parameters are usually called statistical metrics (indices), or model quality indicators. The latter term is more generic since in some cases qualitative characteristics, such as representativeness, completeness and expert assessment, can also be used. Most air quality model evaluations rely on the comparison of paired data of modelled and observed concentrations (varied in time at a fixed location, across space for a given time, or both). However, for some statistical analyses pairing is not required as it is the statistical characteristics of the model that are being compared with the observations. This typically involves parameters related to the frequency (probability) distributions of the model, e.g. percentile values or standard deviations.

Widely used statistical metrics include the mean observed and modelled values, the standard deviations (SDs), the mean normalised bias (MNB), the mean normalised error (MNE), the fractional bias (FB), the root-mean-square error (RMSE), the index of agreement (IA) and the correlation coefficient (R). For a more detailed discussion, see Chang and Hanna (2004) or Canepa and Irwin (2005). It is generally accepted that no single statistical indicator is comprehensive enough to access model performance. Depending on the type of model application, a set of statistical parameters can be defined as more relevant. For example, the US EPA quality indicators for modelling maximum one-hour averaged ozone concentrations include three metrics: normalised accuracy of domain-wide maximum one-hour concentration unpaired in space and time, mean normalised bias of all predicted and observed concentration pairs with concentrations above 60 ppb, and mean normalised gross error of all predicted and observed concentration pairs with concentrations above 60 ppb (US EPA, 1996). As another example, the Unified EMEP Model, developed in order to support regional and transboundary air pollution strategies in Europe at spatial scales from 100 km^2 to 1000 km^2, generally assesses the mean observed and modelled bias as well as the daily mean RMSE and correlation coefficient (Unified EMEP model, 2011; EMEP, 2008a and 2008b).

According to Borrego et al. (2008), every statistical parameter plays a role in the evaluation of model performance and uncertainty estimation, but some of them can be considered more important. The following quality indicators are recommended by Borrego et al. (2008):

- correlation coefficient (R)
- fractional bias (FB)
- root mean square error (RMSE)
- normalised mean square error (NMSE).

A collection of model quality indicators currently used for evaluation of meteorological parameters and concentrations, together with examples of their application is presented in the joint report of COST Action 728 and WMO-GURME (Schluenzen and Sokhi, 2008). These model quality indicators are defined in Annex 2 of this document.

5.4.2 Qualitative analysis (graphical depiction)

While statistical metrics provide quantifiable and comparable results, it is well known to air quality modellers that quantitative indicators alone do not provide a conceptual understanding of how the model is performing. For this reason, qualitative analysis, also referred to as exploratory data analysis, is indispensable. Such an analysis may reveal shortcomings in input data, model setups or model descriptions (see, for example, the COST 732 report on model evaluation case studies (COST 732, 2009)). For this reason, visual aids are necessary and these can provide insight into model performance that can further be assessed in quantifiable ways.

Some of the most widely used graphical depictions in air quality model evaluation include the following.

- **Scatter plots:** paired in time (modelled versus observed) values are plotted against each other in a two-dimensional plot. This is a classical approach and provides a visualisation of the model-observed probability distribution (density of points indicating high frequency). This is often used in conjunction with linear regression and its related metrics, as a quantitative indicator.
- **Quantile-quantile plots:** unpaired in time and separately ranked (modelled v observed) values plotted against each other in two-dimensional space (see, for example, Figure 3.1). A straight line with a 1:1 ratio indicates a shared statistical distribution. These can be used to indicate percentiles and deviations of percentiles.
- **Box and whisker plots:** these can be used to represent some of the statistical characteristics of binned datasets, e.g. when plotting accumulated diurnal or monthly datasets.

- **Residual plots:** usually show the ratio of modelled to observed values, as functions of various physical parameters (Hanna et al., 2003), e.g. the ratio of modelled to observed concentrations as functions of wind speed, mixing height or stability class. Box symbols may be useful when the number of each data bin is large.
- **Stacked bar plot or pie chart:** these are often used to show the proportional distribution, e.g. the chemical speciation of PM, of some value.
- **Soccer goal plot:** displays the mean fractional bias and mean fractional error; used mainly in evaluation studies (Morris et al., 2005).
- **Time series plot:** sequential in time plots of concentrations, model error, etc. Visualisation of time series is important to understanding the prognostic nature of the model paired in time.
- **Taylor diagram:** combines correlation and model error in a single plot applied in model intercomparisons (Taylor, 2001; Vautard et al., 2007; Venkatram, 2008).

Depending on such factors as the range and amount of data, as well as the information to be conveyed, a combination of plots is usually necessary.

5.4.3 Software for statistical model evaluation

Different software packages have been developed and applied for model performance evaluation over the past decades. The following are some of the best-known ones.

1. **BOOT software** (Chang and Hanna, 2005) — statistical package for evaluation of dispersion models. It is part of the Model Validation Kit (Olesen, 1995 and 2005), widely used in the past decade in the framework of the initiative 'Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes' (HARMO, 2011). Along with statistical metrics, there is a possibility for graphical plots as 'exploratory data analyses'. The last update of the package is dated 2007 with the addition of a new parameter — the hit rate, useful for assessing wind vector data.
2. **ASTM Guidance** — ASTM is the US Standard Guide for Statistical Evaluation of Atmospheric Dispersion Model Performance (ASTM, 2000). This procedure implements the idea that the distributions of model predictions and observations 'share' certain fundamental properties, but are inherently different. The fundamental premise is that model results and observations should not be compared directly, and that observations should be properly averaged before comparison (Canepa and Irwin, 2005). The comparison takes places within different regimes, which can be defined according to atmospheric stability, for example. The ASTM package, prepared by J. Irwin and distributed through the HARMO (2011) webpage is designed to assess the performance of transport and diffusion models to simulate the average 'centre-line' concentration values from a point source release (short-range dispersion).
3. **AMET** — the Atmospheric Model Evaluation Tool, developed recently for the US EPA to facilitate the analysis and evaluation of meteorological and air quality models (Gilliam et al., 2005). Currently it is designed to analyse MM5, WRF, CMAQ and CAMx model outputs (i.e. specific output formats of models used in the United States). It includes various statistics along with a number of plots (scatter, box, spatial, time series plots, stacked bar plot, etc.). For meteorological data, it offers the possibility for comparison with data from wind profiler, radio-soundings or aircrafts.
4. **JRC Tool** — In order to facilitate the intercomparison of model results, JRC-IES (Ispra, Italy) has developed an IDL-based visualisation tool that allows for working interactively and offline on the results. Different versions of the tool have been developed for the CityDelta (2011; urban scale), the EuroDelta (2011; regional scale), the POMI (2011, Po-Valley Modelling Inter-comparison Exercise) projects, and under the Task Force on Hemispheric Transport of Air Pollution (HTAP, 2011; global scale). In general, the tool contains a module for validation, a 'Delta' module for the visualisation of the impact of emission reductions, and a module for the visualisation of monthly averaged plane data in both longitude-latitude projection and the EMEP-specific projection. A large number of variables and indicators are available, including:
   (a) variables: meteorological variables, gas-phase species and indicators, aerosol-phase species, wet and dry deposition quantities;
   (b) statistical metrics: mean values, bias, maximum, minimum and standard deviation, correlation coefficient, RMSE, exceedance days;
   (c) graphical depiction: time series, scatter plots, q-q diagrams, frequency analysis, Taylor diagrams, etc.

5.4.4 Conclusions and recommendations on model quality indicators

The experience gained with the application of model quality indicators (MQIs) in different studies has resulted in the following conclusions/ recommendations.

- The selection of the most appropriate MQI depends on model application and purpose.
- The type of selected quantitative statistical metrics depends also on available observations.
- MQIs for concentrations should be air-pollutant-specific and scale-specific, both on the temporal and spatial level.
- The spatial representativeness of both models and observations must be considered when defining MQIs, since observations are point samples whilst modelling results are usually spatial means.
- Visual inspection of the data (exploratory data analysis) should always be carried out prior to applying statistical software, to identify obvious biases and outliers (quick scan on time series, concentration maps)
- Statistical measures provide limited information on model weakness and cannot identify whether the modelled concentrations are correct for the right or wrong reason, i.e. whether the model is capable of capturing the relevant chemical/physical processes. For this reason, statistical analysis is a necessary criterion for model evaluation, but it is not sufficient; it should be supplemented by evaluation studies on different modelling processes (diagnostic and dynamic evaluation, Hogrefe et al., 2008).

5.5 Existing model evaluation documentation and datasets

Documentation is a main issue in the context of quality assurance; it should cover the following aspects:

- description of the quality assurance procedure itself (e.g. evaluation protocol);
- description of the model, both conceptual formulation and numerical implementation;
- description of the required input data and its formatting;
- description of the validation methods applied and the validation dataset;
- an analysis of the validation carried out;
- an analysis of uncertainties (of both individual elements and of the overall system)

Model validation is one of the reporting points in the AQ MDS (Model Documentation System) (EEA, 2011b). The system includes short and long descriptions on more than 120 individual models, their application areas and their status with respect to evaluation and validation. Thus, a user may obtain an overview of the existing models for a specified application. A survey on the evaluation and the functionality of the MDS has demonstrated that users want quantitative information on model uncertainty to be included in the MDS and put emphasis on the necessity for a quality assessment and quality control of the models, following well-defined and harmonised methodologies, that will be valid for all models and model categories (Moussiopoulos et al., 2000a).

