# Guidance on the use of models for the European Air Quality Directive

***A working document of the Forum for Air Quality Modelling in Europe***

**FAIRMODE**

ETC/ACC report

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***Editor***

Bruce Denby[1]

***Contributing authors***

Bruce Denby[1], Emilia Georgieva[6], Steinar Larssen[1], Cristina Guerreiro[1], Liu Li[1], John Douros[2], Nicolas Moussiopoulos[2], Lia Fragkou[2], Michael Gauss[3], Helge Olesen[4], Ana Isabel Miranda [5], Panagiota Dilara[6], Philippe Thunis[6], Sari Lappi[7], Laurence Rouil[8], Anke Lükewille[9], Xavier Querol[10], Fernando Martin[11], Martijn Schaap[12], Dick van den Hout[12], Andrej Kobe[13], Camillo Silibello[14], Keith Vincent[15], John Stedman[15], María Gonçalves[16], Guido Pirovano[17], Luisa Volta[18], Addo van Pul[19], Alberto González Ortiz[20], Peter Roberts[21], Dietmar Oettl[22], Amela Jericevic[23]

[1] Norwegian Institute for Air Research (NILU), Norway. [2] Laboratory of Heat Transfer and Environmental Engineering, Aristotle University, Thessaloniki, Greece. [3] Norwegian Meteorological Institute, Norway. [4] NERI, Denmark. [5] CESAM, University of Aveiro, Portugal. [6] EC-JRC, Ispra, Italy. [7] Finnish Meteorological Institute (FMI), Finland. [8] INERIS, France. [9] European Environment Agency, Denmark. [10] IDAEA – CSIC, Spain. [11] CIEMAT, Spain. [12] TNO Environment and Geosciences, The Netherlands. [13] DG Environment, European Commission, Belgium. [14] Arianet, Milano, Italy. [15] AEA Technology, Harwell, United Kingdom. [16] Barcelona Supercomputing Center, Barcelona, Spain. [17] ERSE, Milan, Italy. [18] UNIBS, Brescia, Italy. [19] RIVM, Bilthoven, The Netherlands. [20] Ministry of Environment and Marine and Rural Affairs, Madrid, Spai. [21] Concawe, Brussels, Belgium. [22] Government of Styria, Austria, [23] Meteorological and Hydrological Service, Croatia

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# Preamble to version 6.2

This is the sixth draft (version 6.2) of the document entitled 'Guidance on the use of models for the European air quality Directive', which is an activity of Working Group 1 of FAIRMODE (http://fairmode.ew.eea.europa.eu/). This document is intended to provide a harmonised focus for modelling activities that are relevant to the Air Quality Directive, providing interpretation, reference and summary information for both authorities and researchers.

This version is the final draft submitted to EEA, with the intention of publication as an EEA technical report. However, the document is still considered to be dynamic and regular updates based on activities, both internal and external to FAIRMODE, will be included in later versions.

It has become clear during the writing of this document that 'consensual guidance' (i.e. guidance to which the significant majority agrees) on air quality modelling and its application for the Air Quality Directive is not yet available. Though a number of other documents and projects have addressed the guidance and recommendation issue, the modelling community is so broad and the applications of models so varied that there is not yet a clear and common understanding of what can be regarded as 'best practise' in modelling. Indeed, within this document we refer extensively to 'good practice' rather than 'best'. There is currently no common understanding of the quality assurance requirements that should be applied to modelling. Indeed, there are still some aspects of the AQ Directive itself that are ambiguous and require further clarification. This document is work in progress and will continue to develop as required to aid the modelling community and its users.

A brief status overview of the document (version 6.2) is as follows:

- Chapters 1 - 4 deal with the interpretation of the new Air Quality Directive (2008/50/EC). Though these chapters are relatively complete they still require further discussion and refinement, particularly in harmonising the document with other guidance documents from the Commission that will be made available in 2010.
- Chapter 5, which deals with quality assessment and uncertainty in air quality models, contains a review of quality assurance aspects and will be further developed as part of the Working Group 2 activities in FAIRMODE to provide effective guidance.
- Chapters 6 – 8 are intended to provide overviews and short examples of existing applications of modelling for the AQ Directive. These chapters will require further input and 'good practise' examples, hopefully resulting from the activities of FAIRMODE and from input from the community. Eventually recommendations and guidance will be provided for the applications.
- Annexes provide a more extensive list of examples and definitions.
    - Annex 1: A selection of 'good practice' examples requiring further selection and addition
    - Annex 2: Quality assurance definitions

# 1 Introduction

In 2008 the new European Air Quality (AQ) Directive was ratified by the European parliament (EC, 2008). This AQ Directive replaced earlier Directives simplifying and streamlining existing provisions, including reporting, and introducing new provisions, in particular new objectives concerning $PM_{2.5}$ and the possibility to postpone the attainment year of some limit values. Whilst previous Directives have based assessment and reporting largely on measurement data, the new AQ Directive places more emphasis on, and encourages, the use of models in combination with monitoring in a range of applications.

Modelling may be used as a tool to supplement monitoring data for assessment purposes when reporting exceedances. 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 when appropriate modelling is also carried out.

Modelling is an important tool on which to base action plans, both short and long term. Applications for postponement require such plans as does reporting when limit values of the AQ Directive are exceeded. Source apportionment, 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.

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 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 best be applied. It also provides background information and guidance on best practices for achieving modelling through example case studies, references and links to other relevant documents.

This guidance document will develop 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 this document can be found on the FAIRMODE website (http://fairmode.ew.eea.europa.eu/). At that site it is also possible to register to participate in FAIRMODE activities and to provide feedback and ask questions through an open forum.

In addition to this Guidance document on modelling a number of other Guidance documents, both existing and under development, are accessible through the European Commission web site on air quality (http://ec.europa.eu/environment/air/quality/). These address a range of other issues relevant to the AQ Directive but may overlap with this document when modelling is involved.

## 1.1 Aims

The major aims of this document are:

- to provide guidance for the use of air quality modelling in regard to the European Air Quality Directive (EC, 2008) 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.

## 1.2 Scope and structure

This document deals with the application of air quality models. These models are mathematical tools used to quantify concentrations of air pollutants as a result of emissions to 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. It is presented as a series of chapters where Chapters 2 – 4 deal with an interpretation and understanding of the AQ Directive, in regard to modelling, Chapter 5 deals with the overarching need for quality assurance of models and Chapters 6 – 8 describe modelling applications and methodologies. An annex provides a number of relevant examples and definitions. The document covers the following topics:

- a summary of the European Air Quality Directive
- an interpretation of the European Air Quality 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 special topics in regard to the AQ Directive when modelling is applied, including assessment of non-anthropogenic contributions to air quality and contributions to PM from road sanding or salting
- definitions of relevant concepts

This document does not provide in depth recommendations or practical solutions to all modelling requirements needed for assessment, however, a number of indicative examples are provided. The reader is instead guided to a number of references where such details may be found.

## 1.3 Audience

This document is intended for use by authorities, consultancies and research bodies involved in air quality assessment and mitigation planning that address the European Air Quality Directive. The major text 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 annexes and references provide broad overviews as well as specific examples to help guide authorities and modellers in these activities.

## 1.4 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 eco-system impacts have been studied. Even though modelling is often seen as being more uncertain than monitoring there are three major reasons for using models 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 meteorological conditions.
- Modelling provides an improved understanding of the sources, causes and processes that determine air quality.

In regard to the AQ Directive there are distinct advantages in using models for reporting, e.g.

- 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 be potentially 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 them, e.g.

- Models require extensive input data, particularly emissions and meteorology, which are not always reliable or easily acquired.
- Models remain uncertain in their predictions and extensive validation is required before models can be applied and believed.
- The ability of models to represent the real world is limited, e.g. spatial resolution and process descriptions. 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 to promote these advantages and to address these disadvantages. In particular, activities in FAIRMODE aimed at the improving and harmonising the quality assurance of models will provide transparency and increased understanding of their applicability.

# 2 Summary of the 2008 Air Quality Directive

The "Directive 2008/50/EC of the European Parliament and of the Council on ambient air quality and cleaner air for Europe" was officially adopted by the European Parliament on the 21 May 2008 (EC, 2008). In addition, reference is also made to the Directive on heavy metals and PAH (EC, 2005), as this is will remain valid. In this guidance document we refer to these two collectively as the 'European Air Quality Directive' or simply the 'AQ Directive'. When necessary, specific distinction between the two will be made.

This chapter summarises the AQ Directive in regard to the 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*.

## 2.1 Concepts and definitions

In this section a number of terms and concepts necessary to understand the AQ Directive are given. Many of these are provided in the AQ Directive already *(Article 2)*, however some terms are not defined and these are also given an interpretation here. The list given here is intended to supplement those provided in the AQ Directive and are listed under topics. These descriptions are intended to guide the reader, for an official interpretation of all terms the reader is referred to the AQ Directive itself.

*Table 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, for every year. These are legally binding. |
| **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 that one tries to avoid. Generally applicable over longer periods, 3 – 5 years. These are not legally binding. |
| **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 (3 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, e.g. particulates, 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 method should be < 100%. |
| ***Other defined concepts*** | |
| **Proportionate measures** | These are not defined explicitly but can be considered to be 'all necessary measures not entailing disproportionate costs' |
| **Contributions from natural sources** | Contributions from emissions not caused directly by human activities. These are: volcanic eruptions, seismic activities, geothermal activities, wild-land fires, high wind events, sea sprays, the atmospheric re-suspension or transport of natural particles from dry regions |
| ***Undefined concepts*** | |
| **Combine** | The text in 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 text in the AQ Directive often refers to a 'supplementary' methods or assessment. Nowhere is this defined but it is understood to refer to all other methods than the use of fixed measurements. The best indicator of the term is given in *Article 7.3a* |

## 2.2 Where does the AQ Directive apply?

The AQ Directive applies everywhere outdoors 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):

a) at any locations situated within areas where members of the public do not have access and there is no fixed habitation

b) on factory premises or at industrial installations to which all relevant provisions concerning health and safety at work apply

c) on the carriageway of roads and on the central reservations of roads except where there is normally pedestrian access to the central reservation.

Note that these exceptions exclude exposure during road transport activities. E.g. the AQ Directive does not cover the environment within a bus but will cover the ambient environment when the public steps out of the bus. It also does not cover cyclists whilst on the road but does cover cyclists on bicycle paths.

In regard to the protection of vegetation and natural eco-systems 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). 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 are provided in Table 2. This includes the limit values, target values, the assessment threshold values, the long term objectives and the information and alert thresholds, as stated in Table 1. Some of these values come with specific conditions so for a 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 limits and levels for the legislated pollutants are provided in Table 3, as stated in Table 1. Some of these values come with specific conditions so for a definitive reference the reader is referred to the AQ Directive itself.

*Table 2. Summary of the air quality directive limit, target, assessment threshold, long term objective, information threshold and alert threshold values for the protection of human health*

| HUMAN HEALTH | Limit or target (t) value | | | | | Assessment threshold values | | Long term objective | | Information (i) and alert thresholds | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Pollutant | Averaging period | Value | Maximum number of allowed occurrences | Margin of tolerance | Date applicable | Upper | Lower | Value | Date | Period | Threshold value |
| $SO_2$ | Hour<br>Day | 350 $\mu gm^{-3}$<br>125 $\mu gm^{-3}$ | 24<br>3 | 43% (150 $\mu gm^{-3}$)<br>none | 2005<br>2005 | none<br>75 $\mu gm^{-3}$ | none<br>50 $\mu gm^{-3}$ | | | 3 hours | 500 $\mu gm^{-3}$ |
| $NO_2$ | Hour<br>Year | 200 $\mu gm^{-3}$<br>40 $\mu gm^{-3}$ | 18<br>0 | 50% in 2000 to 0% in 2010<br>50% in 2000 to 0% in 2010 | 2010<br>2010 | 140 $\mu gm^{-3}$<br>32 $\mu gm^{-3}$ | 100 $\mu gm^{-3}$<br>26 $\mu gm^{-3}$ | | | 3 hours | 400 $\mu gm^{-3}$ |
| Benzene | Year | 5 $\mu gm^{-3}$ | 0 | 100% in 2005 to 0% in 2010 | 2010 | 3.5 $\mu gm^{-3}$ | 2 $\mu gm^{-3}$ | | | | |
| CO | Maximum daily 8 hour mean | 10 $mgm^{-3}$ | 0 | 60% | 2005 | 7 $mgm^{-3}$ | 5 $mgm^{-3}$ | | | | |
| $PM_{10}$ | Day<br>Year | 50 $\mu gm^{-3}$<br>40 $\mu gm^{-3}$ | 35<br>0 | 50%<br>20% | 2010<br>2010 | 35 $\mu gm^{-3}$<br>28 $\mu gm^{-3}$ | 25 $\mu gm^{-3}$<br>20 $\mu gm^{-3}$ | | | | |
| $PM_{2.5}$ | Year | 25 $\mu gm^{-3}$<br>25 $\mu gm^{-3}$ (t) | 0<br>0 | 20% in 2008 to 0% in 2015 | 2015<br>2010 | 17 $\mu gm^{-3}$ | 12 $\mu gm^{-3}$ | 25 $\mu gm^{-3}$ | 2020 | | |
| Pb | Year | 0.5 $\mu gm^{-3}$ | 0 | | 2005 | 0.35 $\mu gm^{-3}$ | 0.25 $\mu gm^{-3}$ | | | | |
| As | Year | 6 $ngm^{-3}$ (t) | 0 | | 2013 | 3.6 $ngm^{-3}$ | 2.4 $ngm^{-3}$ | | | | |
| Cd | Year | 5 $ngm^{-3}$ (t) | 0 | | 2013 | 3 $ngm^{-3}$ | 2 $ngm^{-3}$ | | | | |
| Ni | Year | 20 $ngm^{-3}$ (t) | 0 | | 2013 | 14 $ngm^{-3}$ | 10 $ngm^{-3}$ | | | | |
| B(a)P | Year | 1 $ngm^{-3}$ (t) | 0 | | 2013 | 0.6 $ngm^{-3}$ | 0.4 $ngm^{-3}$ | | | | |
| $O_3$ | Maximum daily 8 hour mean averaged over 3 years | 120 $\mu gm^{-3}$ (t) | 25 | | 2010 | | | 120 $\mu gm^{-3}$ | Not defined | 1 hour<br>3 hours | 180 $\mu gm^{-3}$ (i)<br>240 $\mu gm^{-3}$ |

*Table 3. Summary of the air quality Directive critical, target, assessment threshold and long term objective values for the protection of vegetation.*

| VEGETATION | Critical Level or target value | | | | Assessment threshold values | | Long term objective | |
|---|---|---|---|---|---|---|---|---|
| Pollutant | Averaging period | Value | Margin of tolerance | Date applicable | Upper | Lower | Value | Date |
| $SO_2$ | Calendar year and winter (1 October to 31 March) | 20 $\mu gm^{-3}$ | none | | 12 $\mu gm^{-3}$ | 8 $\mu gm^{-3}$ | | |
| $NO_x$ | Calendar year | 30 $\mu gm^{-3}$ | none | | 24 $\mu gm^{3}$ | 19.5 $\mu gm^{-3}$ | | |
| $O_3$ | May to July | AOT40* 18 000 $\mu gm^{-3} \cdot h$ averaged over five years | | 2010 | | | AOT40* 6000 $\mu gm^{-3} \cdot h$ | Not defined |

* AOT40 (expressed in $\mu gm^{-3} \cdot$ hours) is the sum of the difference between hourly concentrations greater than 80 $\mu gm^{-3}$ (= 40 parts per billion) and 80 $\mu gm^{-3}$ over a given period using only the one-hour values measured between 8:00 and 20:00 Central European Time (CET) each day from 1 May to 31 July each year, for vegetation protection and from 1 April to 30 September each year for forest protection).

# 3 Interpretation 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, however, modelling is only 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**

   - 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.
   - 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)*.
   - Given adequate quality and resolution of the model it can be used to reduce the number of measurements of ozone by 1/3rd *(Annex IX)*.

   This topic will be described in more detail and illustrated with examples in chapter 6 and Annex I.

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, but it is not possible to do 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, neighbouring countries and the contribution from resuspended road sand and salt. Monitoring of these source contributions everywhere in a zone or agglomeration would not be possible so modelling, usually in combination with monitoring, is the most likely methodology that can 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 is a 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. In principle modelling can be used anywhere but unlike monitoring there is no minimum requirement regarding the use of models, i.e. there is no demand that modelling be used at all for the assessment of existing air quality. Concretely, the AQ Directive defines the following situations where models can be applied:

1. Models can always be used to supplement fixed measurement data no matter 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. These are:

- Modelling can be used to supplement monitoring when a zone is in exceedance of the upper assessment threshold
- Modelling can be used in combination with monitoring when a zone is in exceedance of the lower assessment threshold
- Modelling can be used to replace monitoring when a zone is below the lower assessment threshold

3. *Article 9.2 and Annex II.B* goes on to state that, when monitoring data is not available for 5 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 is 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 6.2 and 6.3 of this document. In addition future activities in FAIRMODE will address the question of good practices for combining models and monitoring.

## 3.4 What types of models can be used?

The AQ Directive does not provide any provisions for the actual models to be used. As long as the model complies with the quality objectives (*Annex I*) then it may be applied. The following general 'fit for purpose' criteria should however apply:

- The model has the appropriate spatial and temporal resolution for the intended application
- The model is adequately validated for the particular application and 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 is available

In Table 4 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 EIONET Model Documentation System web site (http://air-climate.eionet.europa.eu/databases/MDS/index_html). In addition COST728 has developed a model inventory (http://www.mi.uni-hamburg.de/Model-Inventory.6295.0.html?&no_cache=1) that provides information on a large number of mesoscale air quality and meteorological models.

Table 4 should be considered to be 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 best modelling practices. The SATURN project (Moussiopoulos, 2003) provided a review of air quality models for use in urban applications. The EU FP6 project Air4EU (Air4EU, 2007) provided a number of reports recommending best practises for the use of models in air quality assessment.

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' (http://www.eea.europa.eu/publications/emep-eea-emission-inventory-guidebook-2009).

*Table 4. 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 – 1000 m)** | **Urban/agglomerate (1 – 300 km)** | **Regional (25 – 10 000 km)** |
| Model type | Gaussian and non-Gaussian parameterised models<br>Statistical models<br>Obstacle resolving fluid dynamical models<br>Lagrangian particle models | Gaussian and non-Gaussian parameterised models<br>Eulerian chemical transport models<br>Lagrangian particle models | Eulerian chemical transport models<br>Lagrangian chemical models |
| Meteorology | Local meteorological measurements<br>Obstacle resolving fluid dynamical models<br>Diagnostic wind field models | Mesoscale meteorological models<br>Localised meteorological measurements<br>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<br>Source specific emissions | Bottom up and/or top down emission modelling<br>Emission process models | Top down emission modelling<br>Emission process models |
| **Compound** | **Local/hotspot** | **Urban/agglomerate** | **Regional/continental** |
| $PM_{10}$ | No chemical processes | Deposition<br>Secondary inorganic particle formation | Deposition<br>Primary (combustion) particles<br>Secondary inorganic and organic particle formation<br>Suspended dust<br>Sea salt |
| $PM_{2.5}$ | No chemical processes | Deposition<br>Secondary inorganic particle formation | Deposition<br>Secondary inorganic and organic particle formation |
| $NO_2$ | Simple photo-oxidant chemistry<br>Statistical/empirical relations | Limited photo-oxidant chemistry<br>Photo-stationary scheme<br>Statistical/empirical relations<br>Deposition | Deposition<br>Full photo-oxidant chemistry |
| $NO_x$ | No chemical processes | No chemical processes<br>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<br>Secondary inorganic particle formation | Deposition<br>Secondary inorganic particle formation<br>Full photo-oxidant chemistry |
| Pb | No chemical processes | Deposition<br>No chemical processes | Deposition<br>Specialised chemical schemes |

| | | | |
|---|---|---|---|
| Benzene | No chemical processes | | Deposition<br>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<br>Specialised chemical schemes | Deposition<br>Specialised chemical schemes |

## 3.5 The spatial and temporal resolution of the models

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

### *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 points out 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:

a) Assessment should occur at sites where the concentrations are highest, e.g. kerbside or close to strong sources, as well as in areas representative of the exposure of the general public, i.e. urban background. However, in regard to the positioning of traffic sites (Annex III.C) 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"*.

b) For industrial areas concentrations should be representative of a 250 x 250 m area and for traffic emissions the assessment should be representative for a 100 m street segment (Annex III.B.1.b).

c) Urban background concentrations should be representative of several square kilometres (Annex III.B.1.c).