The web-based COST 728/732 model inventory (COST 728/732, 2011) provides detailed information on model capabilities, including model validation/evaluation studies according to the following four categories: analytic solutions, evaluated reference dataset, model intercomparison, and additional validation and evaluation efforts. The inventory includes models for the microscale (local street and building level), the mesoscale (urban-regional models) and the macroscale (regional-global); it covers both meteorological and chemical transport models.

A **metadatabase** has been compiled in COST 728 for the purposes of mesoscale model evaluation (Douros et al., 2008). It includes information on available well-documented air quality and meteorological datasets. More on available datasets for model validation can be found in the publication mentioned above.

5.6 Special topics

5.6.1 Evaluation of different modules of the air quality model

Air Quality models are complex systems based on different modules — for calculating emissions, meteorological parameters, transport and dispersion, chemistry and deposition. Meteorological predictions and emission inventories are critical components for the performance of the models. Evaluating the different components of the AQ model is believed to be as relevant as evaluating the full model, since the linkage between the modules has implications for accessing uncertainty. The EPA Guidance (US EPA, 2009) states that each component must be evaluated.

General guidance on QA/QC and uncertainties in constructing an emission inventory is given in the *EMEP/EEA Emission Inventory Guidebook* (EMEP/EEA, 2009). Emission inventories are typically based on a certain amount of assumptions, best guesses and engineers' judgements. To evaluate these estimates, different approaches can be applied: alternative emission assessment, examining the trends in ambient air concentration, inverse modelling and receptor modelling (source apportionment) (Friedrich and Reis, 2004; Pulles and Builtjes, 1998).

In the Amreican framework for model evaluation, the influence of emissions and meteorology on modelled concentrations is studied in the so-called diagnostic evaluation (Dennis et al., 2009). In Europe, the activities of COST Action 728 (COST 728, 2011) have focused on improving meteorological mesoscale models used in atmospheric pollution dispersion studies and on providing methodologies and tools for their evaluation (Schluenzen and Sokhi, 2008).

Evaluation is also needed for the interface that links meteorological output to air quality models. The interface is often used in offline AQ systems, since most meteorological models are not built for air quality simulations and further data elaboration is needed to provide the complete set of parameters required for the air quality model and to adapt the data formats and model projections (Finardi et al., 2005; Baklanov et al., 2007).

Another interface module to be evaluated is related to nested (multiscale) models. Nested models are commonly applied for the study of air quality problems in urban areas. A proper nesting of fine-scale simulations into larger scale simulations is managed by an interface module that has to match grid and resolution differences and possibly different chemical schemes employed in the models. Thus, uncertainties arising from scale interactions also need to be evaluated (Borrego and Gauss, 2007).

5.6.2 *Evaluation of air quality forecast models*

Air quality forecasting, or chemical weather prediction as it is sometimes called, is an area under considerable development and is highly relevant for applications within the AQ Directive. However, the evaluation of forecasts may be different to those for other air quality models. Different metrics related to weather forecasting quality assurance may be more relevant than standard metrics used for the assessment of past-time or near real-time AQ. Currently, the COST action ES0602, Chemical Weather (COST 602, 2011), is investigating aspects of quality assurance including QA tools, methods, criteria, experience and QA requirements for measurement data.

5.6.3 *Evaluation in the case of data assimilation*

Agreement between model solutions and observations can be increased by data assimilation techniques that force model solutions to be more consistent with observations. Data assimilation defines a new atmospheric state by making a weighted average of the observed and modelled state in an intelligent and statistically sound way. Hence, if a model value is more uncertain than an observed value, more weight will be put on the observation, and the assimilated value will tend to get closer to the observed value, and vice versa. However, such techniques have to be carefully applied, particularly in developing the data insertion strategy that controls when and where the observations are assimilated or how strongly they affect the solutions (Amicarelli et al., 2008). Data assimilation may be used for initialising atmospheric states prior to forecasting, or may also be used for AQ assessment purposes (e.g. MACC, 2011).

In the case of assessment, the inclusion of observations in the data assimilation process necessitates the need for validation to be carried out in a different manner than is typical for normal model validation exercises. This is generally achieved through either cross-validation methods (e.g. Horálek et al., 2007), where the assimilation procedure is run a multiple number of times with the exclusion of a different station for each of the runs, or through the separation of the monitoring data into assimilation and validation datasets (e.g. Denby et al., 2008).

Assimilation experiments with the chemical transport model LOTOS-EUROS and their evaluation against independent observations contained in the European air quality database AirBase (EEA, 2011c) demonstrate that assimilation significantly reduces the average residual and RMSE between model and observation for ozone, whereas the annual average is not affected as much (Schaap and Builtjes, 2006). The success of an assimilation experiment is determined by the quality of the input data, the model uncertainty and the correct implementation of the assimilation procedure. Recommendations on data assimilation, based on Air4EU activities (Denby et al., 2007) state as a basic requirement that:

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

5.6.4 *Representativeness of data for model validation*

When comparing monitored to modelled data it is important that both the spatial and temporal representativeness of the two datasets match as closely as possible. Representativeness errors arise when comparing point observations with gridded model averages. Concentrations measured at monitoring sites can differ substantially from average concentrations in the area if pollutant concentration gradients are high. For example, a gridded air quality model with 2 km^2 model resolution cannot be compared to a roadside monitoring site, since the monitoring site represents very local concentrations and not the average concentration over several square kilometres. Therefore, model performance evaluated by comparing between point observations and volume-averaged simulations may not represent how well the model actually simulates air pollution dynamics.

As outlined in Air4EU (2011), this kind of small-scale variation may be several times larger than the pure observation (i.e. instrumentation) error, even for grid cells as small as 1 x 1 km^2. Attention should be paid to the definition of stations' representativeness, specific for different pollutants, and the methodologies to assess it.

Stern and Flemming (2004) have investigated the impact of spatial variability within model grids for model validation. Spangl et al. (2007) have assessed the representativeness and classification of stations. The Air4EU report, 'Representativeness of model outputs and monitoring data' (Air4EU, 2006) also discusses the question of representativeness for both model and monitoring applications.

5.7 Recommendations on the framework for model quality assurance

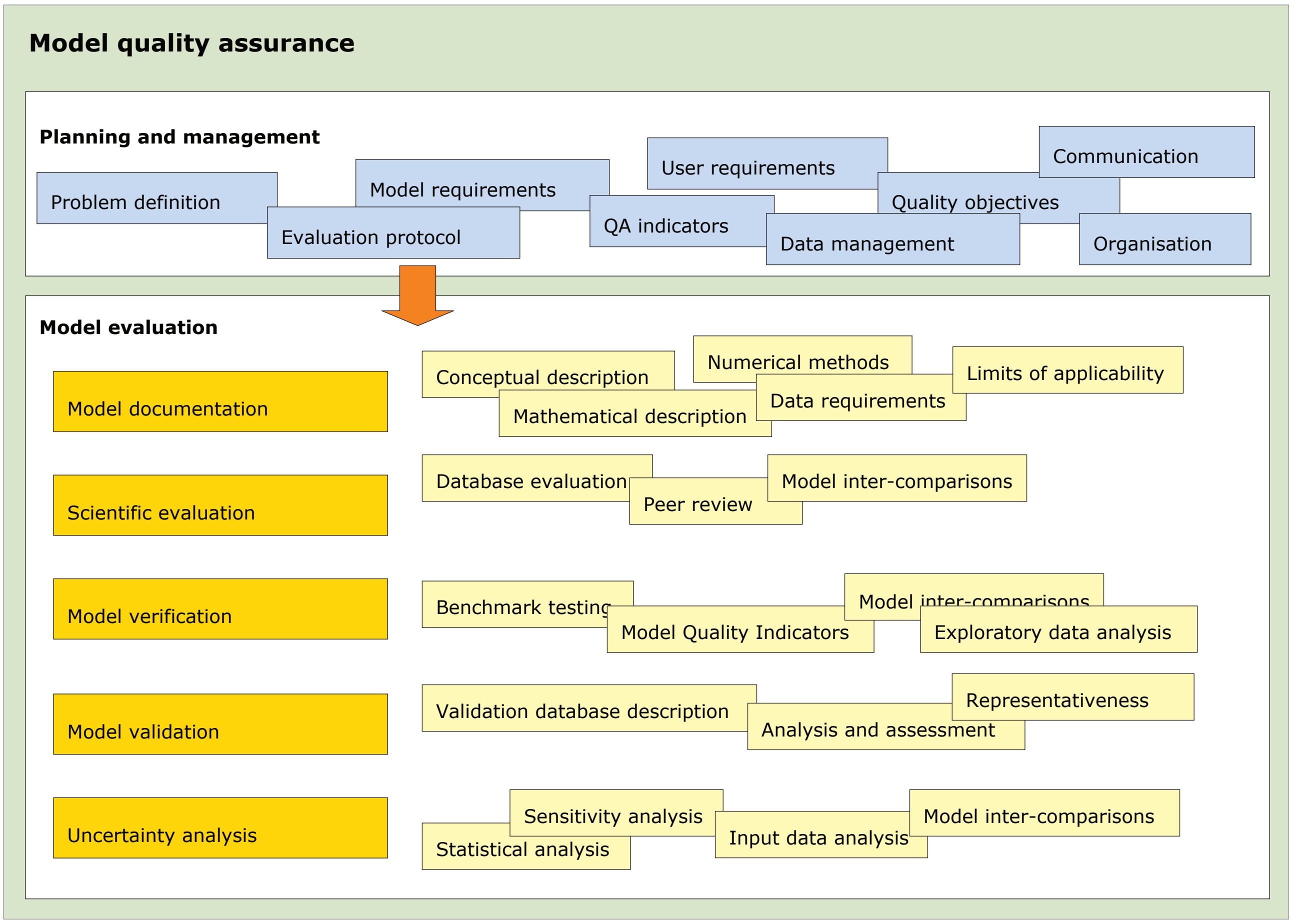
Although there are a range of methods outlined in the literature, they all share a number of common aspects. In this section, we summarise and provide preliminary recommendations on the structure and components of model quality assurance. Experience has shown that the process of model evaluation is intrinsically difficult. Olesen (2001) has listed the problems involved in a structured manner and highlighted the importance of input datasets and of model uncertainty. It is worth noting again that the level of model evaluation depends on the application and the user need. In this regard, even in the AQ Directive, the quality objectives will differ depending on the application, and the resulting methodologies for quality assurance will also necessarily differ.