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 either 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 kerbside or some allowance be 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 between 1.5 – 4 m, the breathing zone (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, but several points representing a 100 m long segment would be required.
- 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 resolution.

In regard to the protection of vegetation and natural eco-systems the AQ Directive is intended to cover regional background levels of pollutants within any zone in areas where eco-systems 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:

a) Assessment should be made more than 20 km away from an agglomeration and more than 5 km away from built up areas or other sources of pollution, e.g. roads with a traffic volume > 50 000 vehicles per day (Annex III.B.2).

b) The area for which the calculated concentrations are valid is 1000 $km^2$, roughly a 30 x 30 km grid (Annex III.B.2).

c) There are exceptions where terrain is complex or small scale eco-systems occur. It is then possible to redefine the representative area to be smaller with a subsequent increase in model resolution (Annex III.B.2).

From a modelling perspective this infers that grid resolutions of 20 - 30 km, or less, are suitable for eco-system assessment. A problem may occur in relation to mixed grids, where emissions from major sources such as major roads or industrial areas in rural areas, are included in a grid that is considered to be rural in nature. Under such conditions Eulerian models of 20 – 30 km 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 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 eco-systems smaller than 1000 $km^2$ or less than 5 km from major sources should be ignored. It is up to the Member States to consider the eco-system 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 $NO_2$, where percentiles are required of hourly means, then in principle a model will need to provide hourly mean concentrations of that pollutant. The same is true for $PM_{10}$, $O_3$, $SO_2$ and CO that all 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, for instance, annual mean $NO_2$ levels to hourly percentiles and apply this to derive the $NO_2$ percentiles. In such a case hourly monitoring data would have been used to develop the relationship.

Table 5 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 eco-systems, as discussed in Section 2.4.

*Table 5. Relation between the AQ Directive temporal averaging period and application region to the model temporal and spatial resolution.*

| Compound | AQ Directive | | Model | |
|---|---|---|---|---|
| | Temporal averaging | Spatial region | Temporal resolution | Spatial resolution |
| $PM_{10}$ | Annual mean<br>Daily mean | Hotspot<br>Urban<br>Rural | Hourly | Individual hotspot<br>1- 5 km<br>10 – 50 km |
| $PM_{2.5}$ | Annual mean | Urban<br>Rural | Annual | 1 – 5 km<br>10 – 50 km |
| Speciated PM | - | Rural | Hourly - Daily | 10 – 50 km |
| $NO_2$ | Annual mean<br>Hourly | Hotspot<br>Urban | Hourly | Individual hotspot<br>1- 5 km |

| | | | | |
|---|---|---|---|---|
| $NO_x$ | Annual mean | Rural | Hourly | 10 – 50 km |
| $O_3$ | 8 hour mean | Suburban<br>Rural | Hourly | 5 – 50 km |
| $SO_2$ | Hourly mean<br>Daily mean<br>Annual mean<br>Winter mean | All | Hourly | All |
| Pb | Annual mean | Hotspot<br>Urban | Annual | Individual hotspot<br>1- 5 km |
| Benzene | Annual mean | Hotspot<br>Urban | Annual | Individual hotspot<br>1- 5 km |
| CO | 8 hour mean | Hotspot<br>Urban | Hourly | Individual hotspot |
| Heavy metals and B(a)P | Annual mean | Hotspot<br>Urban | Annual | Individual hotspot<br>1- 5 km |

## 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. These are represented in Table 6. 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. These are listed as relative uncertainties and a single value of 60% is indicated for all compounds, see Table 6. For modelling the uncertainty is defined in a similar manner to the Air Quality Directive as:

> *"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 precisely for modelling to what the uncertainty will be compared, but states for the measurement uncertainty 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 interpreted to be the same as for the Air Quality 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, but unspecified, way.

### 3.6.1 Mathematical formulation of the AQ Directive quality objectives

As in the previous Directives the wording of this text remains ambiguous. Since values are to be calculated a mathematical formulae is required. As such the term 'model uncertainty' remains open to interpretation. Despite this we suggest the following interpretation that we call, for want of another name, the Relative Directive Error (RDE) and define it mathematically at a single station as follows:

$$RDE = \frac{\left|O_{LV} - M_{LV}\right|}{LV} \qquad (1)$$

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:

$$RPE = \frac{\left|O_p - M_p\right|}{O_p} \qquad (2)$$

where $O_p$ and $M_p$ are the observed and modelled concentrations at the percentile ($p$), used to define the exceedance percentile. The two major differences between the formulations are 1) in the choice of using the closest value to the limit value or using the defined percentile and 2) 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 can be arguments for or 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 will 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 which is shown in Figure 1, which shows the calculation of RDE and RPE for both daily and annual mean $PM_{10}$ concentrations. 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 $\mu gm^{-3}$) is 63. The correspondingly ranked model concentration at the observed limit value is 75 $\mu gm^{-3}$. The resultant RDE will then be RDE = |50 – 75|/50 = 48%. To determine the RPE we see that the 36'th highest observed daily mean concentration is 79 $\mu gm^{-3}$, 29 $\mu gm^{-3}$ above the limit value. The corresponding model 36'th percentile is 108 $\mu gm^{-3}$. From this the RPE = |79 – 108|/79 = 36%. In this example the results are similar 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, but this will depend on the model characteristics. Note that in this example $PM_{10}$ daily mean data has been used, however, there are currently no quality objectives in the AQ Directive for daily mean $PM_{10}$ concentrations.

Also included in Figure 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 agreed to 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 uncertainty there that is

the most important. Any assessment of uncertainty then should be interpretable as an uncertainty around the limit value. i.e. even if there are no data close to the limit value then the expected uncertainty at the limit value should be provided. Unfortunately, determining this may also be subjective .

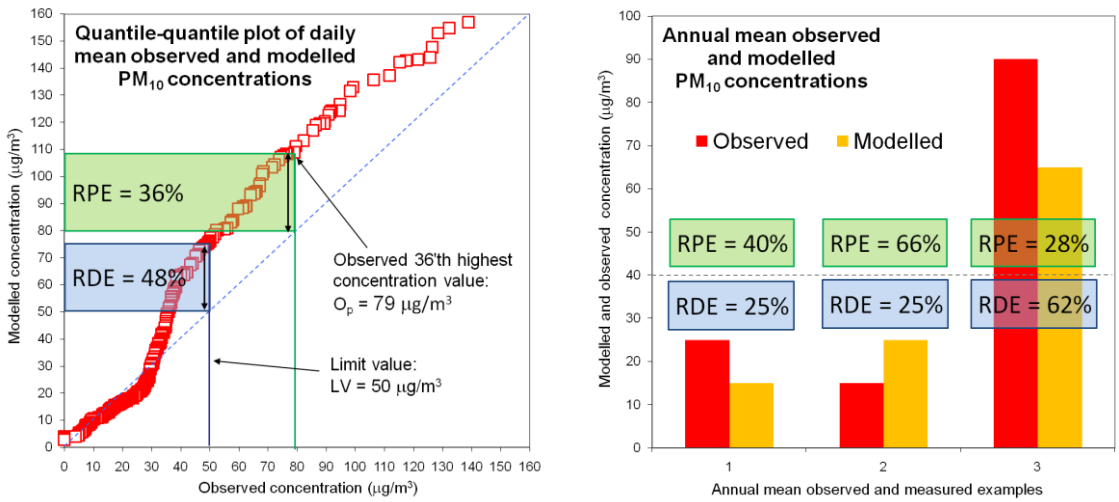


*Figure 1. Left: Quantile-quantile plot demonstrating how to calculate the RDE and RPE for daily mean $PM_{10}$ as described in the text for percentiles. The example is from a traffic station in Oslo, 2003. Right: Bar chart demonstrating how to calculate the RDE and RPE for fictitious annual mean $PM_{10}$ concentrations.*

### *3.6.3 Interpretation 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 to be a clause that allows any outliers, i.e. 10% of the stations, to be excluded from the uncertainty calculation. It is perhaps not intended to be taken absolutely literally, as this will 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 interpretation. Unfortunately there are many urban areas where there are less than 10 stations, especially ones representing the same scale as the model, and as a result the AQ Directive must 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 the following 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 that they are representative for, e.g. 2 x 2 km grid, and as such cannot be expected to provide adequate results on smaller scales, e.g. near roads or industrial sources. Though there can be some discussion concerning how large an area is represented by a monitoring station, common sense can be used if the local environment surrounding the monitoring station is known. If this is not known then station classifications, e.g. traffic, industrial, urban background, etc. can be used to match the models resolution. This is one of the subjects of FAIRMODE activities.

*Table 6. 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 % |

# 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 reporting to the Commission when using models for assessment of existing air quality

The overall requirements for the reporting of air quality assessment to the Commission are provided in Article 27 and Annex I, Section B of the AQ Directive. To aid in such reporting the Commission provides an Excel based questionnaire (http://ec.europa.eu/environment/air/quality/legislation/pdf/questionnaire.xls). To aid in the completion of this questionnaire a guidance document is also provided (http://ec.europa.eu/environment/air/quality/legislation/pdf/guidelines_quest.pdf). This questionnaire is based on the earlier daughter directives, up to and including the 4'th daughter directive on heavy metals (EC, 2005). Assessment reports should be provided within 9 months of the completion of the reporting period. This means that such reports are due by 30 September every year. Following the introduction of the new AQ Directive, new implementing provisions regarding reporting are being developed. These will introduce a new reporting mechanism that will allow the upload of territory resolving maps based on model, or other, calculations.

Most air quality assessments already reported can be found at http://cdr.eionet.europa.eu/ 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. On sheets 8 - 10 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'.

On sheets 19a - 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 submitted 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 then this must be indicated and appropriate referencing included. It is not requested that detailed information be given in the questionnaire itself.

Sheets 21 – 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 given to the methods used to assess the natural contribution to these exceedances. If models have been used then these must be referred to and documentation be made available. These sheets will need to be updated for the new AQ Directive as the range of natural sources has been expanded.

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 Member countries rather than to any justification or assessment of the contribution from another country. However, in any consultation process clearly justified arguments are required and modelling will be invaluable for this.

### *4.1.2 Information required concerning models used for assessment*

The information required concerning any modelling activities that are used for reporting assessment is described in Annex I, Section B of the AQ Directive. 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, population exposed). The remaining information (e.g. uncertainty analysis, description of the methods and results) is too extensive to be included in the questionnaire and is not required by the 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 in 2004 - 2007 (Vixseboxse and de Leeuw, 2008 and 2009) shows that some form of modelling was used by 13 of the 27 Member States to determine the exceedance status in their zones. This was not evenly distributed over the different legislated pollutants with Lead (30.3%), Benzene (21.7%) and CO (17.9%) being the pollutants most frequently reported using modelling, Table 7. The use of modelling for these pollutants has been seen to be increasing. In comparison the use of modelling for the pollutants $SO_2$, $NO_2$, $NO_x$ and $PM_{10}$ between 2004 and 2007 is significantly less at 7 – 10 %. There is no strong trend in their use. Further to these, a number of more extensive examples are provided in Chapter 6 and Annex 1, presenting 'good practise' in model assessment.

*Table 7. EU27 share of zones where exceedances are based to some degree on modelling in 2004 – 2007, taken from Vixseboxse and de Leeuw (2009). Note that there are approximately 1000 zones in total.*

| Exceedance based on modelling | | | 2004 | 2005 | 2006 | 2007 |
|---|---|---|---|---|---|---|
| SO2 | Health | Hr | 13.0% | 12.1% | 10.6% | 10,3% |
| | | Day | 8.0% | 8.8% | 7.7% | 9,7% |
| | Eco | Yr | 21.0% | 14.4% | 7.2% | 6,9% |
| | | Winter | 19.0% | 19.4% | 5.4% | 7,1% |
| NO2 | Health | Hr | 10.0% | 10.3% | 8.5% | 6,1% |
| | | Yr | 12.0% | 10.6% | 4.4% | 10,8% |
| NOx | Veg | Yr | 19.0% | 2.8% | 6.9% | 7.0% |
| PM10 | Day | | 10.0% | 9.3% | 7.2% | 8,1% |
| | Yr | | 9.0% | 8.0% | 6.0% | 7,1% |
| Lead | Yr | | 15.0% | 19.3% | 17.9% | 30,3% |
| Benzene | Yr | | 13.0% | 12.5% | 13.1% | 21,7% |
| CO | Yr | | 14.0% | 9.6% | 11.9% | 17,9% |
| O3 | Health | | 2.1% | 3.3% | 2.0% | 7,1% |
| | Veg | | 2.2% | 3.6% | 2.9% | 6,1% |

## 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 (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 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 in 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 and are also contained 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 new AQ Directive) for the air quality Directive 96/62/EC. A specific 2004/224/EC form, provided as an Excel document, is available for this (http://ec.europa.eu/environment/air/pdf/form_en.xls).

Within this Excel document, are a number of sheets (7 in total) that must be filled in. To help Member States report plans within this form the Commission provides 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 Commission under Decision 2004/224/EC' will soon be available. These documents can be found on the European Commission Environmental website (http://ec.europa.eu/environment/air/quality/legislation/management.htm).

There are a number of points within the management form that are relevant for modelling. These are clearly described in the associated guidance document. The reader is referred directly to this 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 Commission by December 2005. A number of similar background documents concerning plans and programmes may also be found on the CAFE website (http://ec.europa.eu/environment/archives/air/cafe/general/keydocs.htm).

A number of examples of plans and programmes reported to the Commission, and also not yet reported, can be found in Chapter 7 and Annex 1 of this document.

### *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 (http://ec.europa.eu/environment/air/quality/legislation/time_extensions.htm) and in particular provides a document to aid reporting (EC-COM, 2008), including an Excel based form developed from 2004/224/EC. 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 Commission also requires that such plans be drawn up, when appropriate or necessary, and made available to the public and the appropriate organisations (Article 24). The AQ Directive goes on to state in Article 24, section 4 that by June 2010 the Commission will publish a number of best practises of such plans.

### *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 the Member States are encouraged to cooperate with each other to reduce the effects of transboundary air pollution and the Commission should be present and assist during discussions concerning this. There are no formal reporting requirements concerning these activities but the Commission expects to be kept informed of them. 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 as those set out in sections 4.1 and 4.2 above.

### *4.3.1 Annual information to 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. By this it is intended that the relevant information on air quality is 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 model results. It is up to the Member States to define how the information is communicated but it should be in line with that which is reported directly to the Commission.

### *4.3.2 Alert and information threshold information to the public*

On a daily basis Member States are obliged to inform the public first and foremost on any exceedances of the information and alert thresholds (Annex XII and Table 2). 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 information includes:

a) information on observed exceedance(s)

b) 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

c) information on the type of population concerned, possible health effects and recommended behaviour

d) information on preventive action to reduce pollution and/or exposure

In the above list points b) and d) are the most relevant for modelling since they involve the forecasting of air quality for the following day(s) and an 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 to the public*

Also in Annex XVI, article 2 and 3, the AQ Directive indicates the general information on pollutant concentrations that should be made available on a regular basis. Table 8 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). This means, for example, that daily mean values of $PM_{10}$ should be communicated rather than hourly. 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 Air Quality Directive it does not state the required frequency of such information but indicates that updated information should be routinely made available to the public.

*Table 8. 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 |

In general regular reporting to the public occurs through the use of monitoring (see table 9). However, there is no reason why spatially distributed, i.e. through modelling, air quality data 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. Though there are few such near-real time model updates currently available in Europe (PREVAIR currently provides such analysed maps of France for ozone twice daily, www.prevair.org), this task is one of the focus points of MACC (www.gmes-atmosphere.eu/) that intends to provide such information on the European scale.

### *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. In Table 9 a list of these is provided. 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 9. Links to public information web sites for the EEC*

| Country (EEC) | Air quality public information site link | Monitoring information | Modelling information |
|---|---|---|---|
| **Austria** | http://www.umweltbundesamt.at/en/umweltschutz/luft/luftguete_aktuell/ | Daily average | |
| **Belgium** | www.irceline.be/ | Hourly graphs<br>Hourly maps | Three day forecasts for Belgium |
| **Bulgaria** | http://www.icsr.bas.bg/icsrwebsite/departments/rdts/htdocs/index_EN.html | Daily average | |
| **Cyprus** | www.airquality.gov.cy | Hourly graphs | |
| **Czech Republic** | www.chmi.cz/uoco/act/indexe.html | Hourly average<br>Hourly graphs | |
| **Denmark** | http://www2.dmu.dk/atmosphericenvironment/byer/forside.htm | Hourly graphs | 3 day forecasts for Denmark |
| **Estonia** | http://mail.klab.ee/seire/airviro/ | | |
| **Finland** | http://www.airquality.fi<br>http://silam.fmi.fi/AQ_forecasts/v4/index.html | Hourly graphs<br>Hourly maps | 6 hours forecast for Finland |
| **France** | www.prevair.org | Hourly | 1 day French and European forecasts |

| | | | |
|---|---|---|---|
| | | Twice daily maps | Near real time analysis maps |
| **Germany** | www.env-it.de/umweltbundesamt/luftdaten/index.html | Hourly graphs | 3 day ozone forecasts for Germany |
| **Greece** | http://www.minenv.gr/1/12/122/12204/e1220400.html<br>http://lap.phys.auth.gr/gems.asp<br>http://lap.physics.auth.gr/forecasting/airquality.htm | Daily average | General forecasting for Athens<br>3 day forecasting for Athens<br>Daily forecasting |
| **Hungary** | http://members.chello.hu/dasy.kft/forecast/Budapest.htm | Daily map | 2 day forecasting for Budapest |
| **Ireland** | http://www.epa.ie/whatwedo/monitoring/air/ | Hourly graphs | |
| **Italy** | http://www.arpalombardia.it/qaria/doc_DistribSpazialeCalcolata.asp<br>http://www.aria-net.eu/QualeAria | Daily maps<br>Daily graphs | Air quality forecasting for Lombardy region<br>48 hour forecasts of air quality for Italy |
| **Latvia** | | | |
| **Lithuania** | http://stoteles.gamta.lt/ | Hourly average<br>Hourly graphs | |
| **Luxembourg** | http://www.environnement.public.lu/air_bruit/index.html | Hourly average<br>Hourly graphs | |
| **Malta** | http://www.mepa.org.mt/airquality | Hourly average | |
| **Netherlands** | http://www.lml.rivm.nl/ | Hourly maps<br>Hourly graphs | 2 day forecasting for Netherlands |
| **Poland** | http://armaag.gda.pl/en/results.htm | Hourly maps<br>Hourly graphs | |
| **Portugal** | http://www.qualar.org/?page=7&subpage=1&PHPSESSID=c43ac9502aa658b258c016b399430608 | Daily graphs<br>Daily average | 3 day forecasting for Portugal |
| **Romania** | http://www.calitateaer.ro/ | Hourly average<br>Hourly graphs | |
| **Slovakia** | | | |
| **Slovenia** | http://nfp-si.eionet.europa.eu/Dokumenti/GIS/zrak | | |
| **Spain** | http://www.mma.es/portal/secciones/enlaces/enl_auton.htm<br>http://verde.lma.fi.upm.es/wrfchem_eu/<br>http://www.aqforecast.troposfera.org/o3.php<br>http://www.bsc.es/caliope<br>http://pagina.jccm.es/medioambiente/rvca/Dest/principal.htm<br>http://www.gencat.cat/mediamb/qaire/pronostic/pronostic_aire.htm<br>http://gestiona.madrid.org/aireinternet/html/web/ModeloPredictivoAccion.icm?rangoModelo=24&ESTADO_MENU=4_1<br>http://www.ingurumena.ejgv.euskadi.net/r49-n82/es/vima_ai_vigilancia/prevision48.apl<br>http://mca-retemca.ciemat.es/ | General provincial portal for AQ data | 3 day forecasting for Europe<br>3 day forecasting of ozone for Spain<br>2 day forecasts for Europe and Spain<br>Regional forecast for Castilla la Mancha<br>Regional forecast for Cataluña<br>Regional forecast for Madrid<br>Regional forecast for País Vasco<br>General web Portal on Atmospheric |

| | | | |
|---|---|---|---|
| | | | Pollution Modelling in Spain |
| **Sweden** | http://www.slb.mf.stockholm.se/e/<br>http://gems.ecmwf.int/d/products/raq/forecasts/plot_SMHI | Hourly graphs | 2 day forecasting |
| **United Kingdom** | www.airquality.co.uk<br>http://www.airqualityni.co.uk/<br>http://gems.ecmwf.int/d/products/raq/ | Hourly graphs | 1 day forecasts for the UK<br>1 day forecasts for Northern Ireland |
| **Albania** | | | |
| **Bosnia and Herzegovina** | | | |
| **Croatia** | | | |
| **Iceland** | http://www.reykjavik.is/desktopdefault.aspx/tabid-1007 | Hourly average<br>Hourly graphs | |
| **Macedonia FYR** | | | |
| **Norway** | www.luftkvalitet.info | Hourly graphs | Winter forecasts for several cities in Norway |
| **San Marino** | | | |
| **Serbia and Montenegro** | | | |
| **Switzerland** | http://www.bafu.admin.ch/luft/luftbelastung/aktuell/index.html?lang=en | Hourly average<br>Daily graphs<br>Daily maps | |

# 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 develop in parallel with these activities. In the current phase, 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 in Annex 1.5. More detailed information coming from the relevant activities of FAIRMODE, such as further recommendations, examples, specific model evaluation criteria and model validation documentation and datasets will be updated in following versions of this document, leading to clear guidance on the topic of quality assurance.