It is recommended that the following general points should be kept in mind when developing protocols for model evaluation.

- The structure of the evaluation protocol should be common for all scales, but the details in the protocol should be scale specific, target/pollutant specific and application specific.
- The model evaluation protocol should be built upon a broad consensus among the various interested parties relevant to its correctness and suitability. It should be open and easily accessible.
- The datasets needed for model evaluation will differ for the different scales.
- Model evaluation should focus not only on final concentration levels, but also on the different modules (emission and meteorology) relevant for simulation of concentrations.
- A sensitivity analysis, an uncertainty analysis and a model intercomparison should be embedded in the model evaluation process.
- A broadly based model evaluation should be well planned, since the application of evaluation protocols and analysis of the model performance is expensive in terms of computing and labour resources.

In Figure 5.1, many of the elements of quality assurance and model evaluation are visualised. A number of aspects need to be defined in the planning phase, for example the problem definitions and user requirements before model evaluation can be undertaken. These aspects do not necessarily need to be detailed, but they should be known. It may not be necessary or practical, depending on the needs of the application, to address all these elements in the model evaluation. Some methods are common for the different evaluation elements, e.g. model intercomparisons can be used for scientific evaluation, model verification and also uncertainty analysis. The role of the validation database is also important in both model validation and in uncertainty analysis. This schematic outline will be further developed and implemented with Fairmode's continued activities.

Figure 5.1 Visualisation of the different elements involved in model quality assurance



6 Application of models for air quality assessment

This chapter provides an overview of the use of models for assessment purposes and provides a number of examples relevant to the AQ Directive. Other documents, such as the Air4EU reviews of assessment methods (Air4EU, 2011: deliverables D3.1, D4.1 and D5.1) and results from the SATURN project (Moussiopoulos, 2003) also provide background information on assessment methods and examples of AQ assessment. We summarise some of these activities and present a number of more recent examples representing 'good practice' in the use of models for air quality assessment.

6.1 General background and scope

Any air quality assessment using models involves the following main steps:

- screening and identification of likely sources and causes of poor air quality;
- establishment of emission inventories and modelling tools;
- validation and assessment (e.g. source apportionment) of the models and inventories;
- iteration and improvement of the modelling system.

Before such modelling assessment can be carried out, the following data and tools are generally required:

- air quality monitoring data for validation or assimilation;
- meteorological monitoring data for validation, model input parameters for use with diagnostic wind field models;
- emissions inventory;
- other relevant input data dependent on model type, such as background concentrations, land use or traffic data;
- modelling tools for carrying out the assessment (i.e. the air quality model and meteorology);
- analysis tools for validation and assessment.

There are a number of different aims for air quality assessments; this chapter explores the following three:

- assessment for the purpose of reporting exceedances of the AQ Directive or national limit values;
- assessment for the purpose of calculating population exposure and health impacts;
- assessment for identifying source contributions (source apportionment).

Often more than one aim is fulfilled in any given assessment. For instance, any modelling assessment activity that includes emissions from a variety of sources can also be used for source apportionment studies. Any modelling activity looking at AQ Directive limit values can also provide results on national limit values, for example. Indeed, the AQ Directive (see Section 4.1.2) requires both an assessment of exceedances and of the population exposed to these. Since the applications overlap extensively, we have divided the assessments methodologically into assessments where only modelling is used for the reporting (but based on model validation), and assessments where both modelling and monitoring are combined, either through some form of integrated assessment or through data assimilation methods.

Other applications, such as planning and forecasting, are different in aim to these types of assessments, but the tools and much of the methodology are quite similar. For most applications of planning, the model will simply carry out the same calculations as for assessment, but will do so using different emissions. The major difference between planning/forecasting and assessment applications is that, in the case of planning, they predict air quality forward in time, when monitoring data are not available for validation. Applications for planning and forecasting are dealt with separately in Chapter 7 and Section 8.2 of this document, respectively.

The possibility for reporting assessments in the questionnaire is quite limited (see Section 4.1.2) but the AQ Directive requests (Annex I, Section B) a significant amount of information concerning the modelling method. Member States are expected to include documents or links to documents that can provide this information.

6.2 Assessment using models only

Under certain conditions, i.e. when concentrations are below the lower assessment threshold value (Article 6), models alone may be used for assessment. The reality of most reporting in regard to the AQ Directive is, however, that modelling is rarely undertaken in a zone if there are no exceedances. However, there are a range of models that can be used to provide the quality required for assessment.

It is important to note that the application of models when no monitoring data are available should require that the model is validated under similar conditions to those that it is being applied. Though a model may be 'fit for purpose' under one set of conditions and for one particular application, it may be less adequate for another. Though this generally holds true for all modelling, it is of particular importance where there are no monitoring data available to validate the model calculations. An example of where modelling has been applied is provided via the Fairmode website (Fairmode, 2011b; Example 1.1.6). In this case, modelling has been used for CO levels in the United Kingdom because concentrations of this pollutant have persistently been below the lower assessment threshold.

6.3 Integrated assessment using monitoring and modelling

For situations where exceedances are above the lower threshold limit (Article 6), models may be used in combination with monitoring data or, for cases where exceedances are above the upper threshold value, models may be used to supplement monitoring data. There are no clear definitions of what supplement or combine mean. However, 'supplement' is interpreted to mean that modelling is secondary to the monitoring and that 'combined' gives a similar or optimal weight to both the modelling results and the monitoring.

Many modelling applications will use monitoring data for validation purposes. Given that the model is performing within the required quality objectives, the model results can be used in the assessment to fill in the geographical area not covered by measurement data. There is no direct interaction or combination of the monitoring and modelling data, and the modelling results can be considered supplementary in order to provide, for instance, estimates of population exposure.

A number of examples of the assessments mentioned above have been reported to the European Commission. Some of these are described on the Fairmode website (Fairmode, 2011b: Example 1.1). For instance, Copenhagen, Denmark uses an integrated approach to assessment (Example 1.1.1) where both models and monitoring are presented together, and the models are used to extend the geographical coverage of the assessment. Oslo, Norway (Example 1.1.2) uses models to support the monitoring data, making use of these to calculate population exposure above limit values. Long-term assessment of air pollution in Portugal has been carried out using modelling at 10 x 10 km^2, taking into consideration the AQ Directive limit values (Monteiro et al., 2005 and 2007). Results of the modelling exercise were reported to the Portuguese Environment Agency aiming at a first overview of the air quality levels across Portugal.

6.4 Combining monitoring and modelling data

When model and monitoring data, or any other dataset, are combined to provide improved spatial concentration fields, these methods are often referred to as 'data fusion' or 'data assimilation'. Methods that combine various data sources, without directly considering one or the other to necessarily be primary, are often referred to as 'data fusion' or 'data integration' methods. They take any number of datasets and combine these in a range of ways, either through geometric means or based on statistical optimisation methods. For example, it is possible to fuse interpolated monitoring data, satellite data and air quality modelling data into a single integrated map (e.g. Sarigiannis et al., 2004 and Kassteele et al., 2006). The fusing often takes the form of a weighted linear combination of the different data sources, with the weighting being dependent on the estimated uncertainty of each of the sources.

One of the most straightforward methods that can be applied to combine monitoring and modelling data is multiple linear regression, where model concentrations as well as other supplementary data are fitted to the available observations using least squares optimisation (e.g. Horálek et al. (2007); see also Examples 1.1.4 and 1.1.5 in Fairmode (2011b)). Though this provides an unbiased model field, there may still be significant deviations from the observations. This deviation may be accounted for by using residual interpolation of the deviations. In this way, the model field provides the basis for the concentration map and the residual deviations are accounted for by using interpolation methods (e.g. Horálek et al. (2007), Kassteele et al. (2007), Hogrefe et al. (2009), Stedman (2005 and 2007)). Although these methods have been shown to be effective when compared to methods using data assimilation (Denby et al., 2008), they are not confined by any physical or chemical constraints, but rather by statistical ones.

'Data assimilation' methods, on the other hand, are more physically consistent. The methods refer to a modelling technique that incorporates monitoring data directly into air quality model calculations during the modelling process itself (see also Section 5.6.3). It is the measured data that helps guide the model towards an optimal solution, one that is consistent with the physical description provided by the air quality model. The most common type of data assimilation methods applied are variational methods (Elbern et al., 1999), already used extensively in meteorological forecasting, but other methods such as ensemble Kalman filters (van Loon et al., 2000) may also be applied. Data assimilation is now used operationally in air quality forecasting (see Section 7.2), and it is also applied for air quality assessment purposes (Denby et al., 2008; Barbu et al., 2009; Rouïl, 2011). Data assimilation in these forms is most often applied on the regional scale and rarely applied on the urban scale, due to the complexities of the urban environment and the large variability and gradients in emissions.

6.5 Source apportionment using models

Source apportionment is relevant for the AQ Directive in a number of ways, but the major aspect is related to planning. Before any effective mitigation strategy can be undertaken, knowledge of the sources is required. These may include a range of sources within the city or zone, over which the authorities have some form of control (e.g. traffic, heating or industry). It may also include sources outside the zone or outside the country (long-range transport or transboundary air pollution) over which local authorities have no control, but for which international cooperation is required (e.g. the UNECE Convention on Long-range Transboundary Air Pollution (LRTAP Convention)). In this section, we describe modelling methods that are principally aimed at identifying local sources as related to the local assessment of air quality. The contribution of long-range transport is discussed in Section 7.3, as it is more directly related to planning activities. Other special source apportionment topics, e.g. contribution of natural sources and road salt and sand, are discussed in Chapter 8.

Source apportionment studies can make use of both model and monitoring data in order to complement and support the results of both. A range of methods is available, including the following.

- Calculating source contributions from **monitoring** only based on **chemical analysis** and **receptor modelling** (for particulate matter) or by using other statistical assessments of monitoring data, such as wind roses to identify sources. These methods can provide a basic level of information for the larger sources.
- Calculating source contributions based on existing **emission inventories and modelling** alone. This method provides source contributions with the same uncertainty as the models and emission inventories.
- **Inverse modelling**, whereby measured concentrations are coupled to model calculations to infer emission strengths of the contributing sources. This method can provide information on larger sources with the same uncertainty as the models.

The most commonly applied source apportionment method is where models alone are used for the source contribution, and are validated with available information. However, it is essential to keep in mind that any such assessment is dependent on the quality of the model applied and the uncertainty of the emission inventories used. For this reason, it is always recommended to validate the model, wherever possible, for individual source contributions. For the case of particulate matter, this can be achieved to some extent through chemical analysis and receptor modelling, which is a statistical method for attributing chemical profiles (inferring sources) from a time series of chemical analysis data. However, for gaseous pollutants, such as O_3 and NO_2, this is not possible, and sensible conclusions must be drawn from the total concentrations.

6.5.1 Source contributions using models

Assessing source contributions based on modelling is a straightforward application of air quality models. The results of such studies are often included in assessments and action plans submitted to the European Commission. For most applications, source apportionment is carried out in sectors (e.g. traffic or industry) or sub-sectors (e.g. diesel heavy duty or diesel light duty). When the pollutants involved are considered to be non-reactive, source contributions can be determined by separate model runs of the individual sources. However, for chemically reactive species, the source contributions must be defined by making model runs with the full emission inventory and removing each individual source of interest, or some fraction of them, for each run. Note that for non-linear species, the source contributions assessed in this way do not add up to the total contributions when all sources are used. In either case, the number of model runs required is equivalent to the number of sources that are to be assessed.

Many examples of such calculations are available and are used as background information for reporting assessments, making air quality plans or supporting requests for postponement or exemptions if limit values are exceeded. Some examples are provided via the Fairmode website (Fairmode, 2011b; Examples are found under 1.2).

Complex pollutants involving non-linearity and transformations, such as particulate matter, may require extra attention when determining the source contributions. In the case of multiple sources, requiring a large number of model runs, it can be useful to apply special algorithms within the model to assess the source contributions to PM. An example of this is given in Bedogni et al. (2008) who have applied the CAMx model to the Milan region to assess the source contributions of local and regional sources to $PM_{2.5}$ concentrations (Fairmode, 2011b; Example 1.2.7). They use the PSAT algorithm for the source apportionment; this provides an effective method for modelling source apportionment when a large number of sources is used.

6.5.2 *Inverse modelling for assessing emission inventories*

There may be significant uncertainties in emission inventories used in air quality modelling, either due to lack of information on activity rates or to poorly determined emission factors. Typical examples of uncertain sources for particulate matter are fugitive emissions from industrial or agricultural sources, wind-blown dust, non-exhaust traffic emissions or home heating through wood or coal burning. In such cases, effort must be made to quantify these sources more accurately. To do so, inverse modelling methods can be applied, where air quality models are coupled to measured concentrations to infer emission strengths. In the simplest case, where it is known that only one type of source is contributing and the position of the source is well known, inverse modelling is generally a straightforward inversion of concentrations to emissions; this may also be referred to as reverse modelling. However, when multiple sources or non-linear reactions are involved, and if the positions of the emissions are not well defined, then this becomes a more complex issue. Rao (2007) provides an overview of such methods, mostly in regard to regional or global scale modelling where inverse modelling is often applied.

Inverse modelling on the local or urban scale is less frequently applied; a range of methodologies have been used. Basic forms where only one specific source is contributing, e.g. traffic or industry, will simply require a conversion of measured concentrations to emissions using the model. An example of this is Ghenu (2008), who makes use of the OSPM model and traffic and urban background measurements of CO, NO_X and $PM_{2.5}$ to determine the hourly emissions strengths and emission factors in a street canyon in Rouen, France.

When multiple sources are present, but the pollutant is non-reactive, then other basic methodologies may be applied. Examples include the use of multiple linear regression, which Laupsa et al. (2009) used to optimally fit a number of different modelled $PM_{2.5}$ sources in the city of Oslo, Norway. Cosomans and Mensink (2007) also applied a similar method to determine fugitive emissions of PM_{10} from an industrial region in Antwerp, Belgium.

More complex methods can be applied using known data assimilation techniques such as Kalman filters (e.g. Mulholland and Seinfeld (1995)) or variational methods using adjoint equations (e.g. Vautard et al. (2000)). These types of complex methods are closely related to data assimilation methods, since it is often the aim of data assimilation to optimally choose input data, such as emissions, to guide the model towards the observed concentrations. Though many of these methods are complex and require extensive expertise, it is strongly recommended to make independent checks of emission inventories through some form of inverse modelling method, keeping in mind that the quality of the emissions estimate using inverse modelling will not only depend on the quality of the model used but also on how well conditioned the inverse problem is (i.e. how many similar solutions are possible). Uncertainty assessment is an absolute necessity when using inverse modelling methods.

7 Application of models for air quality planning

In addition to assessment, the AQ Directive (2008/50/EC) states (Articles 23, 24 and 25) that when limit or target values are exceeded (plus any relevant margin of tolerance), an air quality action plan is required from the Member States for the effected zone or agglomeration. In regard to O_3 (Article 17), air quality plans are only required 'if appropriate' when the target value is exceeded.

Such plans include longer term **air quality plans** (Article 23), **short-term action plans** in regard to exceedances of alert thresholds (Article 24) and cooperative air quality plans with other Member States when **transboundary air pollution** is seen as the cause of the exceedances (Article 25). These plans are to be reported (Annex XV of the AQ Directive) to the European Commission within two years of the exceedance. The Directive on heavy metals (2004/107/EC) does not explicitly require such plans to be made. Though the use of models is not expressly mentioned in the AQ Directive, it is clear that modelling is an integral part of such planning.