In general, the quality of models is understood in terms of their "fitness for purpose" (Britter, 1994). The modelling experience gives evidence that there are no "good" models or "bad" models, rather that a model is suitable, or not, 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 Annex 2 (Table A2.1) defining the terms used in this document. As a starting point we work with the concepts of quality assurance and model evaluation, which we can generally describe 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 Glossary, URL1).

**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 that it has been designed for (Following the terminology accepted by COST 732, URL2).

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. e.g. 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.

### *5.1.1 EU activities*

Model evaluation has been supported by the EC through both projects and networks of excellence. The following activities have included aspects of model QA and model evaluation:

- European Commissions Model Evaluation Group (1994), Britter (1994), Vergison (1996) developed recommendations on quality assurance protocols for models used in industrial hazardous gas release.

- Initiative on Harmonisation launched in 1991 (URL3) which has for the past decades promoted and encouraged a harmonised approach to model quality assurance.
- EUROTRAC2 – SATURN (URL4) dealing with urban scale models.
- The Review of the Unified EMEP model hosted a model intercomparison study (van Loon, 2004)
- The modelling inter-comparison exercises EuroDelta and CityDelta (URL5, Cuvelier, et al., 2007) carried out by JRC-IES in support of the modelling activities (urban to regional scales) within the CAFE and NECPI programme.
- ACCENT (URL6) aimed at defining protocols and benchmark tests suitable for air quality assessment in regional and global scales.
- COST Action 728 (URL7) working on standardised model evaluation protocol for meso-scale meteorological models.
- COST Action 732 (URL2) on quality assurance of micro-scale (obstacles resolving) meteorological models.
- The Air4EU project (URL8) 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 (URL9) focused also 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,b,c), originally developed for support to emergency response has recently proved useful as a test bench for air quality models within the context of the COST728 activity where it is being used for a variety of case studies.

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

a) Model evaluation guidance and protocol document for micro-scale meteorological models (Britter and Schatzmann, 2007)

b) Model evaluation guidance for meso-scale models (Schluenzen and Sokhi, 2008)

c) Uncertainty analysis - methodologies and recommendations by AIR4EU for models from hot spot through urban to regional scales (Borrego et al., 2006)

d) Models meta-database (ACCENT, COST 732 and COST 728 at UR10 and URL11) and the Model Documentation System (MDS) of the ETC/ACC (URL12).

### *5.1.2 US experience*

The U.S. Environmental Protection Agency (EPA) uses a wide range of models with different complexity for regulatory decision making. The EPA Quality system, defined in 2000, covers also environmental data produced from models (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, (EPA, 2002). In March 2009 the “Guidance on the Development, Evaluation, and Application of Environmental models” was also published (URL14). It presents recommendations and provides an overview of best 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 recognized the necessity for exploring advanced methodologies for model evaluation as well as the necessity to categorize 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 (URL15) is organized around the model evaluation frameworks of Operational, Diagnostic, Dynamic and Probabilistic evaluation (Dennis et al., 2009) that include:

- Operational evaluation: evaluation based on routine observation for both meteorology and air quality. The comparison is mainly focusing on a one-to-one pairing of model output with monitoring data.
- Diagnostic evaluation: investigates the way in which specific physio-chemical 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: characterizing the uncertainty of air quality model predictions and used to provide a credible range of predicted values rather than a single "best-estimate".

Activities are being organized around and across these four themes that will involve the EU and NA modelling communities in a common modelling effort that will feature both NA and 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 slightly differing categories. This section provides an overview of the key elements of model evaluation based on these works.

### *5.2.1 US – EPA: description of model evaluation*

Key elements of *quality assurance* can be described, following the US-EPA (EPA, 2002), as:

- *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, 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 inter-comparison 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 EPA (URL 14) the process of model evaluation addresses four main elements:

1. Soundness of the science underlying a model.
2. Quality and quantity of available data supporting the choice of model.
3. Model corroboration (qualitative and/or quantitative methods for evaluating the degree to which a model corresponds to reality).
4. 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:

1. *Model description* (brief description of the characteristics of the model, intended application range, theoretical background, parameterisations, data used, etc.)
2. *Database description* (complete description of the database to be used for the evaluation of the model, including data uncertainty estimation)
3. *Scientific evaluation* (description of the equations employed to describe the physical and chemical processes that the model has been designed to include)
4. *Code verification* (to analyse whether the conceptual model is correctly implemented in a computerized model, estimation of numerical error)
5. *Model validation* (comparison with experimental data including statistical analysis)
6. *User-oriented assessment* (includes documentation of the code, best practice guidelines)

The above steps of model evaluation have been further elaborated for the purposes of quality assurance of micro-scale meteorological models and for the purposes of evaluation of meteorological and air pollution meso-scale models.

### *5.2.3 EU COST 732: description of model evaluation*

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

1. Scientific evaluation
2. Verification
3. Validation datasets
4. Model validation
5. An operational user evaluation that reflects the needs and responsibilities of the model user.

The document provides a step-by-step guidance for model evaluation addressing both 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 approach. The results are published on the COST732 page (URL2).

### *5.2.4 EU COST 728: description of model evaluation*

The proposed Model Evaluation protocol for meso-scale meteorological models consists of three groups, summarizing the key elements (Schluenzen and Sokhi, 2008). These are:

1. General evaluation (includes model description and user oriented assessment)
2. Scientific Evaluation (includes also database description)
3. 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 best practice guideline.

### *5.2.5 GLOREAM: description of model evaluation*

The model evaluation for regional scales adopted in the framework of the GLOERAM project (Builtjes et al., 2003) includes three different elements:

1. A strategy protocol
2. A core activity of model runs

3. 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 (MQO), 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 mentioned as relevant or necessary for model evaluation. These are uncertainty analysis, sensitivity analysis and model inter-comparisons.

1. *Uncertainty analysis* is the process to characterise 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 given also to the process of communicating uncertainties, especially for decision making. Uncertainty analysis covers a range of activities, including model inter-comparison and sensitivity analysis. More details are given in Section 5.3.
2. *Sensitivity analysis* is a process to understand 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 two fold. It can be used to propagate uncertainty in input parameters for uncertainty assessment and it can be used 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 e.g. in Saltelli et al. (2005).
3. *Model inter-comparison* is the process to assess 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 parameterisations 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 (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):

1. *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.
2. *Input data uncertainty:* related to emissions, observational data (accuracy and representativeness), meteorology, chemistry, model resolution
3. *Inherent variability* due to random turbulence. This refers to stochastic and anthropogenic processes that by nature are not known.

It may be possible to reduce the first component 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, in emissions, in Gaussian regulatory models, in 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, but also other statistical methods can be applied, such as maximum likelihood estimation technique (Koračin et al., 2007), 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 inter-comparison (model uncertainty) and spectral analysis (stochastic variations).

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 recently by Miranda et al. (2008). It includes also 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, URL8). It is recommended to present a qualitative (e.g., graphical representation of time series, 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, while the third one is more comprehensive since it details the total model uncertainty and the contribution of different components. For decision making the second level is appropriate. The following statistical parameters have been recommended: correlation coefficient, fractional bias, root mean square error and normalised mean square error. This is in addition to the parameter according The AQ Directive, see Section 3.6 for the definition of the Relative Directive Error.

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

The following list indicates some of the main methods available for assessing model uncertainty.

- **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 (PDF) 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, e.g. Latin Hyperbole Sampling, are then necessary for implementing the method.
- **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 intercorrelations between various inputs. 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.
- **An ensemble of models** can be used to indicate uncertainty in not just input parameters, as in the Monte Carlo approach, but also in the model formulation. The ensemble of different model outputs can be comprised of different models (multi-model ensemble), different initial and boundary conditions, and/or different model physics modules. Though, 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 among air quality modellers, (Galmarini et al., 2004b,c, Vautard et al.,2008).

- **Model inter-comparisons** and model ensembles are generally similar in the sense that they require output from multiple models. Model inter-comparison, however, are intended to assess not just the uncertainty but the reasons for the variability between models.
- **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 that reflect the PDF of the model results. This method will then include not just model uncertainties but also monitoring, representativeness and stochastic uncertainties. Generally the total model uncertainty is 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 (MQI)

### *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 last 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 (SD), the mean normalized 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 good 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 - normalized accuracy of domain-wide maximum 1-hour concentration unpaired in space and time, mean normalized 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 (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 100-1000 km, generally assesses the mean observed and modelled bias as well as the daily mean RMSE and correlation coefficient (EMEP, 2008).

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 could 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)
- Normalized 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. Statistical metrics may even sometimes be misleading. For this reason qualitative analysis, also referred to as exploratory data analysis, is indispensable. Such an analysis may reveal shortcomings in both input data, model setups or model descriptions (see e.g. the COST 732 report on model evaluation case studies (COST732, 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:

- *Scatter plots:* paired in time (modelled vs. observed) values are plotted against each other in a two dimensional plot. This is a class 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 it's related metrics, as a quantitative indicator.
- *Quantile-quantile plots:* unpaired in time and separately ranked (modelled vs. observed) values plotted against each other in two-dimensional space. 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 data sets, e.g. when plotting accumulated diurnal or monthly datasets.
- *Residual plots:* usually show the ratio of modelled to observed values, as function of various physical parameters (Hanna et al., 2003), e.g. the ratio of modelled to observed concentrations as function 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 USA 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 understand 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:

- *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 Harmonisation initiative. Along with statistical metrics, there is a possibility for graphical plots as 'exploratory data analysis'. The last update of the package is dated 2007 with addition of a new parameter – the Hit Rate, found especially useful for velocity models.
- *ASTM Guidance* – ASTM is the USA 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 for example according to atmospheric stability. The ASTM package, prepared by J. Irwin and distributed through the Harmonisation web page (URL3) 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).

- *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 is designed to analyse MM5, WRF, CMAQ and CAMx model outputs. 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 aircraft.
- *JRC Tool* – In order to facilitate the inter-comparison of model results, JRC-IES (Ispra, Italy) has developed an IDL-based visualization tool which allows working interactively and off-line on the results. Different versions of the Tool have been developed for the CityDelta (urban scale, URL5), the EuroDelta (regional scale, URL16), the POMI (Po Valley – Italy, URL17) and the HTAP (global scale, URL18) projects. In general the Tool contains a module for Validation (i.e. model comparison with observational data), a 'Delta' module for the visualization of the impact of emission reductions, and a module for the visualization of monthly averaged plane data in both longitude-latitude projection and the EMEP-specific projection. A large number of variables and indicators is available and include:
    - Variables: Meteorological variables; gas-phase, and aerosol-phase species, as well as wet and dry deposition quantities.
    - Indicators: Mean values, bias, maximum, minimum, standard deviation, correlation coefficient, RMSE, exceedance days, AOTx, SOMOx, time series, scatter plot, 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 in different studies suggests 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.
- MQI for concentrations should be pollutant specific and scale specific, both temporal and spatial.
- The spatial representativeness of both model and observations must be considered when defining MQI's, since observations are point samples whilst models 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 give little or no 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 alone is a necessary, but not sufficient criteria, for model evaluation. It should be completed 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 context with quality assurance. The documentation should cover the following aspects:

1. Description of the quality assurance procedure itself (e.g. evaluation protocol)
2. Description of the model, both conceptual formulation and numerical implementation

3. Description of the required input data and its formatting
4. Description of the validation methods applied and the validation dataset
5. An analysis of the validation
6. An analysis of uncertainties (of both individual elements and of the overall system)

Model validation is one of the reporting points in the *AQ Model Documentation System* (MDS), developed and maintained by the European Topic Centre on Air Quality and Climate Change (ETC/ACC) and accessible on the internet (URL12). 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 a well defined and harmonized methodology, that will be valid for all models and model categories (Moussiopoulos et al., 2000).

The web based *COST 728/732 model inventory* (URL11) provides detailed information on model capabilities, including model validation/evaluation studies according the following four categories: analytic solutions, evaluated reference dataset, model inter-comparison and additional validation and evaluation efforts. The inventory includes models for the micro-scale, for the meso-scale (regional models) and macro-scale and covers both meteorological and chemical transport models.

A *meta-database* has been compiled in COST 728 (URL10) for the purposes of meso-scale 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 above publication.

## 5.6 Special topics

### *5.6.1 Evaluation of different modules of the air quality model*

AQ models are complex systems based on different modules – emission model, meteorological model, chemical-transport model (CTM). Meteorological predictions and emission inventories are critical components for the CTM performance. 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 (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 emission trend vs. ambient air concentration trends, inverse modelling, receptor modelling (source apportionment) (Friedrich and Reis, 2004, Pulles and Builtjes, 1998).

In the USA 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 (URL7) have put their main effort on improving meteorological meso-scale models used in atmospheric dispersion studies and on providing methodologies and tools for their evaluation (Schluenzen and Sokhi, 2008).

Evaluation is needed also for the interface that links meteorological output to CTM. The interface is often used in off-line AQ systems, since most meteorological models are not built for air quality simulations and the further data elaboration is need to provide the complete set of parameters required for the CTM and 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 (multi-scale) 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 referred to, 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 assessment. Currently the COST action ES0602, Chemical Weather (URL19), 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, those 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 assessment purposes.

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 of the AIRBASE network 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. 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 D7.1.3 (URL8) this kind of error is 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 station's 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 on 'Representativeness of model outputs and monitoring data' M.3 (URL 8) also discusses the question of representativeness for both model and monitoring applications.

## 5.7 Recommendations on the framework for model quality assurance

Though 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. Experiences have 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 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 dependent on the application, and the resulting methodologies for quality assurance may 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 concentrations levels, but also on the different modules (emission, meteorology) relevant for simulation of concentrations.
- A sensitivity analysis, an uncertainty analysis and a model inter-comparison 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 with respect to both computing and labour resources.

In Figure 2 many of the elements of quality assurance and model evaluation are visualised. A number of aspects need to be defined in the planning phase, e.g. problem definitions, user requirements, etc. before model evaluation should 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 elements of model evaluation, e.g. model inter-comparisons 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 during the course of FAIRMODE.

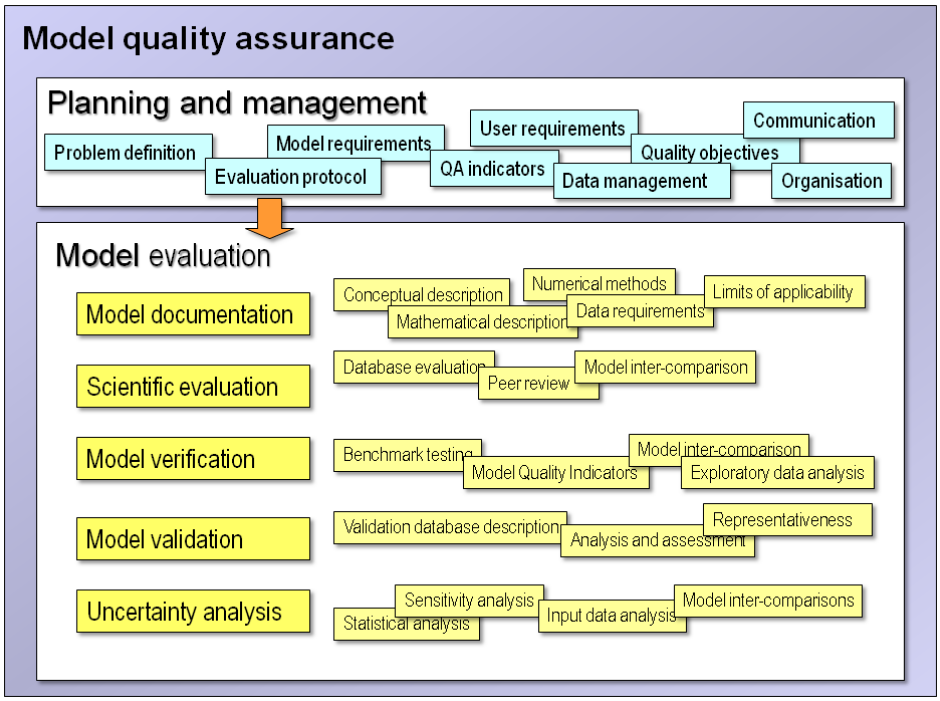


Figure 2. Visualisation of the different elements involved in model quality assurance.

# 6 Applications of models for 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, 2007; 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 assessment. Another European project INTEGAIRE (www.integaire.org), which ended in 2004, collated a range of air quality assessments and best practices for both assessment and planning, some of which are relevant for modelling. 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

The main steps in any air quality assessment using models involves the following:

1. Screening and identification of likely sources and causes of poor air quality
2. Establishment of emission inventories and modelling tools
3. Validation and assessment (e.g. source apportionment) of the models and inventories
4. Iteration and improvement of the modelling system

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

a. Air quality monitoring data for validation or assimilation.
b. Meteorological monitoring data for validation, model input parameters or for use with diagnostic wind field models.
c. Emissions inventory.
d. Other relevant input data dependent on model type, such as background concentrations, land use or traffic data.
e. Modelling tools for carrying out the assessment (i.e. the air quality model and meteorology).
f. Analysis tools for validation and assessment.

There are a number of different aims for air quality assessments and the three dealt with in this chapter are:

1. Assessment for the purpose of reporting exceedances of the AQ Directive or national limit values
2. Assessment for the purpose of calculating population exposure and health impacts
3. 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, etc. Indeed, the AQ Directive (see section 4.1.2) requires both an assessment of exceedances and of the population exposed to these. Since such strong overlap exists between the applications we divide 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 the above type 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 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 is not available for validation. Applications for planning and forecasting are dealt with separately in chapters 7 and 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 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 required quality of assessment.