It should be noted that the AQ Directive also mentions (Article 23.2) that these plans should not be carried out independently of other relevant directives, i.e. there should be consistency between the related directives. These include Directive 2001/80/EC on emissions from large combustion plants (EC, 2001a), Directive 2001/81/EC on national emission ceilings for certain pollutants (EC, 2001b) and Directive 2002/49/EC concerning environmental noise (EC, 2002b). In addition to this consistency between directives, there will also be a range of other local planning measures of relevance to the air quality planning. These include aspects such as local traffic planning (e.g. Lutz (2010)), industrial planning, regional development plans, urban planning and environmental health.

The AQ Directive does not require impact assessments or plans to be carried out prior to any changes in emissions, even though it is clearly to the advantage of authorities to do so. Indeed, such impact assessments are required according to the AQ Directive on the assessment of plans and programmes on the environment (EC, 2001c). For the AQ Directive, air quality plans are only required after exceedances have occurred. In this chapter, we focus on examples of air quality plans for improving air quality where the current limit values are being exceeded. In so doing, we provide examples of the role of models in developing **air quality plans**, in implementing **short-term action plans** and in identifying the contribution of **transboundary air pollution** to the local air quality.

7.1 Air quality plans

In regard to the AQ Directive an air quality plan is a plan to reduce the concentrations of pollutants that are in exceedance of the AQ Directive limit or target values. Reductions in pollutant levels are almost exclusively the result of reduced emissions of either the pollutant itself or of its precursors. However, in the sometimes complex and non-linear reactions that occur in atmospheric chemistry, this is not always the case, i.e. a reduction in some pollutants may lead to an increase in others.

As in many aspects of air quality there are various degrees of complexity and it is necessary, as a first step in the planning process, to try to establish the likely cause of the exceedances and the level of modelling required (if any) to deal with it. This can be more easily determined when there is a clear source leading to exceedances, e.g. road traffic or industrial activities, but this can be more complex, as may be the case with $PM_{2.5}$ where a number of sources and processes can contribute to the observed $PM_{2.5}$ concentrations. It is under such situations that modelling becomes an essential tool for developing and accessing air quality plans.

The main steps in any action plans involve the following:

- screening and identification of likely sources and causes of poor air quality;
- establishment of emission inventories and modelling tools;
- validation and assessment (e.g. source apportionment) of the models and inventories;

- identification of possible measures to reduce emissions;
- development of emission reduction scenarios;
- assessment using models of the emission reduction scenarios;
- iteration of the process to determine optimal reduction scenarios, including the feasibility of the emission scenarios.

The first three steps described above are also the same steps required for carrying out any assessment of air quality using models. In this regard, air quality planning is a clear extension of air quality assessment.

The following examples are provided to illustrate methodologies for using models in air quality plans where these plans have been developed to meet the limit and target values as stated in the AQ Directive. For the most part, models are used for the following activities:

- identifying source contributions from within the zone;
- identifying transboundary or long-range source contributions external to the zone;
- calculating changes in concentrations as a result of different emission scenarios;
- calculating the population exposure, and its changes, under different emission scenarios.

One aspect that is important for many local authorities, but that is beyond their control, is the long-range contribution to local air pollution. This is discussed separately in Section 7.3. Some examples of planning applications are provided via the Fairmode website (Examples are found under 1.3) (Fairmode, 2011b).

7.2 Air quality forecasting for alert thresholds, information for the public, and short-term action plans

In Annex XII of the AQ Directive, levels of information and alert thresholds for SO_2, NO_2 and O_3 are provided. The Member States have an obligation to provide information to the public concerning these levels (Annex XVI). Though purely statistical methods may be applied for determining any future realisation of these threshold levels or higher, air quality models are best suited for forecasting air pollution levels at both the regional and urban scales. In addition, Article 24 of the AQ Directive states that short-term action plans are required if there is a risk that alert thresholds, limit values or target values are to be exceeded. Models are suitable tools for assessing the effects of any short-term measures employed to reduce the air pollution or protect the public as well as for predicting, through forecasts and potential risks of exceedance.

There are a number of established air quality forecasting systems for both regional and urban air quality (see Table 9). A number of these, but not all, can be accessed through the PROMOTE web site (PROMOTE, 2011a). On the European scale, both the PROMOTE (2011b) and GEMS (2011) projects provide a feasibility study related to the use of ensemble forecasts for all of Europe. The GEMS regional-scale forecasts are based on up to seven European air quality models running fully operationally in a number of countries (listed in Table 4.3). As continuation of the PROMOTE and GEMS projects, first pre-operational ensemble forecasts have been provided since the end of 2009 within the MACC project (MACC, 2011) which will be one cornerstone of the planned operational GMES Atmospheric Service.

Model studies have shown that short-term action plans can be effective if they are determined and implemented at least two or three days before the pollution episode occurs. Therefore, the forecasting capacity that provides, in many cases, an assessment on the origin of the episode (e.g. long-range transport, transport of natural species, local emissions and local meteorological conditions) can help in deciding the most appropriate information and emergency measures to be taken. Generally these measures concern road traffic (speed limits and alternating circulation) and industrial emission controls. Despite being recommended in the AQ Directive, use of forecasting results for designing emergency measures is still a new approach that has not been fully adopted by the Member States. Its relevance depends on the forecasting models' quality and accuracy, i.e. their ability to prevent false alarms and missing events. It may be considered that air quality models are not sufficiently mature for this application. However, promising results are now achieved by some systems running over long periods, especially for O_3 (Honoré et al., 2008; Rouïl et al., 2009).

The forecasting capacity of an air quality model is strongly determined by the quality of the meteorological forecasts driving the system, as well as by the accuracy of the emissions inventory used. In particular, the temporal variability of the emissions is generally not well represented in such models, although this is a key point in the occurrence of pollution episodes, particularly those emissions which depend on meteorological conditions (e.g. heating, agriculture, natural emissions and road dust). In regard to meteorology, many whether forecast models are not designed to provide accurate results for typical episodic pollution events, such as low wind speeds, inversions and local recirculation.

7.3 Transboundary and long-range air pollution

Article 25 of the AQ Directive deals with the problem of transboundary air pollution for which local measures will not have an effect. Under such circumstances, cooperation between the Member States is required. Before plans can be made, an assessment of the impact of transboundary air pollution is required to indicate the contribution of other Member States to the local air quality. Regional-scale air quality models are required for such assessments.

7.3.1 Background to long-range transboundary air pollution

Long-range transport of air pollutants is one of the main issues that European Union includes in its legislation. In particular, transboundary air pollution, namely the air pollution generated in one country and being transported to its neighbouring countries, is considered as a major European problem of international political concern. This transfer of pollutant air masses impacts other countries' chances of achieving their environmental and policy objectives, such as meeting air quality standards or reducing pollution below critical levels, according to the AQ Directive. Major emission reductions for SO_2, NO_X, volatile organic compounds (VOCs) and ammonia (NH_3) as adopted in the Gothenburg Protocol (1999) under the LRTAP Convention and EU legislation, primarily Directive 2001/81/EC on national emission ceilings (EC, 2001) with legally binding ceilings for 2010 (EC, 2001c), have reduced the harmful effects associated with the presence of these substances. Those effects are namely their contribution to the formation of photochemical smog, and the acidification and eutrophication of water and soil (e.g. Moussiopoulos et al., 2004). However more recent assessments have also shown that a number of health-related transboundary pollutants, notably particulate matter and ozone, are still at levels harmful to human health (EEA, 2010).

Originally models were developed and used to inform the policy definition processes towards an international agreement on reducing acidification resulting from long-range transboundary air pollution, in particular for the definition of the Protocol to LRTAP Convention on further reductions of sulphur emissions. These pioneering models were created to support the international negotiations, which were the political answer to increased requests from some European countries that raised concerns about the consequences of such transboundary pollution (Gough et al., 1998). Within the framework of the multi-pollutant/multi-effects Gothenburg Protocol (1999), these models have extended their domain of application to photochemical air pollution (ozone). Currently, the Gothenburg Protocol is under revision, aiming at more stringent emission ceilings for SO_2, NO_X, VOCs and NH_3 to be met by 2020, the introduction of a 2020 emissions ceiling for $PM_{2.5}$, updated technical annexes, guidance documents and aspirational emission reduction targets for 2050. The NEC Directive revision has been put on hold until (most probably) 2013.

Though the LRTAP Convention concentrates on European contributions to air pollution, there is also a hemispheric component to this. The most recent report from the Task Force on Hemispheric Transport of Air Pollution (HTAP, 2011) on the intercontinental transport of air pollution provides an overview of this contribution.

Models are the most relevant tools to obtain reliable information about the magnitude of long-range transport of air pollution due to current emissions and possible future changes under various emission and climate scenarios. In order to provide such updated information, models have been developed that realistically describe transport, transformation, and deposition processes, particularly focusing on source-receptor relationships. Evaluation and model intercomparison initiatives organised in response to requests from the LRTAP Convention help in building confidence in such models for policy applications. Examples are:

- the Task Force on Measurement and Modelling of the EMEP programme (TFMM, 2011; EMEP, 2011)
- the European Commission, e.g. CityDelta (CityDelta, 2011)
- the Fairmode initiative (Fairmode, 2011a)
- the scientific community, e.g. the AQMEII project (AQMEII, 2011).

7.3.2 European transboundary assessments

Various methods using modelling, monitoring and combinations of these can be applied to assess the transboundary contributions to air pollution.

The EMEP model is one of them (EMEP, 2011) that provides support for the LRTAP Convention. EMEP carries out source-receptor calculations every year to identify the transboundary contributions within Europe; this information can be used to support air quality plans between Member States (see Fairmode 2011b, Example 1.2.3). The status reports, technical notes, and country reports focusing on each party to LRTAP Convention are issued by the Meteorological Synthesizing Centre — West annually and are made available on the Internet (MSC-W, 2011). The purpose of the annual EMEP status reports is to provide an overview of the status of transboundary air pollution in Europe, tracing progress towards existing emission control protocols, and supporting the design of new protocols when necessary. An additional purpose of these reports is to identify problem areas and new findings of relevance to LRTAP Convention. Further, annual reports on transboundary transport of particle matter (e.g. Yttre et al., 2009) are produced based on both modelling and monitoring data.

7.3.3 *National, regional and city-based assessments of long-range transport*

Independent of the Europe-wide assessments, there are also a number of national, regional and city-level assessments dealing with the contribution of long-range transport. In the case of cities, this is often referred to as the contribution from the regional background. It is of primary concern to city authorities since these contributions are outside their administrative jurisdiction, even though the source may be within the national borders (e.g. Lutz, 2010).

An important use of models is the evaluation of different emission reduction scenarios in terms of their efficiency in improving regional and local air pollution levels, by considering distant air pollutant emission sources. Particularly in the case of O_3, it should be taken into account that an emission intervention which is effective on the regional scale may not necessarily be effective for a city and its surroundings. A methodology for this purpose is presented in a paper by Moussiopoulos et al. (2000), in which three regional emission reduction scenarios were assumed to be valid also for the emission situation in the urban areas of Athens, Greece and Stuttgart, Germany and the corresponding emission inventories were compiled. The EMEP MSC-W ozone model was used to calculate the regional scale ozone distribution, while local-scale transport and chemical transformation processes were analysed with the OFIS model (Moussiopoulos et al., 2000b). Both the regional- and the local-scale simulations were performed for a base case (1990 situation) and three emission reduction scenarios. The significance of regional-scale emission reductions was demonstrated by performing a second series of simulations assuming that the emission interventions were implemented only at local scale. The results revealed that ozone exposure in conglomerations like the ones considered in this study depends on both urban- and regional-scale influences. Urban VOC emission control was found to be effective in reducing O_3 primarily on the local or urban scale, whereas urban NO_X control would cause an increase of urban peak O_3 while contributing to an effective reduction of regional ozone.

In order to establish how current air quality standards can best be met now and in the future, it is necessary to understand the cause of PM_{10} episodes. In a relevant study (Malcolm et al., 2000), the United Kingdom's Met Office's dispersion model, NAME (Jones et al., 2007), has been used to model hourly concentrations of sulphate aerosol for 1996 at a number of British locations. The model output has been compared with measured values of PM_{10} or sulphate aerosol at these sites and used to provide information on the contribution of long-range transport to local levels. Another study on the long-range transport of particulate matter emitted directly into the air (primary PM) uses a simple atmospheric transport model to estimate the contribution of primary PM to PM_{10} and $PM_{2.5}$ concentration across Europe (ApSimon et al., 2001). The resulting population exposure is compared with that of secondary particulates (i.e. PM formed in the atmosphere), and it is found that both primary and secondary contributions will be significantly reduced with the implementation of new protocols under the LRTAP Convention (LRTAP Convention, 2011).

8 Special topics

There are a number of special topics that require some extra attention. In this chapter, these are mostly related to assessing the contributions of natural sources or other 'non-harmful' sources, as described in the AQ Directive. Article 2.15 and Article 20 of the directive deal with the contribution of natural sources to exceedances of the limit values. Where limits are exceeded, it is possible to subtract the contribution of natural sources from the hourly, daily or annual mean concentrations (derogation). To determine this, both monitoring and modelling may be employed. Examples given of natural sources in Article 2.15 include volcanic eruptions, seismic activities, geothermal activities, wild-land fires, high-wind events, sea sprays, or the atmospheric re-suspension or transport of natural particles from dry regions. Recently a technical document (Marelli, 2007) was published on the topic of natural sources. A respective guidance document on this, as well as on assessing salt and sanding contributions, is currently under development. These documents are available through the European Commission web portal (EC, 2011a).

In general, assessing the contribution of natural and other sources is best performed using an integrated approach, whereby modelling and monitoring are used in a complementary fashion. For example, increased concentrations due to emissions from natural sources such as volcanic eruptions or wild-land fires will often be visible in the measurement data. To assess what type of event has occurred, models (for example including back trajectories modelling) and satellite data can be used to identify the source regions and confirm the origin (e.g. MACC, 2011). Often emissions of these natural sources are poorly known and so any forward modelling and prognosis of such events will need to be quantified in combination with monitoring data.

Based on the analysis of the air quality questionnaires from 2007 by Vixseboxse and de Leeuw (2009), for example, four Member States (Greece, Spain, Cyprus and Portugal) claimed PM_{10} derogation on the basis of natural events, and five Member States (Estonia, Latvia, Lithuania, Slovakia and Finland) due to winter sanding. The following sections deal chiefly with the use of modelling for a number of these sources.

8.1 Assessing the contribution of winter sanding or salting of roads to PM exceedances

Article 21 of the AQ Directive allows for the subtraction of the winter sanding and salting contributions to PM_{10} when exceedances occur. This is most relevant to the PM_{10} daily mean limit value but may also be applied to the annual mean concentrations. If a Member State can adequately show that exceedances of the daily mean limit value are caused by road salt and sanding activities, these days are not included in the exceedance assessment.

The European Commission provides guidance on this in 'Guidance on assessing the contribution of winter-sanding and -salting under the EU Air Quality Directive' (EC, 2011a). In the document, the use of air quality models is not recommended for this application since emission models, needed to quantify the salt or sand contribution to PM, are not capable of simulating this emission source. Instead they recommend monitoring of chlorine to assess the salt contribution. No preferred or recommended method is provided for winter sanding. However, chemical analysis and the application of receptor modelling are suggested as a methodology.

There are a small number of road-dust emission models available that could be further developed for this type of application. These include the US EPA model AP-42 (EPA, 1993), and the non-exhaust emission models developed by Omstedt et al. (2005) and Tønneson (2003). Road-dust emissions are currently more uncertain than exhaust emissions, due to the strong dependence of re-suspension on road surface conditions (e.g. surface wetness) and on the lack of knowledge concerning road surface dust loadings. Though these models have been shown to provide reasonable estimates of total road dust emissions, after adjustment to local factors (e.g. Omstedt et al. (2011)), they cannot be applied to quantify salt emissions; also, only the model from Omstedt includes a treatment for sanding. Even in that case, no direct validation of the contribution of sanding to PM concentrations has been carried out.

In summary, the current set of emission models used to calculate road dust and other non-exhaust contributions to PM are not presently capable of providing the required information for assessing the contribution of winter sanding and salting to daily mean PM_{10} exceedances; therefore, monitoring and statistically based methods are currently recommended. This situation may change in the future as new models are developed.

8.2 Assessing the contribution of wind-blown and Saharan dust events to PM exceedances

Article 20 states that exceedances caused by natural contributions will not count as exceedances for the purpose of the AQ Directive. In Article 2.15, one of the natural sources is described as being the 'atmospheric re-suspension or transport of natural particles from dry regions'. This is generally understood to refer to Saharan dust events but may include any such event. It does not in principle include wind-blown dust events caused by human activities such as agriculture or mining activities. As with road salting and sanding, wind-blown dust events are most relevant for the PM_{10} daily mean limit values due to their episodic nature.

The European Commission has developed a guidance document on natural contributions that has been made available through the European Commission website (EC, 2011a). This guidance document is based on a prior technical document (Marelli et al., 2007). For the particular case of Saharan dust episodes, this document recommends using back trajectory modelling, Saharan dust forecasts, satellite data and ground-based measurement data to identify such events. It is not recommended to use modelling alone as a method for quantifying Saharan dust outbreaks, but rather to use monitoring methods after the events have been identified, using both models and monitoring data. A recent document (Querol et al., 2009) describes a comprehensive methodology that combines the above aspects and allows for a quantitative assessment of the contribution of Saharan dust outbreaks to PM_{10} exceedances. This methodology is summarised on the Fairmode website (Fairmode, 2011b; Example 1.2.5).

In principle, models can be used to quantify the contribution of wind-blown dust for applications involving the AQ Directive if the models can be shown to fulfil the uncertainty criteria as laid out in the AQ Directive for daily mean PM_{10} concentrations. In practice, however, quantifying daily mean PM_{10} concentrations to the required level of uncertainty (50 %) using only models is not currently feasible; their use together with monitoring data, both satellite and ground based, is necessary to reduce the uncertainty.