It is important to note that the application of models when no monitoring data is 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 is generally true for all modelling it is of particular importance where there is no monitoring data available to validate the model calculations. An example of where modelling as been extensively applied and the number of monitoring stations reduced by 50% is provided in A1.1.6. In this case, modelling has been extensively applied for carbon monoxide in the UK because concentrations of this pollutant have been persistently 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 models and the monitoring.

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

A number of examples of such assessments are reported to the Commission. Some of these are described in Annex 1.1. For example, Copenhagen uses an integrated approach to assessment (Example A1.1.1) where both models and monitoring are presented together, and the models are used to extend the geographical coverage of the assessment. Oslo (Example A1.1.2) 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 also been carried out using modelling at 10 x 10 km, taking into consideration the Air Quality Directive limit values (Monteiro et al., 2005, 2007). Results of the modelling exercise were reported to the Portuguese Agency aiming at a first overview of the air quality levels for all of 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 then 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 optimization 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; 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 data sources.

One of the most straightforward methods that can be applied to combine monitoring and modelling data is multiple linear regression, where model concentrations, and also other supplementary data, are fitted to the available observations using least squares optimization (e.g. Horálek et al., 2007), see also Example A1.1.4 and

A1.1.5. 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). Though 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. Data assimilation refers to a modelling technique that incorporates monitoring data directly into air quality model calculations during the modelling process itself. It is the measured data that helps guide the model towards an optimal solution, and one that is consistent with the physical description provided by the air quality model. The most common type of data assimilation applied are variational methods (Elbern et al., 1999), which are 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). Data assimilation in these forms is most often applied on the regional scale and is 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 on 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, industry), or may 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 co-operation is required (e.g. CLRTAP). In this section we describe modelling methods that are principally aimed at identifying local sources as these are related to the local assessment of air quality. In Section 7.3 the contribution of long range transport is discussed 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. There is a range of methods available including:

1. 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, e.g. wind roses, to identify sources. These methods can provide a basic level of information for the larger sources.
2. 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.
3. **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 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 done to some extent through chemical analysis and receptor modelling (dependent on the uniqueness of the chemical profile of the contributing sources) but for gaseous pollutants, such as ozone 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 Commission. For most applications source apportionment is carried out in sectors (e.g. traffic, industry) or sub-sectors (e.g. diesel heavy duty, diesel light duty, etc.). When the pollutants involved are considered to be linear (e.g. non-reactive species) then source contributions can be determined by separate model runs of the individual sources. However, for non-linear 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 plans or supporting requests for postponement or exemptions. Some examples are provided in Annex 1.2.

Complex pollutants involving non-linearities 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 CAMx to the Milan region to assess the source contributions of local and regional sources to $PM_{2.5}$ concentrations (Annex 1.2.7). They use the PSAT algorithm for the source apportionment which provides an effective method for modelling source apportionment when a large number of sources are 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 consumption rates or 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 this 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, then 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 but 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. Cosomans and Mensink (2007) also applied a similar method to determine fugitive emissions of $PM_{10}$ from an industrial region in Antwerp.

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 (i.e. how many similar solutions are possible) the inverse problem is. 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) then an air quality action plan is required from the Member States for the effected zone or agglomeration. In regard to ozone (*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 co-operative 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*) to the commission within 2 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 explicitly 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 the 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, 2002). 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, industrial planning, regional development plans, urban planning, environmental health, etc..

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 then 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.

A good practice database was previously developed in the INTEGAIRE project (www.integaire.org/indexuk.html) that concluded in 2004. Within this database are a number of summarised examples and recommendations for developing and assessing action plans.

## 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 assessing air quality plans.

The main steps in any action plans involve the following:

1. Screening and identification of likely sources and causes of poor air quality
2. Establishment of emission inventories and modelling tools
3. Validation and assessment (e.g. source apportionment) of the models and inventories
4. Identification of possible measures to reduce emissions
5. Development of emission reduction scenarios

6. Assessment using models of the emission reduction scenarios
7. Iteration of the process to determine optimal reduction scenarios, including the feasibility of the emission scenarios

The first 3 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 it's 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 in Annex 1.3.

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

In Annex XII levels of information and alert thresholds for $SO_2$, $NO_2$ and ozone 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, air quality models are well 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, 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 (www.gse-promote.org/services/localAQ_sub.html). On the European scale both PROMOTE (http://wdc.dlr.de/data_products/projects/promote/IAQ) and GEMS (http://gems.ecmwf.int/d/products/raq/) projects provide a feasibility study related to the use of ensemble forecasts for all of Europe. These forecasts are based on an integrated ensemble of up to eight European air quality models running fully operationally in a number of countries (most are listed in table 9). As continuation of the PROMOTE and GEMS projects, operational ensemble forecasts will be provided by the end of 2009 within the MACC project (Monitoring Atmospheric Composition and Climate – FP7, www.gmes-atmosphere.eu/) which will be the cornerstone of the future GMES Atmospheric Service (Global Monitoring for Environment and Security). Such regional scale forecasts are useful information for providing regional scale concentrations, particularly in regard to compounds such as ozone, but also provide background contributions for urban scale forecasts.

Model studies have shown that short term action plans can be effective if they are decided 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, 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, alternating circulation) and industrial emission controls. Though it is recommended in the AQ Directive, use of forecasting results for designing emergency measures is still a new approach and not fully adopted by the Member States. Its relevance depends on the forecasting models' quality and accuracy, meaning their ability to avoid 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 ozone (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 forecasts 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 co-operation 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 an assessment.

### *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' possibilities to reach their environmental and policy objectives, such as meeting air quality standards or reducing pollution load below critical levels, according to the AQ Directive. Major emission reductions for $SO_2$, $NO_x$, VOCs and ammonia as adopted in the Gothenburg Protocol under the Convention on Long Range Transboundary Air Pollution (CLRTAP) and EU legislation, primarily the Directive 2001/81/EC on National Emission Ceilings (EC, 2001c), have reduced the harmful effects associated with the presence of these substances, namely their contribution to the formation of photochemical smog and the acidification and eutrophication of water and soil (Moussiopoulos et al., 2004). However more recent assessments have also shown (EEA, 2005) that a number of health related transboundary pollutants, notably particulate matter and ozone, are still at levels harmful to human health.

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 the Convention on Long-Range Transboundary Air Pollution (LRTAP) 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, Castells and Funtowicz, 1998). Within the framework of the Gothenburg Protocol (multi-pollutants/multi effects), these models have extended their domain of application to photochemical air pollution (ozone) and even more recently (the Gothenburg Protocol and the NEC Directive being revised) to primary and secondary particulate matter.

Though CLRTAP 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 on the hemispheric transport of air pollution (URL1) 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 as well as due to 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 CLRTAP (e.g. the task Force on measurement and Modelling of the EMEP program), the European Commission (e.g. City Delta or the FAIRMODE initiative) or the scientific community (e.g. the AQMEII project) help in building confidence in such models for policy applications.

### *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. EMEP is one such model that provides support for the CLRTAP.

EMEP carries out source-receptor calculations every year to identify the transboundary contributions within Europe and this information can be used to support air quality plans between Member States (see example A1.2.3). The status reports, technical notes, and country reports focusing on each Party to the Convention are issued by MSC-W annually and are freely available on the internet at http://www.emep.int/mscw/mscw_publications.html. 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 the Convention. In addition annual reports on transboundary transport of particle matter (e.g. Yttre et al., 2009) are produced based on both modelling and monitoring data.

Though EMEP is supported by the CLRTAP, other studies of transboundary air pollution are regularly carried out by national and local authorities to assess the contribution of long range transport.

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

Independent of the European wide assessments carried out 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.

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 taking into account distant pollutant emission sources. Particularly in the case of ozone, 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 the 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 and Stuttgart 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 ozone fine structure (OFIS) model. 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 as the ones considered in this study depends on both urban and regional scale influences. Urban VOC control was found to be effective in reducing ozone primarily on the local or urban scale, whereas urban $NO_x$ control would cause an increase of urban peak ozone 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, Derwent and Maryon, 2000), the UK Met Office's dispersion model, NAME, has been used to model hourly concentrations of sulphate aerosol for 1996 at a number of UK 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 primary PM over Europe (ApSimon, Gonzalez del Campo and Adams, 2001) uses a simple atmospheric transport model to estimate the contribution of primary particulate material to $PM_{10}$ and $PM_{2.5}$ concentration across Europe. The resulting population exposure is compared with that of secondary particulates, and it is found that both primary and secondary contributions will be significantly reduced with the implementation of new protocols under the Convention on Long-Range Transboundary Air Pollution (CLRTAP).

# 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 AQ 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 and a guidance document on this, as well as on assessing salt and sanding contributions, is currently under development and is expected in 2010. These documents, when completed, will be available through the Commission web portal (http://ec.europa.eu/environment/air/quality/).

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 monitoring data. To assess what type of event has occurred, models (such as back trajectories modelling) and satellite data can be used to identify the source regions and confirm the origin. Often emissions are poorly known of these natural sources and so any forward modelling and prognosis of these 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), four Member States (CY, GR, ES, and PT) claimed $PM_{10}$ derogation on the basis of natural events and five Member States (EE, FI, LT, LV and SK) 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 as well. If a Member State can adequately show that exceedances of the daily mean limit value are caused by road salt and sanding activities then these days are not included in the exceedance assessment.

The Commission will provide guidance on this in 'Guidance on assessing the contribution of winter-sanding and –salting under the EU Air Quality Directive' (http://ec.europa.eu/environment/air/quality/). In the draft version of that 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 and no preferred or recommended method is provided for winter sanding. However, chemical analysis and the application of receptor modelling is 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). However, none of these have been applied to quantify salt emissions and they only implicitly treat the effect of sanding. They also do not currently have the required level of certainty in predicting daily mean $PM_{10}$ concentrations.

The current set of emission models used to calculate road dust and other non-exhaust contributions to PM are not capable of providing the required information for assessing the contribution of winter sanding and salting to daily mean $PM_{10}$ exceedances and so monitoring and statistically based methods should be applied. This may, however, change in the future as new models are currently under development.

## 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 target values due to their episodic nature.

The Commission is currently developing a guidance document on natural contributions 'Guidance on the quantification of the contribution of natural sources under the EU Air Quality Directive' that will be available in 2010 through the Commission web site (http://ec.europa.eu/environment/air/quality/). This guidance document is based on a prior technical document (Marelli et al, 2007). For the particular case of Saharan dust episodes it is recommended in that document to use 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 for this, 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 in A1.2.5.

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 practise, however, quantifying daily mean $PM_{10}$ concentrations to the required level of uncertainty (50%) using only models is not currently feasible and 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 in Annex 1.

Saharan dust forecasts are currently carried out by the University of Athens using the SKIRON forecasting system (http://forecast.uoa.gr/dustindx.php), the Earth Sciences Division of the Barcelona Supercomputing Center (BSC) using the BSC-DREAM8b model (www.bsc.es/projects/earthscience/DREAM/), the Monterey National Research Laboratories aerosol page (www.nrlmry.navy.mil/aerosol/) and the Tel-Aviv University Weather Research Center (http://wind.tau.ac.il/dust8/dust.html). A number of, but not all, regional scale air quality models, such as CHIMERE (Vautard et al., 2005), also contain modules that describe wind blown dust emissions.

Back trajectory modelling may be carried out with a number of models. Models commonly used for such applications including 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 being *"sea sprays".* Such events also 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 Commission will also provide guidance on this contribution in the future document 'Guidance on the quantification of the contribution of natural sources under the EU Air Quality Directive' (http://ec.europa.eu/environment/air/quality/), 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 $Cl^-$ or $Na^+$ 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 applied. In the first Van Jaarsveld and Klimov (2009) applied the OPS-ST model and in the second Manders et al. (2009) have applied the LOTOS-EUROS model to calculate sea salt contributions using a model resolution of approximately 6 km. These model applications are described in the example A1.2.7. 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 – 3. However, the long term average concentrations (over five 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 models for sea salt (e.g. Unified EMEP model and CHIMERE). 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 km or 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 observations.

Forecasts for sea salt are also available, e.g. the Tel-Aviv University Weather Research Center provides sea salt forecasts (http://wind.tau.ac.il/salt-ina/salt.html) 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 km) 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 it's contribution leads to exceedances. This source is also addressed in the 'Guidance on the quantification of the contribution of natural sources under the EU Air Quality Directive'. The draft of that Guidance document importantly 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 States 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 that includes the use of validated air quality modelling and back trajectories, combined with satellite and ground based monitoring as well as chemical analysis.

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 estimates possible 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 (URL1), 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.

There are a number of ongoing studies and projects dealing with wild land fires, particularly in countries such as Portugal, France, Finland and Greece where there can be significant episodic contributions from forest fires. e.g.

Miranda (2004), Hodzic et al. (2007) and Miranda et al. (2008). An example is provided in A1.2.2. 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 an emerging evidence that smoke from widespread wildfires in Portugal in summer 2003 contributed to the high ozone levels measured at the air quality monitoring stations in Paris (Hodzic et al., 2006). In the scope of the COST728 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 USA 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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http://www.unece.org/env/lrtap/ExecutiveBureau/Air.Pollution%20Studies.No.16.Hemispheric%20Transport.pdf

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## Relevant links to the European Commission

European Commission Environment and Air homepage http://ec.europa.eu/environment/air/index_en.htm

European Commission Environment and Air homepage for reporting plans http://ec.europa.eu/environment/air/quality/legislation/management.htm

# Annex 1: Example case studies

In this Annex a number of more detailed examples are provided that illustrate the use of models for carrying out assessment, planning and source apportionment studies. These examples have either been directly provided by the modelling community or have been extracted from publications

This guidance document has sort to include examples for the following range of applications:

1. Where models are used in combination with measurements for AQ Directive assessments (A1.1)
2. Where only models are used for AQ Directive assessments (A1.1)
3. Where models are used for source apportionment studies including the following special topics (A1.2)
    a. Assessing the contribution of transboundary air pollution
    b. Assessing the contribution of winter sanding or salting of roads to PM exceedances
    c. Assessing the contribution of wind blown and Saharan dust events to PM exceedances
    d. Assessing the contribution of sea salt to PM exceedances
    e. Assessing the contribution of wild-land fires to PM exceedances
4. Where models are used for air quality planning to attain the limit and target values (A1.3)
5. Where models are used to determine the risk of exceedance of the alert threshold and/or developing short term action plans to prevent this (A1.4)
6. Examples of model validation or evaluation exercises and protocols (A1.5)

The contributions are summaries only but provide references for further reading.

## A1.1 Examples for air quality assessment and exposure

### *A1.1.1 Integrated Monitoring and Assessment in Urban Air Quality Management in Copenhagen, Denmark*

Integrated Monitoring and Assessment (IMA) is defined as the combined use of measurements and model calculations. The use of IMA has been the guiding principle for assessment of air quality and deposition in Denmark within different areas. A comprehensive overview of the Danish approach to IMA is provided by Hertel et al. (2007). This example focuses on how IMA is applied in urban air quality assessment and management in Copenhagen, Denmark. The city of Copenhagen has about 600,000 inhabitants and the Greater Copenhagen Area has about 1.8 million inhabitants.

The National Environmental Research Institute (NERI) operates the Danish Urban Air Quality Monitoring Programme that is designed to fulfil the requirements in the EU AQ Directive on air quality assessment and management, and at the same time supports air quality modelling requirements. The measurements are used to determine actual levels and trends, to obtain process understanding, and for the development and validation of air quality models. The results from the air quality and receptor models are used in the interpretation of measurements e.g. for source apportionment to determine the emission contribution from different vehicle categories. Analyses of street and urban background concentrations have revealed that the direct emission of $NO_2$ from traffic has increased in recent years. Air quality models also predict this trend due to an increase in the number of diesel-powered passenger cars and heavy-duty vehicles with particle filters that increase direct $NO_2$ vehicle emissions. The model calculations are used to extend the geographical coverage beyond the few monitoring locations. Further, the air quality models are applied to carry out scenario studies of future pollution loads, e.g. assessment of the impacts of various emission reduction strategies.

NERI has developed a decision-support GIS tool for management of urban air quality and human exposures known as AirGIS (Jensen et al. 2001). The system integrates air pollution dispersion models, digital maps, national and local administrative databases, regional and meteorological data, and a Geographic Information

System (GIS). The system uses the Danish Operational Street Pollution Model (OSPM) (Berkowicz 2000a) and the Urban Background Model (UBM) (Berkowicz 2000b), digital maps on roads with traffic data, registry data for buildings, and it applies a GIS. The EU COPERT IV emission model is integrated into the OSPM model to provide emission data. One of the unique features of AirGIS is that it is able to generate street configuration and traffic data for the OSPM model based on digital maps. This enables estimation of air quality levels at a large number of locations in an automatic and effective way. All necessary input data for AirGIS has been developed to allow calculation of air quality levels at any street location in Denmark.

In recent years, air quality modelling at selected streets in urban areas has been an integrated part of the Urban Air Quality Monitoring Programme that provides annual reports on the air quality situation in Denmark (Kemp et al. 2008). Measurements at the two street monitoring stations in Copenhagen have shown that the EU limit value for annual mean of $NO_2$ in 2010 (plus margin of tolerance) has been exceeded in recent years, and also the limit value for annual mean of $PM_{10}$ in 2005 has been marginally exceeded. Due to these compliance problems several studies with focus on $NO_2$ have been conducted that have mapped air quality levels at selected streets in Copenhagen in 2010, 2015 and 2020 and assessed abatement measures (Jensen et al., 2005). The analyses evaluate urban background concentrations as well as street concentrations at 138 street canyon locations with Average Daily Traffic 15,000 – 65,000.

The studies go beyond traditional air quality assessment as an integrated and comprehensive traffic modelling and air quality modelling approach is used. This approach assesses the impact of different abatement measures and evaluates the feasibility of the measures for solving compliance problems. The abatement measures have included (a) traffic management (b) reductions in transport by toll ring or road pricing, and (c) cleaner transport emission technologies as part of an environmental zone. The studies have shown that the $NO_2$ limit value in 2010 is expected to be exceeded in 65 out of 138 streets which will drop to no, or few, exceedences in 2020 due to penetration of more stringent vehicle emission standards already adapted. Requirements of cleaner emission technology e.g. SCR $NO_x$ catalysts (Selected Catalytic Reduction) on heavy-duty vehicles is the most effective measure to ensure compliance in 2010 whereas traffic management and economic measures have limited potential for reduction of exceedences. Few compliance problems are expected for $PM_{10}$ in 2010 and beyond.

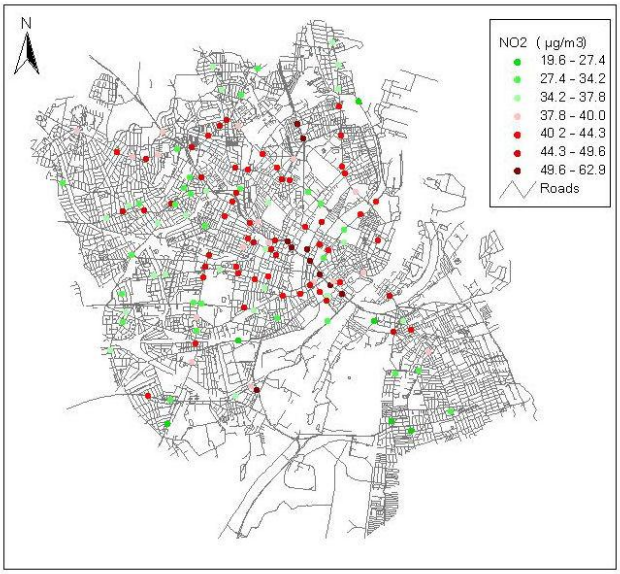


*Figure 1. Annual mean of $NO_2$ in 2010 modelled with AirGIS at 138 selected busy street canyons in Copenhagen*

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### *A1.1.2 Dispersion, Source apportionment and Exposure Calculations of $PM_{10}$, $NO_2$ and Benzene in Oslo and Trondheim for 2007*

The Norwegian Institute for Air Research has calculated the outdoor concentration levels of $PM_{10}$, $NO_2$ and C6H6 (Benzene) for the winter season (January through April, and October through December) for 2007. Ambient air concentrations and population exposure have been calculated both in the positions of buildings located close to the main road network, and within a two-dimensional grid domain (quadratic 1 km2 grid size).

The inhabitants of the representative buildings are assigned to the building point concentrations, while the remaining population is assigned concentration values computed in the grids containing the location of their home address. The exposure calculations have been performed with respect to the goals defined in the ”National Air Quality Targets”(Statens forurensningstilsyn 1998). These targets specify that during a one year period the following limits should be met: no more than 8 hours (hourly mean) of $NO_2$ concentration levels above 150 µg/m3, no more than 7 days (daily mean) of $PM_{10}$ concentration levels above 50 µg/m3, and the yearly averaged Benzene concentration should not exceed 2 µg/m3. The total exposure results for Oslo and Trondheim for 2007 (and 2005) are summarized in Table A.

*Table A: Number of people exposed to exceedances of the goals defined in the “National Air Quality Targets” for* $PM_{10}$, $NO_2$ *and Benzene in Oslo and Trondheim for 2007. Results for 2005 are given in parenthesis.*

| | OSLO | TRONDHEIM |
|---|---|---|
| **$PM_{10}$** | 186 744 (235 849) | 4994 (20 914) |
| **$NO_2$** | 4193 (652) | 85 (40) |
| **Benzene** | 6224 (31585) | 0 (0) |

When considering the exposure estimate presented in Table A, it should be noted that relatively small changes in the calculated concentration levels can result in large changes in the numbers of inhabitants exposed to exceedances. This is especially the case when grid square concentrations in proximity to the target value are computed. For the building points and grid squares in which exceedances of the “National Air Quality Targets” have been found, the relative contribution from the main source categories have also been estimated. When performing this source apportionment calculation, only hours (for $NO_2$) and days (for $PM_{10}$) contributing to the exceedances have been considered, and the final estimate is the average percent contribution from the various sources. No source apportionment estimate was performed for Benzene in this study.

The average source contribution (in percent) to the exceedances in Oslo are summarized in Tables B and C. Since only buildings in the vicinity of the main roads have been treated separately as building points, the exceedances in these points are naturally influenced by traffic. The main source for exceedances is clearly road traffic for both components. For $PM_{10}$, domestic wood combustion is the second most dominant local source.

*Table B: Source contribution (percentage) to the exceedances of the “National Air Quality Targets” for* $NO_2$ *for Oslo in 2007.*

| Calculated in | Domestic wood comb. | Traffic | Regional background | Other sources |
|---|---|---|---|---|
| Building points | 0.06 | 93.52 | 0.18 | 6.25 |

*Table C: Source contribution (percentage) to the exceedances of the “National Air Quality Targets” for* $PM_{10}$ *for Oslo in 2007.*

| Calculated in | Domestic wood comb. | Traffic | Regional background | Other sources |
|---|---|---|---|---|
| Building points | 20.68 | 72.26 | 4.60 | 2.46 |
| Grid squares | 29.71 | 62.29 | 3.90 | 4.10 |

Sundvor, I., L.H. Slørdal and S. Randall (2009). Dispersion and Exposure Calculations of PM10, $NO_2$ and Benzene in Oslo and Trondheim for 2007. NILU Report OR 9/2009. http://www.nilu.no/index.cfm?ac=publications&folder_id=4309&publication_id=22930&view=rep

### *A1.1.3 Street level modelling for regulatory purposes in Antwerp*

Another example of a model application for the estimation of the contribution of main streets in urban air quality is the AURORA (Air quality modelling in Urban Regions using an Optimal Resolution Approach) case study. The integrated air quality box model AURORA was used, in combination with an emissions module, for the assessment of $NO_2$, $SO_2$, $PM_{10}$, CO and benzene concentrations against the legislated values, in 11 selected street canyons in the city of Antwerp. These pollutants were selected as their concentrations should not exceed legally set limit values according to the EU AQ Directive. Model results for all pollutants except for $NO_2$ showed good agreement with measurements from a measurement station located in one of the evaluated street canyons and were within the uncertainty range given by the guidelines in the EU AQ Directive. Regarding contribution from traffic to the ambient concentrations of each of the pollutants considered, the statistical analysis revealed a high variability between the different streets in the case of $NO_2$, CO and benzene, but not for $SO_2$ and $PM_{10}$, thus indicating a more important contribution from the urban and regional background for the last two pollutants. This analysis is particularly useful for regulatory purposes, as it highlights the areas where local abatement measures would have the maximum impact on ambient air pollutant levels.

C. Mensink, A. Colles, L. Janssen, J. Cornelis (2003) Integrated air quality modelling for the assessment of air quality in streets against the council directives, Atmospheric Environment, 37, 5177–5184.

### *A1.1.4 Combined use of monitoring and modelling data for European wide exposure estimates*

As part of the activities of the European Topic Centre for Air Quality and Climate Change for the European Environment Agency, methods for producing European wide maps of legislated air pollutants have been developed. Maps are currently produced every year at 10 km resolution covering all of Europe for $PM_{10}$ and ozone, and irregularly for $NO_2$, $SO_2$ and $PM_{2.5}$ (EEA, 2009; Horálek et al., 2007).

As part of the mapping development a number of methods have been tested. These can be summarised in the following three groups:

1. Spatial interpolation using monitoring data only (geostatistical interpolation methods based on kriging).
2. Combination of monitoring data and chemical transport model (EMEP) data using linear regression, followed by kriging of its residual.
3. Combination of monitoring data, EMEP model data and other supplementary meteorological and land use data using a multiple linear regression, followed by kriging of the residual.

The uncertainty of the mapping methods was assessed using a number of statistical metrics, e.g. root mean square error, by cross-validation. In cross-validation, the spatial interpolation for each measurement point is computed through the use of all available information except the information from that one point. The procedure is repeated for all points. Maps made using method 3 were found to be consistently better than the other two methods. In addition to maps of concentrations, uncertainty maps were also produced. These were based on the residual kriging variance.

The interpolated $PM_{10}$ maps suggest that the number of Europeans exposed to annual mean concentrations of $PM_{10}$ above the annual limit value (40 $\mu gm^{-3}$) was more than 9 % of the total population in 2005. The results also indicate that about 28 % of the European population were exposed for more than 35 days to $PM_{10}$ concentrations of above 50 $\mu gm^{-3}$ (the AQ Directive limit value) in 2005.

The number of premature deaths per million inhabitants attributable to $PM_{10}$ exposure (the EU-27 as a whole) was estimated to range from 510 to 1150 cases per million, with a best estimate of 830 deaths per million (median). The observed range is mainly a result of the differences in $PM_{10}$ concentrations over Europe, and partly of the differences in age distributions and baseline mortalities. Measured particulate matter (PM) concentrations in Europe have not shown, in general, any downward tendencies over the period from 2000 to 2005. The number of 830 premature deaths per million inhabitants corresponds to about 373 000 premature deaths in the EU-25 countries

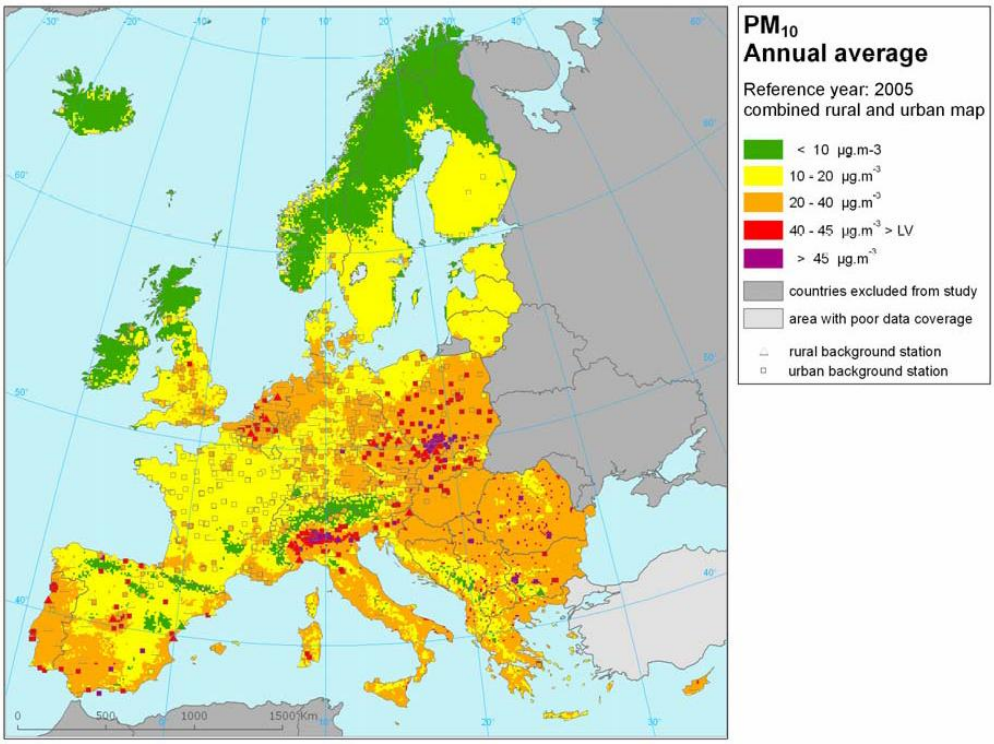


*Figure 1. Annual mean $PM_{10}$ maps generated using multiple linear regression and residual kriging using topography, meteorology and air quality modelling data. Station data are shown as squares (urban) and triangles (rural). Resolution of the map is 10 km and the reference year is 2005 (Horálek et al. 2007).*

Horálek, J.; Denby, B.; de Smet, P. A. M.; de Leeuw, F. A. A. M.; Kurfürst, P.; Swart, R.; van Noije, T., (2007). Spatial mapping of air quality for European scale assessment. ETC/ACC Technical paper No 2006/6. http://air-climate.eionet.europa.eu/docs/ETCACC_TechnPaper_2006_6_Spat_AQ.pdf

Fiala J., Bruce Denby, Jan Horálek, Pavel Kurfürst, Peter de Smet,Frank de Leeuw and Anke Lükewille (2009). Spatial assessment of PM10 and ozone concentrations in Europe (2005). Technical report No 1/2009. http://www.eea.europa.eu/publications/spatial-assessment-of-pm10-and-ozone-concentrations-in-europe-2005-1

### *A1.1.5 Air quality assessment in Spain using a combination of modelling and measured data from stations*

In Spain, air quality assessment has been carried out following the requirements of the European legislation. Since 2002, the Air Pollution Unit of CIEMAT and the Environment Ministry of Spain have collaborated in applying models and ground based measurements to generate more consistent maps of air quality (Martín et al., 2005 and Vivanco et al, 2008). The methodology has been developed and improved during the past years using more suitable models and methods.

During the last 4 years, the models used were the CHIMERE model (Vautard et al, 2003) along with the MM5 meteorological model. Boundary conditions were provided using GFS analysis data and monthly concentrations estimated with the LMDz-INCA model. Emissions were derived from the 50 x 50 $km^2$ EMEP emission database disaggregated with land use information (GLFC-NASA) for finer resolution. This model system has been validated in Spain showing quite good performance for several pollutants (Vivanco et al, 2009).

Two domains are used: a large one covering most of Europe, North Africa and part of North Atlantic Ocean with a resolution of 0.5º x 0.5º, and a smaller one covering the Iberian Peninsula and the Balearic Islands with 0.2º x 0.2º grid cells. Models are run for complete years and hourly, daily, winter and yearly averaged data from several pollutants ($O_3$, $NO_2$, $PM_{10}$, $PM_{2.5}$, CO and $SO_2$) along with the number of exceedances for every grid cell are computed.

Results from the models are combined with measurements to provide maps giving a more complete representation of the air quality in Spain. In the last year a new method has been applied for combining models and measured data from stations. The method consists of using linear regression and kriging interpolation to correct the model results, improving the fit to the observations. It was separately applied to the rural and urban air pollution yielding maps for each case, which are then combined by taking into account the distribution of rural and urban areas in the domain (Martín et al, 2009). It has been tested for the annual mean of $PM_{10}$ for 2004 in Spain (figure 1). Research for improving this method is still ongoing. It will be applied to update the air quality assessment maps of the last four years and for the coming years. This information is being prepared for the Spanish Environment Ministry.

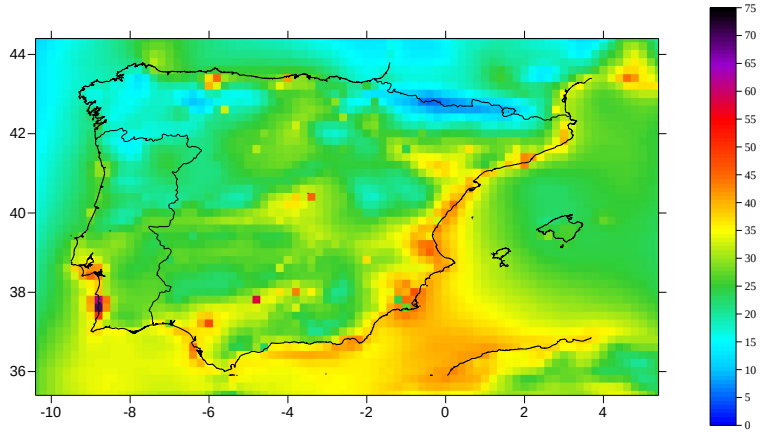


*Figure 1. Final $PM_{10}$ concentration map ($\mu g.m^{-3}$) resulting from the merger of the rural map, produced using linear regression and kriging methods, and the urban map, produced using kriging methods and population density as a surrogate indicator for urban areas.*

Martín F., I. Palomino, M. G. Vivanco. (2005). Aplicación de un modelo de dispersión para la evaluación de la calidad del aire en España. Año 2004 y actividades del 2º semestre de 2005. Informe para la Dirección General de Calidad y Evaluación Ambiental. Ministerio de Medio Ambiente. CIEMAT. Ref: 07/2005.

Martín F., I. Palomino, M. G. Vivanco. (2009). Application of a method for combining measured data and modelling results in air quality assessment in Spain. Revista de Física de la Tierra. ISSN: 0214-4557 (Accepted and in press)

Vautard, R., Martin, D., Beekmann, M., Drobinski, P., Friedrich, R., Jaubertie, A., Kley, D., Lattuati, M., Moral, P., Neininger, B., Theloke, J., 2003. Paris emisión inventory diagnostics from ESQUIF airborne measurements and a chemistry transport model. J. Geophys. Res. 108 (D17), 8564–8585.

Vivanco M. G., I. Palomino, F. Martín y B. Casado (2008). Evaluacion de la calidad del aire en España utilizado modelización combinada con mediciones. Reevaluación año 2005. Acuerdo de Encomienda de Gestión entre el Ministerio de Medio Ambiente y Ciemat para la Aplicación de la Modelización en la Evaluación de la Calidad Del Aire en España. Informe para la Dirección General de Calidad y Evaluación Ambiental. Ministerio de Medio Ambiente. CIEMAT. Ref: 12/2007.

Vivanco M.G, I. Palomino, R. Vautard , B. Bessagnet and F. Martín, L. Menut, S. Jiménez (2009). Multi-year assessment of photochemical air quality simulations over Spain. Environmental Modelling & Software, 24 (2009) 63–73

### *A1.1.6 Assessment of CO when concentrations are below the lower assessment threshold*

During 2008, there was a major restructuring and rationalisation of the national monitoring network in the United Kingdom (Automatic Urban and Rural Network, AURN) to ensure compliance with the then new AQ Directive. The re-structuring followed a 5-year re-evaluation of the Article 5 assessment undertaken during 2007, which showed that concentrations of carbon monoxide had decreased and were below the lower assessment threshold

(LAT) in many zones and agglomerations and hence, monitoring was no longer required. Hence, the monitoring requirement in Annex V and Annex IX was reduced by 50%, in compliance with Article 7. However, even in some of these cases monitoring was retained, over and above the AQ Directive requirements, in order to satisfy the following:

- Good geographic coverage of monitoring throughout the UK
- Provide data for model validation
- Provide data for air pollution forecasting
- Continuity of data at long-running sites.

Altogether 26 sites measuring carbon monoxide were retained in the AURN; the Annex V requirement was for just 8 sites. Details of the re-evaluation of the monitoring requirements in the United Kingdom can be found in Stevenson et al., (2009).

As monitoring is no longer required by the AQ Directive below the LAT, carbon monoxide concentrations are estimated by modelling (as a supplementary assessment methodology). The main modelling features are summarised below (see Grice et al., 2008 for further details ).

Annual mean carbon monoxide concentrations are predicted for each 1 km x 1 km square throughout the United Kingdom by means of a Gaussian dispersion model. The modelled annual mean concentrations are corrected for bias by regressing against the measured concentration. In addition, the annual mean concentration for all major roads is derived from an empirical relationship between the roadside increment ($mg.m^{-3}$) and the emission rate from each road. The modelled maximum of 8-hour concentrations is derived from the modelled annual mean concentration using the relationship between the measured annual mean and maximum 8-hourly concentration values.

Figures 1 shows comparisons of the modelled and measured maximum 8 hour CO concentrations for background and roadside locations. The national network sites used to calibrate the models are shown in addition to the verification sites (sites from non-national network sites, not used to calibrate the model).