Two examples where models have been used to help identify and quantify the contribution of wind-blown dust from the Sahara, relevant for the AQ Directive, are Mircea et al. (2008) and Mitsakou et al. (2008). These examples are summarised on the Fairmode website (Fairmode, 2011b).

Saharan dust forecasts are currently being carried out by the University of Athens, Greece using the SKIRON (2011) forecasting system, the Earth Sciences Division of the Barcelona Supercomputing Center (Italy) using the BSC-DREAM8b model (BSC, 2011), the Monterey National Research Laboratories Aerosol Page (NRL, 2011) (USA) and the Tel Aviv University Weather Research Center (TAU WeRC, 2011) (Israel). Some regional-scale air quality models, such as CHIMERE (Vautard et al., 2005) also contain modules that describe wind-blown dust emissions. On the European scale, the pre-operational atmospheric service of the European GMES programme, MACC, provides forecasts using several regional air quality models (ensemble approach — MACC, 2011).

Back trajectory modelling may be carried out with a number of models. Models commonly used for such applications include FLEXTRA and FLEXPART (Stohl et al., 2002 and Stohl, 2009) and HYSPLIT (ARL, 2009). Both these models have been used for a variety of applications related to the origin of natural emissions.

8.3 Assessing the contribution of sea salt to PM exceedances

Another natural source that is not considered to contribute to exceedances in Article 20 of the AQ Directive is sea salt. In Article 2.15, this is described as 'sea sprays'. Such events tend to be episodic, occurring with high winds, and are most relevant for the PM_{10} daily mean target values. However, it is possible that in coastal regions, the annual mean limit value for PM_{10} can be exceeded as a result of the contribution of sea salt.

The European Commission provides guidance on this contribution in its respective document (EC, 2011a), with background technical information provided in Marelli (2007). As in the case of wind-blown dust, it is recommended to base assessment of sea salt contributions primarily on monitoring data, e.g. measurement of Chloride (Cl^-) or sodium (Na^+) with appropriate corrections, and use models as secondary information to support assessment of the air mass origin through back trajectories, or to provide information on the spatial distribution of sea salt.

However, there have been a number of studies that have applied modelling as a primary source of information for assessing the contribution of sea salt to PM_{10} exceedances. The best examples of these have been carried out in the Netherlands, where two separate modelling studies have been carried out. In the first, Van Jaarsveld and Klimov (2009) applied the OPS-ST model; in the second, Manders et al. (2009) applied the LOTOS-EUROS model to calculate sea salt contributions using a model resolution of approximately 6 x 6 km^2. These model applications are described in on the Fairmode website (Fairmode, 2001b; Example 1.2.7). Generally, the modelling studies remain quite uncertain on the temporal scale of one day, with estimated uncertainties in salt concentrations of between a factor of 2 and 3. However, the long-term average concentrations (over 5 years) are better represented and have been found to have an uncertainty of around 15 % (Van Jaarsveld and Klimov, 2009).

In addition to the LOTOS-EUROS model, a number of other regional-scale models also contain emission modules for sea salt, for example the Unified EMEP Model (2011) and CHIMERE (2011). However, due to the strong gradient of sea salt concentrations from the coast inland, the resolution of these models needs to be of the order of 10 x 10 km^2 less to capture these gradients adequately. In any case, if such models are applied for sea salt calculations, they should be well validated, or applied in combination with measurement observations.

Forecasts for sea salt contributions are also available, e.g. the Tel Aviv University Weather Research Center provides sea salt forecasts (TAU WeRC, 2011) for the Mediterranean region using the same model (DREAM) that is applied for wind-blown dust forecasts. However, this model has too coarse a resolution (~ 35 x 35 km^2) to capture the strong gradient close to the coast.

8.4 Assessing the contribution of wild-land fires to PM exceedances

'Wild-land fires' are also included in Article 20 of the AQ Directive as a natural source that can be discounted when its contribution leads to exceedances. This source is addressed in a respective Guidance document published by the Commission (EC, 2011). Importantly, the document addresses the definition of the source 'wild-land fires' and 'forest fires', since many fires are the result of human activities related to agricultural and other land use activities. In this regard, 'wild-land fires' are defined as:

> 'The burning (naturally or man-induced) of non-managed and managed-forests and other vegetation, excluding agricultural burning of stubble, etc.'

This definition leads to the conclusion that in many instances, wild-land and other fires cannot be treated as natural and so cannot be subtracted from exceedances when the sources are within a Member State's own country. However, the draft Guidance document on natural sources goes on to state:

> 'If a Member State suffers high PM concentrations due to forest fires outside its own country, it may still be appropriate to subtract the contribution from the fires of the total PM levels for compliance purposes. Other provisions of the AQ Directive such as Article 26 on transboundary pollution may also apply in such a case.'

As a result it is well worth determining the contribution of these sources for reporting and planning purposes if they are considered to have a significant impact on air quality. The draft Guidance document on natural sources recommends an integrated approach to determining the contribution of wild-land fires; this includes the use of validated air quality modelling and back trajectories, combined with satellite and ground-based monitoring, as well as chemical analysis of airborne particulate matter.

When air quality models are used, it is important to validate these with observed data, either ground or satellite based, and to use the best possible estimates for the wild fire emissions. To quantify wild-land fire emissions, explicit knowledge of the burned area, burning period, fuel characteristics, fire behaviour, fuel consumption, and pollutant specific emission factors are required (Ottmar et al., 2009). Estimates of emissions at the European scale are already available (Barbosa et al., 2009), based on the

EU fire database (JRC, 2011), which contains data provided each year by individual Member States for each fire event, burned area maps obtained through satellite images, and a map of fuel types. In addition to this emission information, some aspects, such as plume rise of the wild fires, are currently uncertain.

The MACC Global Fire Emissions service, as part of the GMES Atmosphere Service, provides global emissions from biomass burning as input for some of the other MACC products and to the general public. The emissions are calculated in real time and retrospectively from satellite-based observations of open fires (for example wildfires and human-ignited grassland and forest fires; MACC, 2011)

In Europe, there are a number of ongoing studies and projects dealing with wild-land fires, particularly in countries such as Greece, France, Portugal and Finland where there can be significant episodic contributions from forest fires, e.g. Miranda (2004), Hodzic et al. (2007) and Miranda et al. (2008a). An example is provided on the Fairmode website (Fairmode 2011b; Example 1.2.2). Sofiev et al. (2009) applied an operational system for the assimilation of satellite information on wild-land fires for the needs of air quality modelling and forecasting. Some of these studies show the contribution of transboundary pollution from wild-land fire episodes. For instance, there is emerging evidence that smoke from widespread wildfires in Portugal in summer 2003 contributed to the high O_3 levels measured at the air quality monitoring stations in Paris, France (Hodzic et al., 2006). In the scope of the COST 728 (2011) action joint case studies, a modelling exercise is currently being undertaken using wildfire emissions derived from satellite images processing for Europe and for two specific episodes (April–May 2006, and August 2006). In the United States, a recent collaborative and coordinated effort to model smoke impacts, the BlueSky Smoke Modelling Consortium, was established, in order to develop and apply real-time smoke modelling to support fire operations and smoke management (Ferguson et al., 2001; Sestak et al., 2002).

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Annex 1 List of abbreviations

Air4EU	FP6 project: Air quality assessment for Europe
AirBase	Public air quality database system of the EEA
AMET	Atmospheric Model Evaluation Tool
AP-42	Compilation of Air Pollutant Emission Factors from US EPA
AQ	Air quality
AQMEII	Air Quality Model Evaluation International Initiative
ASTM	American Society for Testing and Materials
BSC-DREAM	Dust Regional Atmospheric Model from the Barcelona Supercomputing Center
CAMx	The Comprehensive Air quality Model with extensions
CFD	Computational Fluid Dynamics
CHIMERE	A multi-scale model for air quality forecasting and simulation; Developed at IPSL/LMD, INERIS and LISA in France
CityDelta	Intercomparison of long-term model responses to urban-scale emission-reduction scenarios
LRTAP Convention	Convention on Long-range Transboundary Air Pollution
CMAQ	Community Multiscale Air Quality Modeling System
COST 602	European Cooperation in Science and Technology Action: Towards a European Network on Chemical Weather Forecasting and Information Systems
COST 728	European Cooperation in Science and Technology Action: Enhancing mesoscale meteorological modelling capabilities for air pollution and dispersion applications
COST 732	European Cooperation in Science and Technology Action: Quality Assurance and Improvement of Micro-Scale Meteorological Models
CTM	Chemical Transport Model
DG Environment	Directorate-General for the Environment
EC	European Commission
EEA	European Environment Agency
Eionet	European Environment Information and Observation Network
EMEP	European Monitoring and Evaluation Programme
ETC/ACM	Topic Centre on Air Quality and Climate Change Mitigation
EU	European Union
EuroDelta	Inter-comparison of regional model responses to emission-reduction scenarios
EUROTRAC 2	The EUREKA project on the transport and chemical transformation of trace constituents in the troposphere over Europe; second phase
Fairmode	Forum for air quality modelling in Europe
FLEXPART	Lagrangian particle dispersion model developed by Andreas Stohl
FLEXTRA	Lagrangian atmospheric trajectory model developed by Andreas Stohl
FP6	Sixth European Union Framework Programme for Research and Technological Development
GEMS	Global and regional Earth-system (Atmosphere) Monitoring using Satellite and in-situ data
GLOREAM	GLObal and REgional Atmospheric Modelling. A subproject under EUROTRAC-2
GMES	Global Monitoring for Environment and Security
HARMO	International conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
HTAP	Hemispheric Transport of Air Pollution
HYSPLIT	Hybrid Single Particle Lagrangian Integrated Trajectory Model
IDL	Interactive Data Language
JRC	Joint Research Centre