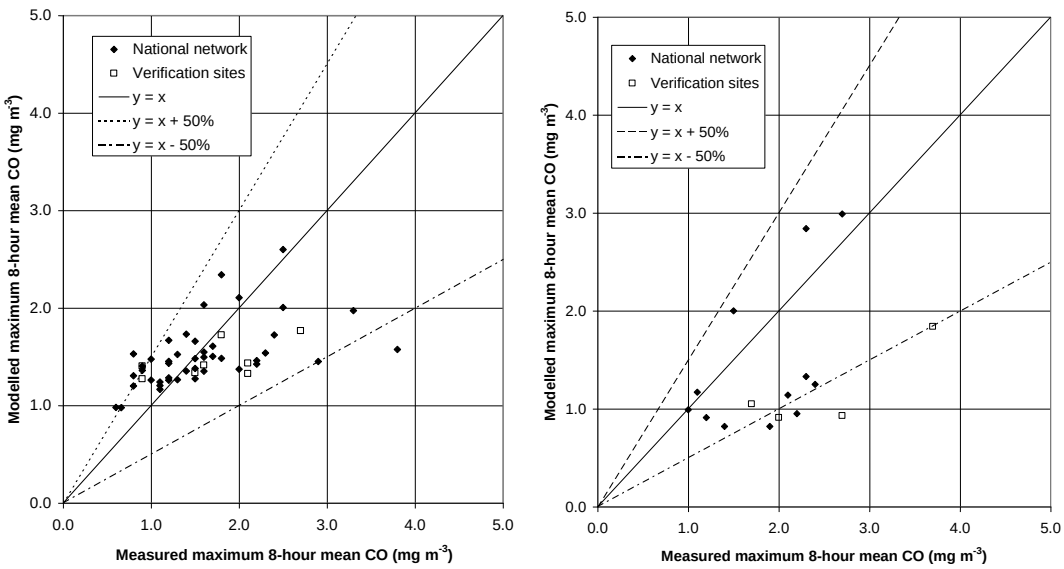


*Figure 1. Verification of background (left) and roadside (right) maximum 8-hour mean CO model 2007.*

Stevenson Ken, Rachel Yardley, Brian Stacey and Richard Maggs (2009) QA/QC Procedures for the UK Automatic Urban and Rural Air Quality Monitoring Network (AURN). AEAT Report No: AEAT/ENV/R/2837. http://www.airquality.co.uk/reports/cat13/0910081142_AURN_QA_QC_Manual_Sep_09_FINAL.pdf

Grice, Susannah, Sally L Cooke, John R Stedman, Tony J Bush, Keith J Vincent, Martyn Hann, John Abbott, Andrew J Kent (2008) UK air quality modelling for annual reporting 2007 on ambient air quality assessment under Council Directives 96/62/EC, 1999/30/EC and 2000/69/EC. AEAT Report: ED48208 Issue 1. http://www.airquality.co.uk/reports/cat09/0905061048_dd12007mapsrep_v8.pdf

### *A1.1.7 Calculation of annual mean $NO_2$ concentrations in the United Kingdom*

Annual mean concentrations of $NO_X$ and $NO_2$ are calculated at urban background, rural background, industrial and roadside locations throughout the United Kingdom. Concentrations are derived using the Pollution Climate Model (PCM), a modelling system that has evolved over many years to take account of the developments in emission inventory compilation, for example, the increasing contribution of primary $NO_2$ from diesel traffic, and the latest understanding of atmospheric dispersion and air pollutant chemistry (Grice et al., 2008). The PCM for $NO_X$ is comprised of a number of sub-models, these are shown below:

| **Sub model** | **Method** |
|---|---|
| Large point sources | Gaussian dispersion modelling |
| Small point sources | Based on Chimney Height Memorandum |
| Rural background concentrations | Monitoring at rural locations |
| Area sources (1 km x 1 km emission) | Dispersion kernels |
| Road link | Traffic increment at roadside |

Background concentrations are derived for each 1 km x 1 km square with the roadside increment added to account for contributions from local major road traffic sources. Monitoring data provides a key component to the modelling method with calibration occurring for the area source model and the road link increment. The roadside increment at roadside locations is estimated from the road $NO_X$ emission using empirically derived adjustment factors that take into account the effect of road speeds, road width and proximity of buildings on dispersion. These adjustment factors are highest for roads with lower traffic flows reflecting the poorer dispersion conditions near such roads.

Maps of $NO_2$ concentrations are derived from the $NO_X$ concentrations maps using the oxidant-partitioning model. This model describes the complex inter-relationships between NO, $NO_2$ and ozone as a set of chemically coupled species (Jenkin, 2004; Murrells et al., 2008). This approach provides additional insights into the factors controlling ambient levels of $NO_2$ (and $O_3$), and how they may vary with $NO_X$ concentration, regional oxidant concentration and primary $NO_2$ emission fractions.

Figures 1 shows the $NO_2$ concentration at background and roadside monitoring sites in 2008. Both the national network sites used for calibration and the verification sites (sites not used to calibrate the models) are presented. The lines representing y = x – 30 % and y = x + 30% show the concentration estimates fall within the required DQO specification. However, the agreement is poorer at roadside locations reflecting the larger uncertainties in modelling roadside concentrations.

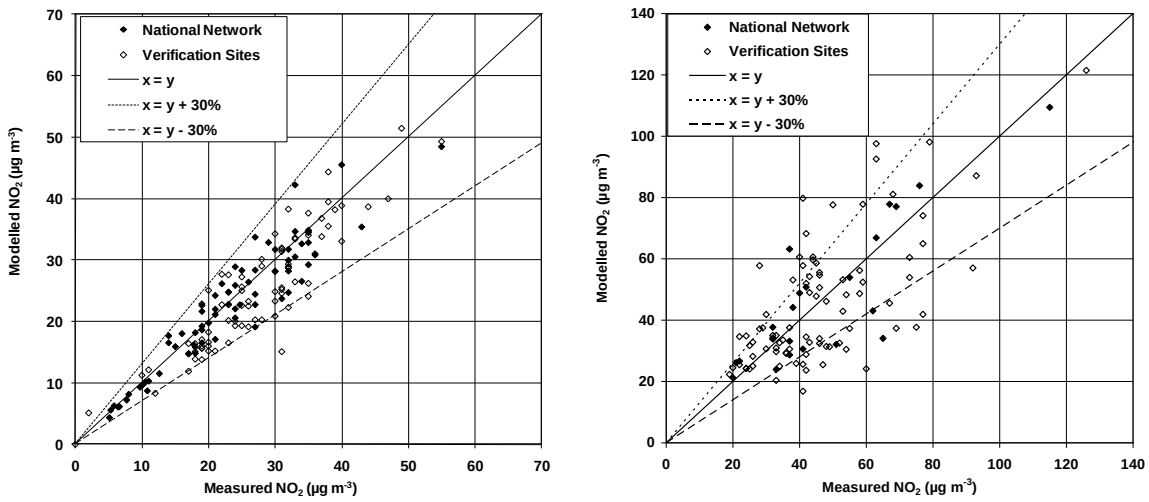


*Figure 1. Left: $NO_2$ model validation at background sites for 2008. Right: $NO_2$ model validation at roadside sites for 2008.*

Grice, S.E., Lingard, J.J.N., Stedman, J.R., Cooke, S.L., Yap, F.W., Kent, A.J., Bush, T.J., Vincent, K.J., and Abbott, J.A., (2009). UK air quality modelling for annual reporting 2008 on ambient air quality assessment under Council Directives 96/62/EC, 1999/30/EC and 2000/69/EC. A report produced for Department for Environment, Food and Rural Affairs, Welsh Assembly Government, the Scottish Government and the Department of the Environment for Northern Ireland. Report number AEAT/ENV/R/2859 Issue 1

Jenkin, M.E. (2004). Analysis of sources and partitioning of oxidant in the UK—Part 1: the NOx-dependence of annual mean concentrations of nitrogen dioxide and ozone. Atmospheric Environment 38 5117–5129.

Murrells. T, Cooke, S., Kent, A. Grice, S., Derwent, R., Jenkin, M., Pilling, M. Rickard, A. and Redington, A. (2008). Modelling of Tropospheric Ozone First Annual Report. Report to The Department for Environment, Food and Rural Affairs, Welsh Assembly Government, the Scottish Executive and the Department of the Environment for Northern Ireland. Report number AEAT/ENV/R/2567 Issue 1. http://www.airquality.co.uk/reports/cat07/0804291542_ED48749_Ann_Rep1_2007_tropospheric_ozone_final_AQ03508.pdf

## A1.2 Examples for source apportionment, transboundary air pollution and related studies

### *A1.2.1 Assessment of the contribution of Saharan dust to $PM_{10}$ exceedances in Greece*

An example study that demonstrates the use of modelling tools in determining the contribution of Saharan dust transport, for air quality assessment as well as source apportionment, is the study by Mitsakou et al. (2008). The contribution of Saharan dust transport to PM pollution levels in several urban areas in Greece is quantified, in order to determine how much of this contribution leads to air quality exceedances though several seasons over a four year period. This is important as intense episodes of Saharan dust transport to southern European countries may result in exceedances of the air quality limit and target values set by the air quality Directive. In this particular study, the SKIRON modelling system was applied to assess the contribution of Saharan dust to $PM_{10}$ concentration values of urban areas in Greece for the period between 2003 and 2006. The atmospheric modelling system SKIRON is a modified version of the ETA/NCEP regional atmospheric model, in which a module for describing the desert dust cycle in the atmosphere is embedded. The desert dust cycle module includes several state-of-the-art parameterisations in order to realistically describe the production, transport and removal processes of the dust cycle. Measurements in the form of monthly $PM_{10}$ averages from four monitoring stations were used to evaluate model results.

The modelling results showed that the maximum contribution of Saharan dust transport to local air quality occurs during the transition spring and autumn periods, as a result of synoptic wind patterns favouring dust transport. The spatial distribution also varies, with concentrations of mineral dust particles decreasing from the south (the city of Heraklion receiving the highest amount of transported dust) to the north. Therefore, the fraction of dust to $PM_{10}$ concentration varied significantly depending on the location. Model simulations in most of the studied areas revealed that natural dust transport may contribute by much more than 20% to the annual number of exceedances.

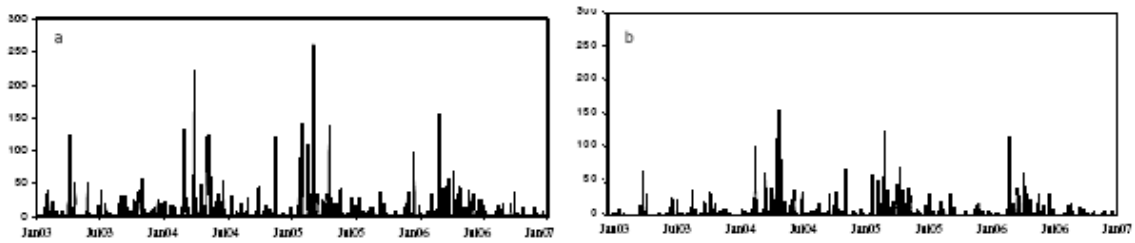


*Figure 1. Contribution of transported* $PM_{10}$ *for (a) Heraklion, (b) Athens as calculated by SKIRON for the period 2003-2006. Vertical axis is in* $\mu g/m^3$.

Mitsakou C., G. Kallos, N. Papantoniou, C. Spyrou, S. Solomos, M. Astitha, and C. Housiadas (2008) Saharan dust levels in Greece and received inhalation doses, Atmospheric Chemistry and Physics, 8 (3), 11967-1996.

### *A1.2.2 Air quality modelling used to determine the contribution of forest fires to $PM_{10}$ in Portugal*

Summer 2003 was one of the most severe fire seasons experienced during the last decades in southern Europe and, in particular, over Portugal, due to persistent extreme fire conditions and as a consequence, unusual air pollutant concentrations were registered in several monitoring stations. In this sense, the year 2003 used as a study case to evaluate the impact on air quality of forest fire emissions. The forest fire emissions were estimated using a simplified methodology, which includes emission factors for each pollutant (CO2, CO, CH4, NMVOC, $PM_{2.5}$, $PM_{10}$ and $NO_x$), burning efficiency, fuel loads and burned area (in terms of forest types and shrubs). Emission factors were based on specific southern European emissions factors, considering the most suitable for Mediterranean ecosystems and for the Portuguese land use types. The selected fuel load was based on the National Forest Inventory. The result of this emission estimation indicates that the fraction of forest fire emissions, relative to the annual total of anthropogenic emissions, represents a significant percentage for major pollutants, principally for CO (40%) and PM (20-30%).

Two modelling systems (MM5-CHIMERE and LOTOS-EUROS) were applied over the mainland Portugal domain, first without considering forest fire emissions and second by adding the hourly estimated emissions, for the entire summer season. Figure 1 shows the spatial differences between both simulations obtained for both modelling systems, for one of the most critical days (August 3) concerning daily values for $PM_{10}$.

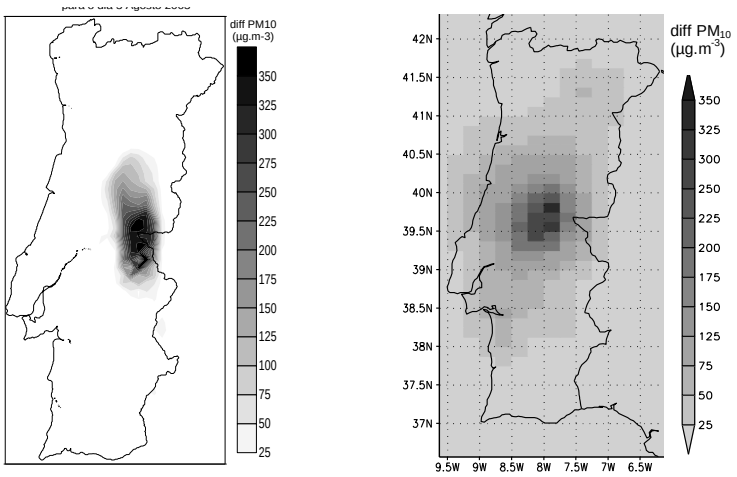


*Figure 1. Spatial differences (µg.m$^{-3}$) between simulation with and without forest fire emissions, for $PM_{10}$ daily averages on August 3rd, 2003. Left CHIMERE and right LOTOS-EUROS.*

Comparison between model results and air quality measurement data shows a significant performance improvement when forest fires are taken into account and allow the quantification of differences in the levels of pollutants when forest fires occur. $PM_{10}$ values can reach differences on the order of 30% for specific monitoring sites, enhancing the importance and the influence of this type of emissions in the local to regional air quality.

The root mean square error (RMSE) between modelled and observed $PM_{10}$ concentrations was determined for the simulations. This quality indicator improves considerably when forest fires are included, reaching differences in the order of 21% (CHIMERE) and 16% (LOTOS-EUROS) for $PM_{10}$ depending on the region considered. On average, uncertainty based on RMSE is always under 50% for both modelling systems.

Miranda A.I., Monteiro A., Martins V., Carvalho A., Schaap M., Builtjes P., Borrego C. (2008) Forest fires impact on air quallity over Portugal. Air Pollution Modeling and Its Application XIX. pp. 190 – 198. Eds. C. Borrego and A.I. Miranda. Springer Nederland www.springerlink.com/content/g1h2122721t0jvp3/

### *A1.2.3 Application of the EMEP model for determining transboundary contributions to air quality*

The mandate of EMEP (European Monitoring and Evaluation Programme, http://www.emep.int ) is to provide sound scientific support for the Convention on Long-range Transboundary Air Pollution (LRTAP), in particular in the areas of atmospheric monitoring, modelling, emission inventories/projections, and integrated assessments. Each year EMEP provides information on transboundary pollution fluxes inside the EMEP area (including all countries that have signed the Convention, and their surroundings), relying on information on emission sources and monitoring data provided by the Parties to the Convention. In 2008 the EMEP area has been extended to include the EECCA countries (Eastern Europe, Caucasus, and Central Asia).

An integral part of the annual EMEP reports are the Source-Receptor matrices, which respond to two fundamental questions about transboundary air pollution. These are: where do the pollutants emitted by a country or region end up and where do the pollutants in a given country or region come from?

In order to arrive at these tables a large number of model runs are performed with the EMEP model of MSC-W (Meteorological Synthesizing Centre - West). The EMEP model is an offline chemical transport model with detailed chemistry for the troposphere and well-tested parameterisations of dry and wet deposition. The source code of the model is open and can be downloaded from http://www.emep.int/OpenSource/index.html .

From 2008 the meteorological data from the ECMWF (European Centre for Medium-Range weather forecasts) have been used to drive the model. In each model run the emission of one chemical species (or group of species) from one country is reduced by 15%, and the effect of this emission reduction on the country itself and other countries are assessed in terms of air quality and depositions. As an example, Figure 1 shows the effect of a reduction in oxidised nitrogen emissions of Germany on Europe and the main contributors to oxidised nitrogen deposition in Germany.

The status reports, technical notes, and country reports focusing on each Party to the Convention are issued by MSC-W annually and are freely available on the internet at http://www.emep.int/mscw/mscw_publications.html. 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 the Convention.

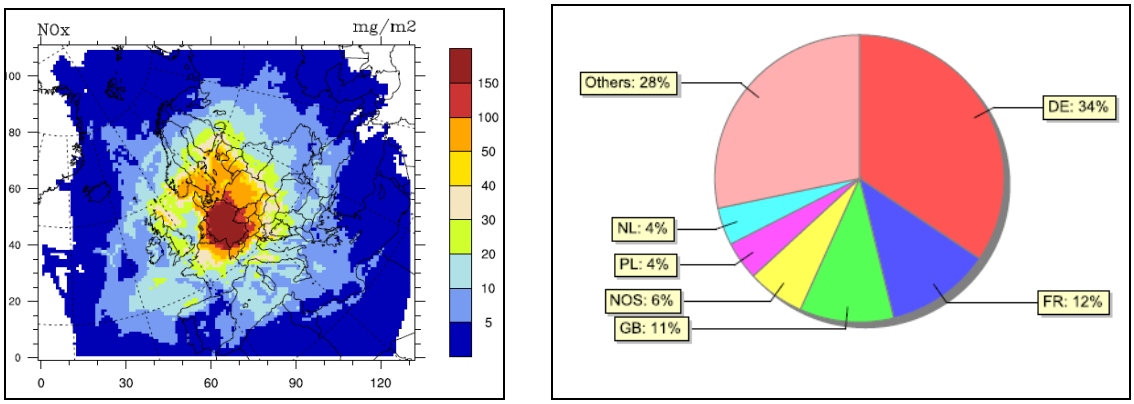


*Figure 1. Left: Contribution of emissions from Germany to oxidised nitrogen deposition in the EMEP domain, unit: mg(N)/m². Right: The main contributors to oxidised nitrogen deposition in Germany, unit: (%) (NL: Netherlands, PL: Poland, NOS: North Sea, GB: Great Britain, FR: France, DE: Germany)*

### *A1.2.4 Analysis of the impact of shipping emissions on air quality in Spain*

Most of the efforts for improving the air quality in Europe are related to the atmospheric pollutant emissions from industry, energy, residential and road traffic sectors. Over the past decades emissions of pollutants such as $SO_2$, ozone precursors and PM from these sectors have been decreasing significantly. Partly as a result of this, other sectors such as shipping are becoming very relevant. It is well known that shipping is an important source of soot, PM, $NO_x$ and $SO_2$ and it has been almost unaffected by regulations for air pollution abatement.

Spain has very intense shipping traffic along its Mediterranean coast, especially in the Strait of Gibraltar, and the North-western and Northern coasts are also strongly affected by North Atlantic routes. The emission of $NO_x$, $SO_X$ and TSP from international shipping close to the Spanish coast is 10 times higher than the national shipping and emissions much higher than aviation sources.

A study devoted to investigate the impact of shipping on the air quality of Spain, especially in the coastal regions, has been carried out by the Atmospheric Pollution Unit of CIEMAT (Vivanco et al, 2008). The CHIMERE model was used to simulate the dispersion of several pollutants for 2003 as a reference year. A European domain with 0.5º resolution was used to feed a nested Iberian Peninsula domain with 0.2º resolution. Boundary conditions for the European domain are from the LMDz-INCA monthly climatology for gaseous concentrations and from GOCART model for particulate species. Emissions were derived from the annual totals of the EMEP database for 2003. These were disaggregated taking into account the high resolution land use information (GLFC-NASA) in order to achieve higher resolution emission data according to CHIMERE requirements. The MM5 model was used to obtain meteorological input fields. The simulations were carried out for a coarse domain and a finer one, with respective resolutions of 36 km and 19 km.

The CHIMERE model was run for 2003 with all the emissions (scenario A) and also switching off the shipping emissions (scenario B). The difference between model predictions for the two scenarios provided an estimate of the contribution of shipping to the air pollution levels, especially in coastal areas with higher ship traffic intensity such as the Straits of Gibraltar and North-western coast of Spain.

The impact on air quality levels and exceedances of standards was determined for the main regulated pollutants: $PM_{10}$, $O_3$, $NO_x$ and $SO_2$.

The main results of the study are:

- The impact of shipping emissions is mainly in coastal regions and islands but it is different for every pollutants. The most affected area is close to the Straits of Gibraltar (figure 1).
- Some inland impacts appear in Southern regions, especially for $SO_2$, but the concentrations are generally low with no impact on limit value exceedances.
- The seasonal effect for $PM_{10}$ and $O_3$ has been estimated with no impact in winter, but intense impact in the summer. Less impact on $NO_2$ is seen in the summer. Secondary aerosol formation is the cause of summer impact for $PM_{10}$.
- In the case of $O_3$, some complex effects have been estimated. It seems that a $NO_x$ saturation regime in areas close to the Straits of Gibraltar and Barcelona Port provides lower $O_3$ levels.
- Shipping was estimated to produce:
    - No exceedances for $SO_2$ and $NO_2$
    - Exceedences for the information threshold $O_3$ for Northern, North-western and North-eastern coastal areas and Balearic Islands, and less in some few areas (close to Barcelona and offshore Western coast of Iberian Peninsula).
    - A number of exceedances for $PM_{10}$ in Mediterranean, southern and south-western coasts.

In spite of the coarse resolution of this study, local impacts in areas close to large ports (Barcelona, Bilbao, etc) are detected, but a higher resolution study is needed to quantify these areas further. These results are not definitive because only 1 years meteorology has been used.

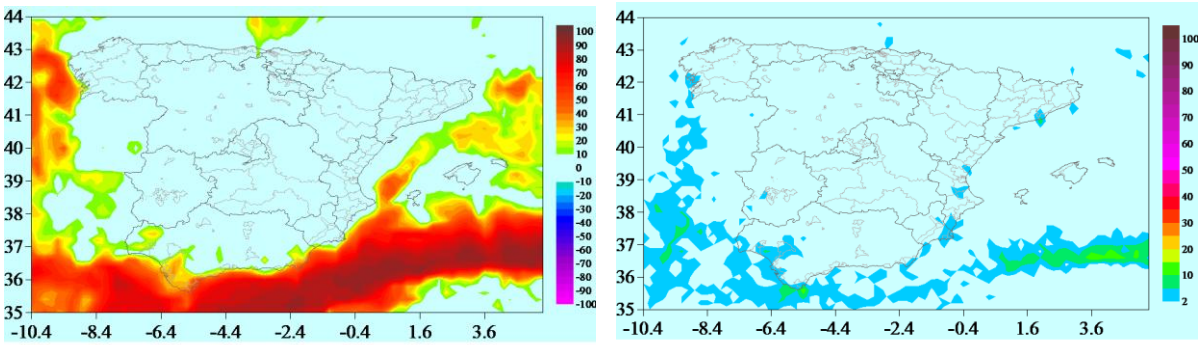


*Figure 1. Hourly maximum concentration of $NO_2$ (left) and estimated exceedances of the daily limit value of $PM_{10}$ (right) due to shipping for 2003 in Spain.*

Vivanco M.G., Azula O., I. Palomino and F. Martín (2008). Analysis of the impact of the shipping emissions on air quality in Spain. Harbours, Air Quality and Climate Change 2008. Rotterdam, (Netherlands), 29-30 May, 2008.

### *A1.2.5 Assessing the contribution of African dust outbreaks to annual PM levels and $PM_{10}$ exceedances of the daily limit value of 50 µg/m$^3$*

According to the AQ Directive (EC, 2008), article 20, some natural events such as Saharan dust episodes, may increase markedly the PM levels over the usual background concentrations, originating in many cases that exceed of the daily limit value of $PM_{10}$ of 50 µg/m$^3$, as established in the AQ Directive. The report of the European Commission Working Group on Particulate Matter titled 'Guidance to member states on PM10 monitoring and intercomparisons with the reference method' (http://ec.europa.eu/environment/air/pdf/finalwgreporten.pdf ) proposes a series of techniques and research tools which could be used to identify the contributions of natural events to measured $PM_{10}$ levels, including the detection of these kind of episodes using aerosol modelling tools, satellite imagery, back-trajectories analysis, and also PM composition studies. These methodologies are appropriate to identify this kind of event, but the quantification of the contributions to the $PM_{10}$ levels is not properly determined with these tools. Modelling tools on these issues have still to improve to give quantitative data with precision enough to be applied to the legal standards. However, these are basic to identify the dust outbreak episodes.

Spain and Portugal jointly developed a methodology to quantify the contributions of the African dust outbreaks at regional background (RB) locations in the Iberian Peninsula, and the Balearic, Canary, Azores and Madeira Isles. Modelling tools (such as SKIRON simulations, DREAM-BSC model outputs, NAAPs NRL model outputs, HYSPLIT-4 back trajectory analysis), satellite imagery data from MODIS and SeaWIFS project, and PM measurements from a dense monitoring RB stations are combined to this end. The daily net dust load in $PM_{10}$ or $PM_{2.5}$ attributable to an African episode can be obtained by subtracting the daily RB level from the $PM_{10}$ or $PM_{2.5}$ concentration value at a RB station. The daily RB level can be obtained by applying a monthly moving 40th percentile to the $PM_{10}$ or $PM_{2.5}$ time series at a RB station after a prior extraction of the data coincident with African dust transport. For days with influence of African dust, the dust load is given by the difference between the daily $PM_{10}$ values minus the daily $PM_{10}$ RB levels. This method allows us to quantify the net African dust load without chemical speciation. The description and justification of this methodology can be found in Escudero et al. (2007).

This methodology allows the monitoring networks to distinguish those exceedances originating from these African dust outbreaks from those originating from other causes (Figure 2). In addition, with this methodology it is possible to quantify the mean annual contribution of the African dust to the $PM_{10}$ or $PM_{2.5}$ annual means (Figure 2, as an example). As demonstrated by Querol et al. (2009a) this methodology may be also used in all southern Europe. A detailed description of the methodology can be found in Querol et al. (2009b).

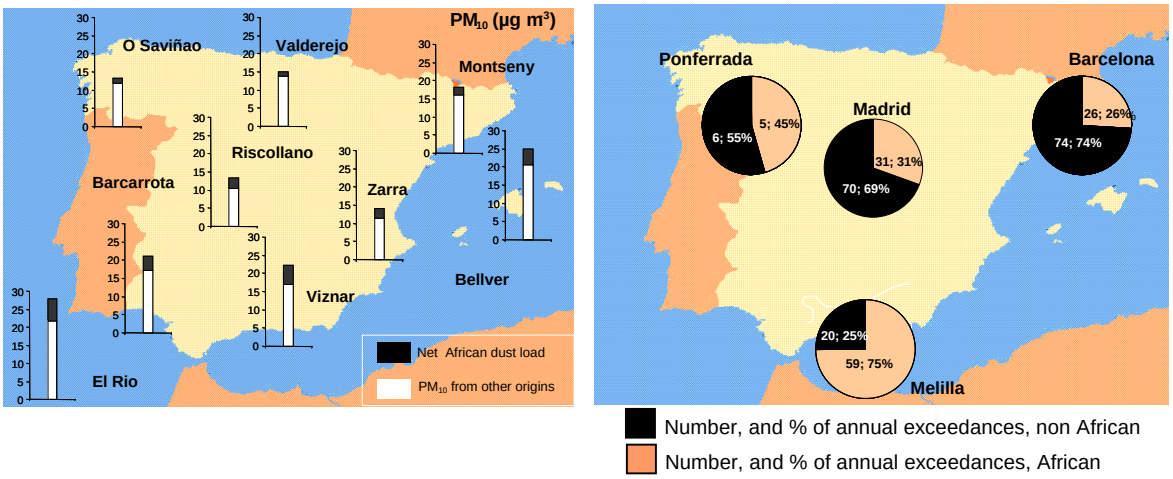


*Figure 1. $PM_{10}$ mean annual contribution of African dust over the Iberian Peninsula, the Canaries and the Balearic Isles. The map (left) shows the contribution of African dust to the bulk $PM_{10}$ annual levels measured at regional background sites. In the map (right) the partitioning between the African caused number of daily exceedances of the $PM_{10}$ daily limit value in selected urban monitoring sites is shown for 2007.*

Escudero M., Querol X., Pey J., Alastuey A., Pérez N., Ferreira F., Alonso S., Rodríguez S. & Cuevas E., 2007. A methodology for the quantification of the net African dust load in air quality monitoring networks. Atmospheric Environment, 41, 5516-5524.

Querol X., Alastuey A., Pey J., Pandolfi M., Cusack M., Pérez N., Viana M., Moreno T., Mihalopoulos N., Kallos G. Kleanthous S. (2009a). African dust contributions to mean ambient PM10 mass-levels across the Mediterranean Basin. Atmospheric Environment 43, 28, 4266-4277.

Querol X, X. Querol, A. Alastuey, J. Pey, M. Escudero, S. Castillo, A. Gonzalez Ortiz, M. Pallarés, S. Jiménez, A. Cristóbal, F. Ferreira, F. Marques, J. Monjardino, E. Cuevas, S. Alonso, B. Artíñano, P. Salvador, J. de la Rosa (2009b). METHODOLOGY FOR THE IDENTIFICATION OF NATURAL AFRICAN DUST EPISODES IN PM10 AND PM2.5, AND JUSTIFICATION WITH REGARDS TO THE EXCEEDANCES OF THE PM10 DAILY LIMIT VALUE. In press, Minsitry of the Environment of Spain. http://www.idaea.csic.es/attachments/103_Methodology%20for%20natural%20episodes-rev%20final.pdf

### *A1.2.6 Source apportionment of particulate matter concentrations in the Milan area*

Complex pollutants involving non-linearities and transformations, such as particulate matter, may require extra attention when determining the source contributions. In the case of multiple sources, that require 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 CAMx (ENVIRON, 2006) to the Milan region to assess the source contributions of local and regional sources to PM2.5 concentrations. They use the PSAT algorithm (Wangstrom et al., 2008) for the source apportionment which provides an effective method for modelling source apportionment when a large number of sources are used. This algorithm provides information on the current source contributions but not on the effect of any reduction or increase in a particular source.

The CAMx chemical and transport Eulerian model has been applied over a 300 x 300 $km^2$ domain focused on the Milan area (Northern part of Italy) for the whole 2004. Model results have been analysed by means of the PSAT (Particulate Source Apportionment technology) at the Milan receptor, in order to discriminate the contribution of several key emission sectors such as road transport, domestic heating and agriculture, also distinguishing the most emitting area of Milan from the surroundings (Figure 1).

The city of Milan accounts for 18% of the PM2.5 contribution, while the whole metropolitan area (Critical zone) is responsible for 34%. The regional contribution produced by the remaining part of the domain covers about 50% of the yearly mean and is mainly due to the North Lombardy area (27%). Finally, it is worth noting the considerable contribution of boundary conditions (16%). This fraction should account for the large scale transport phenomena but, actually, it takes into account also the remaining part of the Po valley, not included in the computational domain. The importance of this contribution indicates that the study area should be extended in order to better discriminate the whole basin scale contribution (i.e. the regional background) from the long range

transport. The results obtained highlight that road transport is the most relevant sector (29%), followed by domestic heating (15%) and agriculture (14%).

The analysis of the evolution of Milan plume contribution at different receptors highlighted that the influence of the city emissions is around 20% at the local receptor, but drops down to less than 3% within a radius of 40 km from the city centre. The results also confirmed that local scale policies might have a very limited effect on the local air quality.

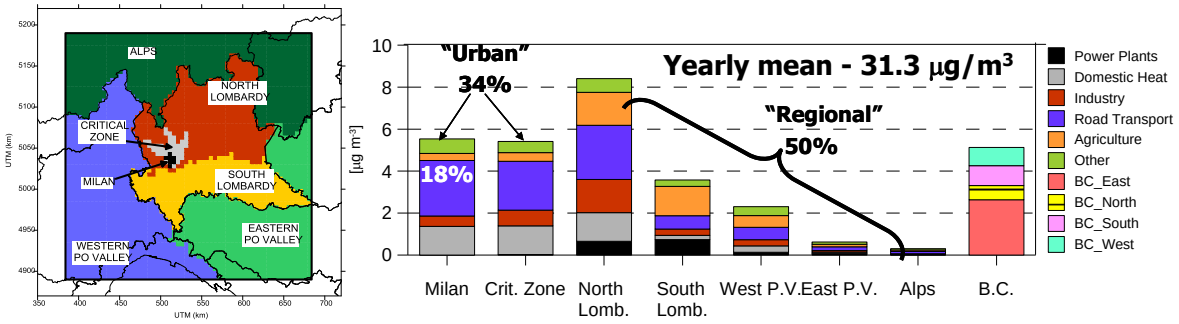


*Figure 1. Left: definition of the emission areas within the computational domain. Right: contribution of each emission area and group to the PM2.5 yearly mean concentration at the Milan receptor.*

Bedogni, M., S. Casadei and G. Pirovano (2008). ASSESSING THE CONTRIBUTION OF THE MAIN EMISSION SOURCES TO PARTICULATE MATTERCONCENTRATIONS IN THE MILAN AREA. Proceedings of the 12th International Conference on Harmonisation within Atmospheric Dispersion for Regulatory Purposes, Cevtat, Croatia. 598 – 602

ENVIRON Corporation, 2006: User's guide to the Comprehensive Air quality Model with extension (CAMx) version 4.42. Technical report.

Wagstrom, K.M., Pandis, S.N., Yarwood, G., Wilson G.M., Morris, R.E, 2008. Development and application of a computationally efficient particulate matter apportionment algorithm in a three-dimensional chemical transport model. Atmospheric Environment 42, 5650– 5659.

### *A1.2.7 Assessment of sea salt contribution to exceedences of $PM_{10}$ in The Netherlands*

In 2005 the Dutch National Guideline (Staatscourant, 2007; based on Hoogerbrugge et al., 2005) was issued that allows the subtraction of the annual average concentration and exceedance days resulting from sea salt for all of the Netherlands. This estimate of the reduction of exceedance days is calculated using the measured Chloride concentrations on 5 locations and for 4 years (2000-2003). Based on this data an average reduction of 6 days was estimated and because no clear separation was possible between the various locations the average is applied for the whole country. Because of the large uncertainties in this study (estimated as 50 %) the yearly measurement of Sodium in $PM_{10}$ was started on 6 locations to enable more accurate estimates in the future.

Later two model studies were applied. In the first Van Jaarsveld and Klimov (2009) applied the OPS-ST model, a short term variation of the Dutch National model OPS which is a Gaussian based Lagrangian trajectory model. They calculated annual means that agreed well with monitored Cl- concentrations but could only explain around 50% of the daily mean variability. In addition, though the annual mean contribution of sea salt to $PM_{10}$ at coastal stations was found to be up to 20%, the contribution of sea salt to daily mean exceedances was limited to just a few days. On average over a seven year period this was less than 2 days per year. This is due to the fact that episodic peaks in sea salt contributions to $PM_{10}$ are not, or even negatively, correlated with total $PM_{10}$ concentrations. i.e. air quality is generally good when strong winds blow from the sea, exactly the conditions that lead to strong sea salt emissions.

In the other example from The Netherlands, Manders et al. (2009) applied the LOTOS-EUROS model to calculate sea salt contributions in The Netherlands using a model resolution of approximately 6 km. Their results arrive at similar conclusions to those of Van Jaarsveld and Klimov (2009) but they emphasize that due to the episodic nature of sea spray events there is a large inter-annual and spatial variability in the contribution of sea salt to exceedances. They argue that calculations of the exceedances should be carried out on a year by year basis and should in principle be spatially varying in nature. The other important aspect brought out in the

modelling is that on a daily mean basis the emission model for sea salt has a likely uncertainty of a factor of 2 – 3 (Figure 1.).

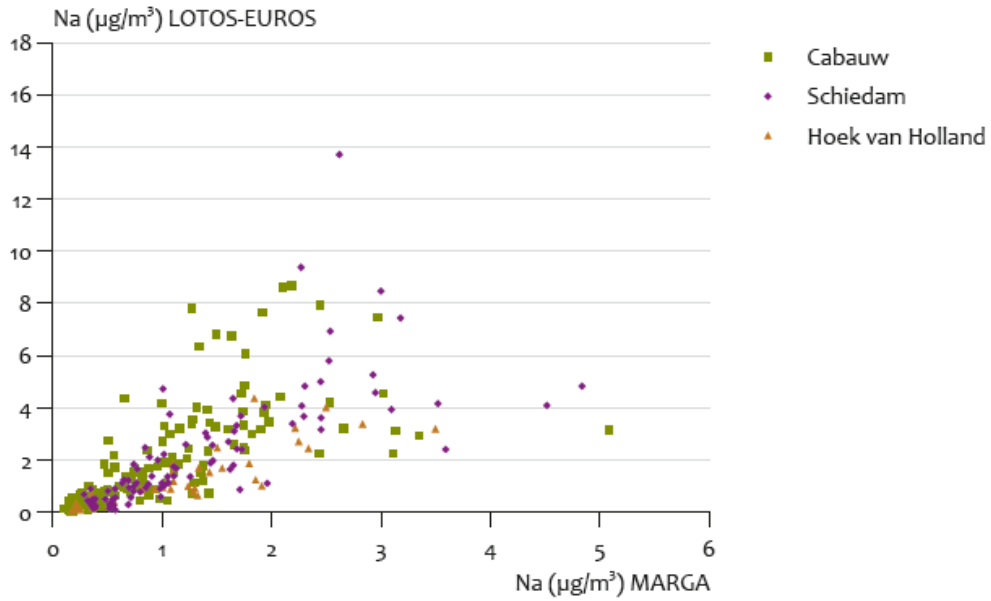


*Figure 1. Observed (MARGA instrument) and modelled (LOTOS-EUROS) daily mean sodium (Na) concentrations taken from three sites in The Netherlands for the period August 2007 to September 2008 (Manders et al.,2009).*

Hoogerbrugge, R. Matthijsen, J., van Jaarsveld, H., Schaap, M., Denier van der Gon, H. (2005) Recommendation for a preliminary guideline for the correction of PM10 concentrations for the sea salt contribution (Aanbeveling voor een voorlopige regeling voor de correctie van fijn stof (PM10) concentraties voor de bijdrage van zeezout, in Dutch), www.rivm.nl/milieuportaal/dossier/fijnstof/bronnen

Manders, A.M.M., M. Schaap, M. Jozwicka, F. Van Arkel, E.P. Weijers, J. Matthijsen (2009). The contribution of sea salt to PM10 and PM2.5 in the Netherlands. Publication of the Netherlands Research Program on Particulate Matter. Report 500099004. http://www.rivm.nl/bibliotheek/rapporten/500099004.pdf

Staatscourant, (2007). Regulation on air quality assessment 2007 (in Dutch): Regeling van de Minister van Volkshuisvesting, Ruimtelijke Ordening en Milieubeheer van 8 november 2007, nr. LMV 2007.109578, houdende regels met betrekking tot het beoordelen van de luchtkwaliteit, Staatscourant,13 november 2007, nr. 220 / pag. 21. (http://www.infomil.nl/contents/pages/22907/regelingbeoordeling_publicatieinclusieftoelichting.pdf ).

Van Jaarsveld, J.A. and Klimov, D. (2009). Modelling the impact of sea-salt particles on the exceedances of daily PM10 air quality standards in the Netherlands. Int. J. Environment and Pollution, in press. Original proceedings document also available at http://www.harmo.org/Conferences/Proceedings/_Cambridge/publishedSections/Op241-245.pdf

### *A1.2.8 Modelling and source apportionment of primary $PM_{10}$ for the city of Graz, Austria*

In Graz the limit value for $PM_{10}$ of 50 µg/m³ according to the AQ Directive EC/50/2008 is exceeded at several monitoring stations more than 35 days a year. For instance, at the monitoring station Graz Don Bosco, where usually the highest $PM_{10}$ concentrations are registered in Austria, the daily mean of 50 µg/m³ was exceeded 120 times in 2006. In order to better understand the contributions of various sources to the $PM_{10}$ pollution and to be able to assess the impact of reduction measures, a comprehensive modelling study has been performed for the greater Graz area. This study among others has also been used to apply for postponement of the attainment deadline for $PM_{10}$.

Within the frame of the European funded LIFE Project KAPA GS (2004-2008), a methodology for modelling the $PM_{10}$ concentration with a very high resolution (10m x 10m) at the urban scale has been developed. After a first successful application for the city of Klagenfurt the method has in this study being applied to the city of Graz (~250.000 inhabitants) in Austria (Oettl, 2008). Based on existing emission inventories for traffic including resuspension of road dust, domestic heating, and industry, simulations for the spatial distribution of $PM_{10}$ have

been performed using the Lagrangian particle model GRAL (Graz Lagrange Model), which is coupled with the mesoscale prognostic model GRAMM (Graz Mesoscale Model). The latter has been operated with a horizontal resolution of 300m x 300m, while the whole modelling domain was 27km x 39km.