JRC-IES	JRC - Institute for Environment and Sustainability
LOTOS-EUROS	Atmospheric chemistry transport model from RIVM and TNO, The Netherlands
MACC	Monitoring Atmospheric Composition and Climate
MDS	Model Documentation System
MM5	The PSU/NCAR mesoscale model (version 5)
MQO	Model Quality Objective
MRDE	Maximum Relative directive Error
MSC-W	Meteorological Synthesizing Centre - West
NAME	Numerical Atmospheric-dispersion Modelling Environment. Dispersion model from the UK met office
OFIS	Ozone Fine Structure model
OPS-ST	Operational Priority Substances Short Term model
OSPM	Operational Street Pollution Model
PAH	Polycyclic aromatic hydrocarbon
PDF	Probability distribution function
POMI	Po-Valley Modelling Intercomparison Exercise
PROMOTE	Protocol Monitoring for the GMES Service Element: Atmosphere
PSAT	Particulate matter source apportionment technology: Algorithm used in CAMx for carrying out source apportionment of PM.
QA/QC	Quality assurance and quality control
RDE	Relative Directive Error
RPE	Relative Percentile Error
SKIRON	Meteorological model from the University of Athens, Greece
UNECE	United Nations Economic Commission for Europe
UNESCO	United Nations Educational, Scientific and Cultural Organization
UNESCO-CEPES	The UNESCO European Centre for Higher Education
US EPA	United States of America Environmental Protection Agency
VOC	Volatile Organic Compounds
WMO-GURME	The World Meteorological Association Global Atmospheric Watch Urban Research Meteorology and Environment Programme
WRF	Weather Research and Forecasting Model

Annex 2 Quality indicators for meteorological and air quality model evaluation

Table A2.1 Quality indicators

Parameter	Formula	Ideal value	Meteorology	Air quality
Average observed value	$\overline{O} = \frac{1}{N}\sum_{i=1}^{N} O_i$		√	√
Average modelled value	$\overline{P} = \frac{1}{N}\sum_{i=1}^{N} P_i$	Same as $\overline{O}$	√	√
Error	$E_i = P_i - O_i$	0.0	√	
Mean absolute error (USA-EPA mean absolute gross error)	$MAE = \frac{1}{N}\sum_{i=1}^{N} \lvert E_i \rvert$	0.0	√	
Standard deviation of measurements	$\sigma_o = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(O_i - \overline{O})^2}$		√	√
Standard deviation of modelled results	$\sigma_P = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_i - \overline{P})^2}$	Same as σ_o	√	√
BIAS	$BIAS = \frac{1}{N}\sum_{i=1}^{N} E_i = \overline{P} - \overline{O}$	0.0	√	
Average normalised absolute BIAS	$ANB = \left(\frac{\overline{P} - \overline{O}}{\overline{O}}\right)$	0.0		√
Mean normalised BIAS	$MNB = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{O_i}\right)$	0.0		√
Mean normalised error (in USA-EPA mean normalised gross error)	$MNE = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\lvert P_i - O_i \rvert}{O_i}\right)$	0.0		√
Standard deviation of error	$STDE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}[(P_i - \overline{P}) - (O_i - \overline{O})}$	0.0	√	√
Fractional Bias	$FB = \frac{(\overline{P} - \overline{O})}{0.5(\overline{P} + \overline{O})}$	0.0		√
Geometric mean bias	$MG = \exp(\frac{1}{N}\sum_{i=1}^{N}\ln P_i - \frac{1}{N}\sum_{i=1}^{N}\ln O_i$	1.0		√
Geometric variance	$VG = \exp((\frac{1}{N}\sum_{i=1}^{N}\ln P_i - \frac{1}{N}\sum_{i=1}^{N}\ln O_i)^2$	1.0		√
Skill variance	$SKVAR = \frac{\sigma_P}{\sigma_O}$	1.0	√	√

Table A2.1 Quality indicators (cont.)

Parameter	Formula	Ideal value	Meteorology	Air quality
Root mean square error	$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2}$	0.0	√	√
Normalised mean square error	$\mathrm{NMSE} = \frac{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2}{\overline{P}\,\overline{O}}$	0.0		√
Correlation coefficient	$r = \left[\frac{\frac{1}{N}\sum_{i=1}^{N}(O_i - \overline{O})(P_i - \overline{P})}{\sigma_O \sigma_p}\right]$	1.0	√	√
Coefficient of variation	$CV = \frac{STDE}{\overline{O}}$	0.0		√
Fraction of predictions within a factor of two of observations	$FAC2 = \frac{1}{N}\sum_{i=1}^{N} n_i$ $n_i = \begin{cases} 1 \text{ for } 0.5 \leq \left\lvert\frac{P_i}{O_i}\right\rvert \\ 0 \text{ else} \end{cases}$	1.0		√
Hit rate	$H_c = \frac{1}{N}\sum_{i=1}^{N} n_i$ $n_i = \begin{cases} 1 \text{ for } \frac{E_i}{\lvert O_i\rvert} \leq A \text{ or } \lvert E_i\rvert \leq DA \\ 0 \text{ else} \end{cases}$ A – desired relative accuracy DA minimum desired absolute accuracy	1.0	√ For the DA for temperature, dewpoint, wind and pressure, see the table below	√
Index of agreement	$IOA = 1 - \frac{\sum_{i=1}^{N}(P_i - O_i)^2}{\sum_{i=1}^{N}\left[\lvert P_i - \overline{P}\rvert + \lvert O_i - \overline{O}\rvert\right]}$	1.0		√
Unpaired peak concentration accuracy	$A_u = \frac{P_{max} - O_{max}}{O_{max}}$ P_{max} , O_{max} are unpaired maxima (no timing/ spacing considered)	0.0		√
Spatially-paired peak concentration accuracy	$A_s = \frac{P_{max,x} - O_{max,x}}{O_{max,x}}$ $P_{max,x}$, $O_{max,x}$ are maxima paired in space (but not in time)	0.0		√

Table A2.1 Quality indicators (cont.)

Parameter	Formula	Ideal value	Meteorology	Air quality
Hit ratio	$A_s = \frac{P_{max,x} - O_{max,x}}{O_{max,x}}$ with: a: forecast event yes, observed event yes b: forecast event yes, observed event no, c: d: forecast event no, observed event no	1.0	√	
False alarm ratio	$FAR = \frac{b}{a+b}$	0.0	√	
Direction weighted wind error	$DIST = \frac{1}{N}\sum_{i=1}^{N}\sqrt{((u_{pi} - u_{oi})^2 + (v_p$	0.0	√	
Probability of detection	$POD = \frac{a}{a+c}$	1.0	√	
Gross error	$GE = \frac{1}{N}\sum_{i}^{N}\lvert P_i - O_i \rvert$		√	

Note: P_i denotes predicted values, O_i denotes observed values, and N the number of values considered.

Source: Adapted from COST 728 (Schluenzen and Sokhi, 2008)

Table A2.2 Desired Accuracy (DA)

Variable	Temperature (°C)	Dew point depression (°C)	Wind speed (ms^{-1})	Wind direction	Pressure (hPa)
Desired accuracy (DA)	± 2	± 2	± 1 for ff <10ms^{-1} ± 2.5 for ff >10ms^{-1}	± 30°	± 1.7

Note: See Schluenzen and Sokhi (2008) for more details.

Table A2.3 Benchmarks for meteorological mesoscale model evaluation

Parameter	Measure	Benchmark
Wind Speed		
	RMSE	< 2 m/s
	Bias	< ± 0.5 m/s
	IOA	≥ 0.6
Wind Direction		
	Gross Error	< 30 deg
	Bias	< ± 10 deg
Temperature		
	Gross Error	< 2 K
	Bias	< ± 0.5 K
	IOA	≥ 0.8
Humidity		
	Gross Error	< 2 g/kg
	Bias	< ± 1 g/kg
	IOA	≥ 0.6

Note: Suggested by Emery et al. (2001) and Tesche et al. (2002), and included in the EPA Draft Guidance on meteorological model evaluation (2009).

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