GRAMM has been initialised using a simple statistics of 5 wind speed classes, 36 sectors of wind direction, and Pasquill-Gifford stability classes. The latter has been used to obtain the vertical profile of potential temperature. For each, out of several hundreds of such characterised dispersion conditions, a steady-state wind field and subsequently a steady-state concentration field has been computed. 16 meteorological stations have been used to compare simulated and observed wind direction frequencies as well as wind speeds. Apart from 12 permanent air quality monitoring stations (AQM) routinely operated, an additional 9 particle counters for $PM_{10}$, $PM_{2.5}$ and $PM_1$ (GRIMM) were available for comparison purposes.

It was found that due to extremely poor dispersion conditions in the basin of Graz, $PM_{10}$ levels can reach or even exceed that of megacities. A fairly good agreement between modelled and observed average $PM_{10}$ concentrations could be achieved, although significant uncertainties arose for each step of the whole model chain (emission inventory, wind field-, and air quality simulations).

It was calculated that traffic is the most significant source of $PM_{10}$ in the centre of Graz and at nearby busy roads, while domestic heating may become the dominant source in suburban areas. Especially non-exhaust emissions are comparatively high, as became evident from road measurements in Graz and Klagenfurt, and additional chemical analyses of $PM_{10}$ filters. There is also some observational evidence of locally generated secondary PM (e.g. ammonium nitrate) at least in the city of Graz.

One major outcome of this study has been that it is practically impossible to meet the limit value for the daily mean $PM_{10}$ concentration due to the poor dispersion conditions. For instance, to meet the limit value at the monitoring site Graz-Süd, it would be necessary to cut down traffic emissions and emissions from domestic heating by 100 %, if there are no other measures taken to reduce the background $PM_{10}$ (long-rang transport and secondary aerosols).

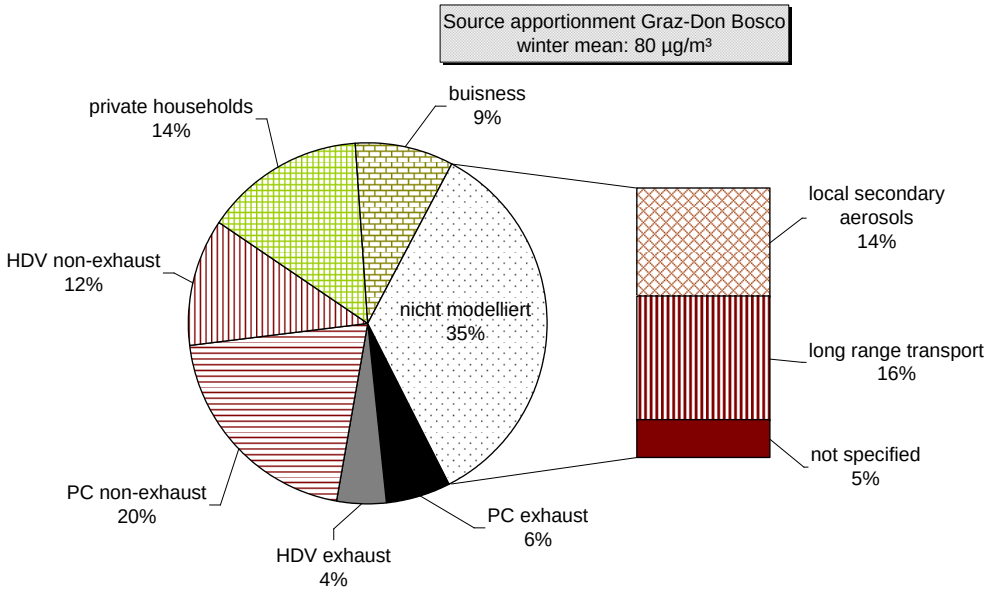


*Figure 1. Example of a source apportionment based on the simulations with GRAL for the AQM station Graz-Don Bosco for the winter months in 2006 (Jan-Feb, Dec)*

Oettl, Dietmar (2008). MODELLING OF PRIMARY PM10 CONCENTRATIONS FOR THE CITY OF GRAZ, AUSTRIA. Proceedings of the 12th International Conference on Harmonisation within Atmospheric Dispersion for Regulatory Purposes, Cevtat, Croatia. 375 - 379

## A1.3 Examples for planning

### *A1.3.1 Plan for the air quality improvement in the Metropolitan Area of Barcelona.*

The Plan for the air quality improvement affects 40 municipalities of the Metropolitan Area of Barcelona. This region was decreed as zone of special protection due to the large number of exceedances of the limit value of $NO_x$ and $PM_{10}$ pollutants. The Plan defines 73 measures to reduce the emissions of these atmospheric pollutants according to its contribution to each emission source. One of the 73 measures was to reduce the emissions of pollutants from private, public and freight transport by reducing the speed limit on highways accessing Barcelona. As a first stage, the vehicle speeds were limited to 80 km/h on the access routes to Barcelona. In order to evaluate the impact of this measure on the air quality, a modelling study was carried out by the Earth Sciences Department of the Barcelona Supercomputing Center (BSC).

The main objective of the study was to analyse the impact of such measure on the air quality. A state-of-the-art modelling system was used, consisting of a high resolution emission model (HERMES; Baldasano et al., 2008), a mesoscale meteorological model (WRF; Michalakes et al., 2005) and a chemical transport model (CMAQ; Byun and Schere, 2006). Emissions from power plants, industries, domestic sector, traffic, airports, harbours, and biogenic were considered.

The air quality of the area under study was simulated for the full year 2008 by assimilating hourly traffic measurement information of vehicle density and speed from 125 traffic stations, and compared with equivalent traffic data from the year 2007 (before enforcing the new speed limit) using only 2008 meteorology. The results obtained show an average reduction in the emissions of $NO_x$ of 4% and a reduction in $PM_{10}$ emissions of 3.7% (figure 1). This reduction is due to reduction of speed and decrease of the traffic congestion as a result of the speed limit measure.

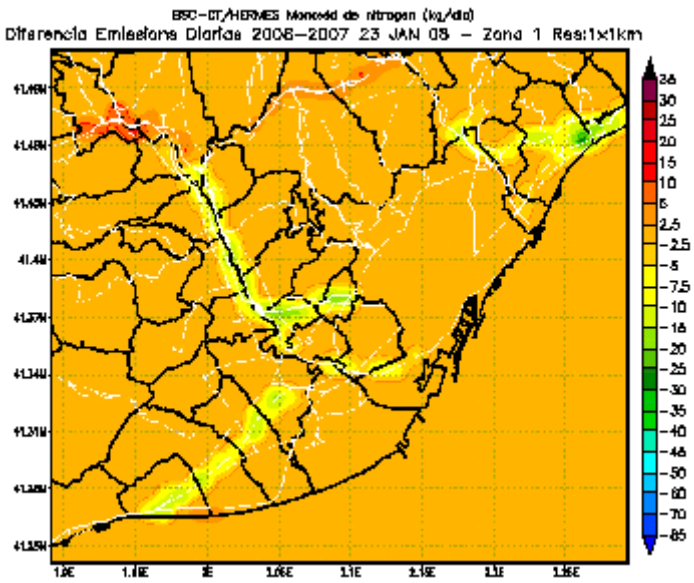


*Figure 1. Difference between daily emissions 2008-2007 based on the speed reduction scenario*

The effects of the measure on air quality predicted by the model affects mainly areas close to the roads, where reductions on $NO_2$ and $PM_{10}$ levels are between 4.3 - 7.5% and 2.0 - 3.1% on 24-hr average concentration, respectively. In spite of some local $O_3$ increases, the $O_3$ levels in most of downwind areas remain practically unchanged.

The detailed emission model along with assimilated information, in this case from vehicular traffic specifically developed for the study area, and the high spatial resolution used in the modelling system (1 $km^2$, 1h) provides the necessary tools for urban scale air quality planning.

Baldasano J.M., L. P. Güereca, E. López, S. Gassó, P. Jimenez-Guerrero (2008). Development of a high-resolution (1 km x 1 km, 1 h) emission model for Spain: the High-Elective Resolution Modelling Emission System (HERMES) . Atmospheric Environment, 42 (31): 7215-7233, doi:10.1016/j.atmosenv.2008.07.026. ISSN: 1352-2310, October 2008.

Baldasano J.M., P. Jiménez-Guerrero, E. López, M. Gonçalves, A. Soret (2009a) Effects on air quality of 80 km h-1 speed limit in the Barcelona Metropolitan Area (Spain). ETTAP09, Toulouse (France) 2-4 June

Baldasano, J.M., López, E., Jiménez, P., Jorba, O., Soret., A., Gonçalves, M. (2009b). Eectos en la calidad del aire por la introducción de la limitación de velocidad a 80 km/h en las vías de acceso a Barcelona. Departamento de Ciencias de la Tierra (BSC-CNS) para el Departament de Medi Ambient i Habitatge, Generalitat de Catalunya. Barcelona, Febrero 2009.

Byun, D.W., Schere, K.L. (2006). Review of the governing equations, computational algorithms and other components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System, Applied Mechanics Reviews, 59(2), 51-77.

Michalakes, J., Dudhia, J., Gill, D., Henderson, T., Klemp, J., Skamarock, W., Wang, W. (2005). The Weather Research and Forecasting Model: Software architecture and performance. Proceedings of the Eleventh ECMWF Workshop on the Use of High Performance Computing in Meteorology, Zwiefhofer, W. and Mozdzynski, G. (Eds.), World Scientific, 156-168.

### *A1.3.2 The MINNI Project: An Integrated Assessment Modelling System For Policy Making over Italy*

In 2002, the Italian Ministry of the Environment decided to sponsor the project presented by ENEA for the development of the national Integrated Assessment Modeling system (the MINNI Project, Zanini et al., 2005). The objective of the project is to support policy makers in the elaboration and assessment of air pollution policies at international, national and local level, by means of the more recent understandings of atmospheric processes. The MINNI Project consists of two main components:

1. A multi-pollutant Atmospheric Modeling System (AMS) simulating air pollution dynamics and multiphase chemical transformations, providing hourly concentrations and annual depositions of SO2, NOx, NH3, PM10 , PM2.5 and O3, with a spatial resolution ranging between 20 and 4 km.
2. A complete Integrated Assessment Model (IAM) derived from RAINS-Europe (Regional Air Pollution Information and Simulation, Amann et al., 2004). With a built-in Atmospheric Transfer Matrix (ATM) calculated by AMS, RAINS-Italy provides emission scenarios, abatement costs and impact assessment scenarios.

The two components complement each other, offering a powerful tool that provides policy makers with detailed analyses, where requested, tailored to the specific national or local needs. AMS may feed RAINS-Italy with fine resolution ATMs and/or different meteorological year based ATMs. RAINS-Italy may feed AMS with a projected emission vector, regarding future scenarios, to develop expected detailed deposition/concentration maps.

The AMS is based on the Flexible Air Quality Regional Model (FARM, Gariazzo et al., 2007; Silibello et al., 2008), that is a three-dimensional Eulerian chemistry transport model (CTM) implementing the aero3 aerosol module (Binkowski, 1999) and different SAPRC chemical schemes (Carter, 1990; Carter, 2000). Boundary conditions for the selected years are provided by the EMEP Unified model (EMEP, 2003) running over the continental-scale for the same simulation periods. Meteorological fields have been obtained by means of the prognostic and non-hydrostatic model RAMS (Cotton et al., 2003) using a 2 way nested grid system, with an outer grid covering large part of the Central Europe and the Mediterranean Sea and inner grids including the target areas, with resolutions of 48, 12 and 4 km. ECMWF (European Centre for Medium Weather Forecast) analysis fields and surface input data and four-dimensional data assimilation technique (nudging) have been used to force RAMS simulations towards the atmospheric reference state, given by observed data. The emission subsystem is based on the Italian and European emission inventories and also includes the maritime emissions. The hourly input needed by the air quality model, on the computational grids, and for the chemical species of interest, have been provided on the basis of a set of activity specific thematic layers, time modulation curves and speciation profiles (NMVOC and PM). A similar procedure was applied to the emissions of the neighbouring countries, starting from the EMEP European inventory. More than 150 Italian large emission sources have been treated as “point sources” taking into account the plume rise effects.

In Figure 1 are reported, for the year 2005, the $NO_2$ yearly averages computed over Italy (20 km resolution) and the five macro-regions (4 km resolution). Products coming from the MINNI Project are made available by the Ministry of Environment to support local authorities air quality assessment and management activities.

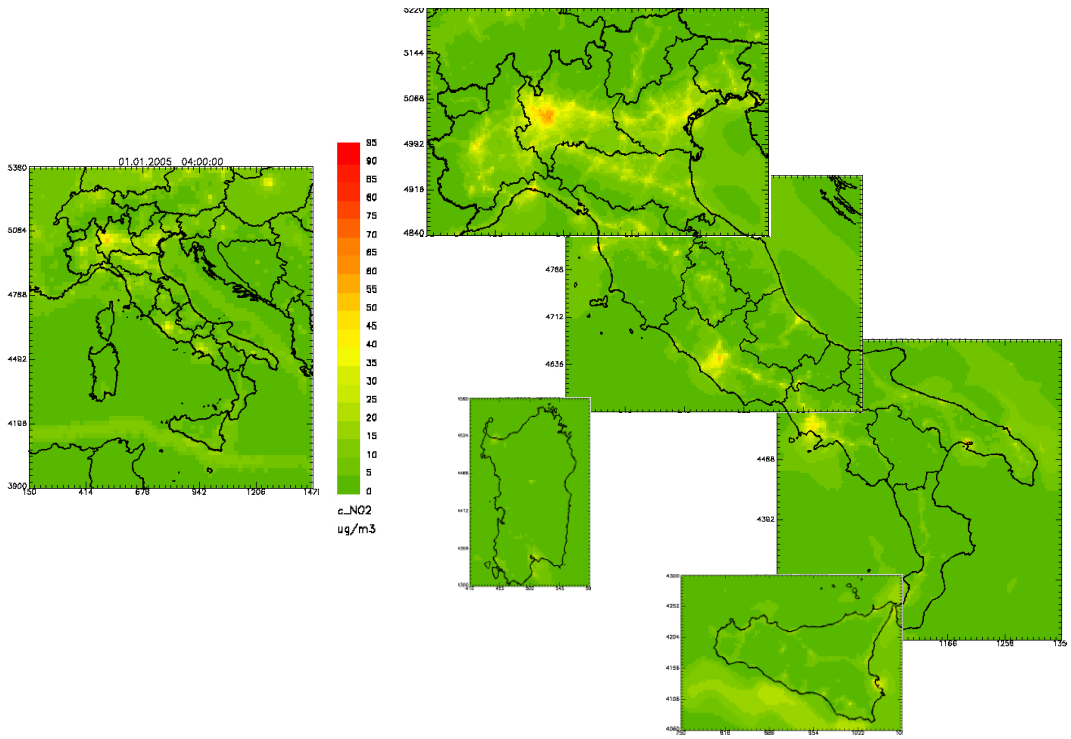


*Figure 1. $NO_2$ annual mean (2005) at 20 km (left) and 4 km (right) resolution*

Binkowski F. S. (1999) The aerosol portion of Models-3 CMAQ, Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. Part II, Chapters 9-18, D.W. Byun, and J.K.S. Ching (Eds). EPA-600/R-99/030,National Exposure Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC, 10-1-10-16.

Amann M., Cofala J., Heyes C., Klimont Z., Mechler R., Posch M., Schöpp, W. (2004) Rains Review 2004, IIASA Interim Report, February 2004.

Carter W.P.L. (1990) A detailed mechanism for the gas-phase atmospheric reactions of organic compounds, Atmos. Environ., 24A, 481-518.

Carter W.P.L. (2000) Implementation of the SAPRC-99 chemical mechanism into the MODELS-3 framework. Report to the USEPA, January 29, 2000.

Cotton, W.R., Pielke R. A., Walko R. L. , Liston G. E., Tremback C. J., Jiang H., McAnelly R. L., Harrington J. Y., Nicholls M. E., Carrio G. G. and McFadden J. P. (2003) RAMS 2001: Current status anf future directions, Meteorol. Atmos. Phys., 82, 5-29.

EMEP Co-operative Programme for Monitoring and Evaluation of the long range transmission of air pollutants in Europe, (2003), Transboundary acidification, eutrophication and ground level ozone in Europe. Part I: Unified EMEP model description, EMEP status Report 1/2003.

Gariazzo C., Silibello C., Finardi S., Radice P., Piersanti A., Calori G., Cucinato A., Perrino C., Nussio F., Cagnoli M., Pelliccioni A., Gobbi G.P., Di Filippo P. (2007). A gas/aerosol air pollutants study over the urban area of Rome using a comprehensive chemical transport model. Atmospheric Environment, 41, 7286-7303.

Silibello C., Calori G., Brusasca G., Giudici A., Angelino E., Fossati G., Peroni E.; Buganza E. (2008) Modelling of PM10 Concentrations Over Milano Urban Area Using Two Aerosol Modules. Environmental Modelling and Software, 23, 333-343.

Zanini G., Pignatelli T., Monforti F., Vialetto G., Vitali L., Brusasca G., Calori G., Finardi S., Radice P., Silibello C. (2005) The MINNI Project: An Integrated Assessment Modeling System For Policy Making. In Zerger, A. and Argent, R.M. (eds) MODSIM 2005 International Congress on Modelling and Simulation. Modelling and Simulation Society of Australia and New Zealand, December 2005, pp. 2005-2011. ISBN: 0-9758400-2-9.

### *A1.3.3 Evaluation of the effects in urban air quality by using natural gas vehicles in Barcelona and Madrid urban areas (Spain).*

Road transport is known to be the largest contributor to anthropogenic emissions in many European urban areas, for example Barcelona and Madrid (Spain). There is a broad range of management options to reduce the

on-road transport emissions and air quality modelling constitutes a valuable tool for assessing the effects of different strategies. The Earth Sciences Department of the Barcelona Supercomputing Center applied the WRF-ARW/HERMES/CMAQ Eulerian modelling system (Michalakes et al., 2005; Baldasano et al., 2008; Byun and Schere, 2006) to evaluate the effects on the urban air quality in Barcelona and Madrid of an eventual introduction of natural gas vehicles with fleet renewal. The high spatial resolution applied (1 $km^2$, 1 h) and the detailed emission scenarios are important factors for providing meaningful results on the urban scale. Seven emissions scenarios were defined, based on the year 2004, where realistic changes in the use of natural gas in the vehicle fleet were introduced and the impact of these scenarios assessed.

The $NO_2$, $PM_{10}$ and $SO_2$ average concentrations decreased with the natural gas vehicle introduction, up to 6.1%, 1.5% and 6.6% in Barcelona and up to 20.6%, 8.7% and 14.9% in Madrid, respectively. Although an increase in $O_3$ average levels, up to 1.3% in Barcelona and up to 2.5% in Madrid were observed, this was due to the $NO_X$ reduction in VOC-controlled areas.

The variation in concentrations was mainly affected by two factors: the vehicle fleet composition of the urban areas, which affects the emissions change, and the specific atmospheric dynamics they have. For $SO_2$ and $PM_{10}$ reductions, the most effective single scenario was the introduction of 50% of NGV instead of the oldest commercial vehicles (Figure 1). This also reduced $NO_2$ concentrations in Barcelona. However in Madrid the lowest levels for these pollutants were attained when substituting 10% of the private cars. (Gonçalves et al., 2009a, 2009b).

The main conclusion extracted from this work is that the air quality improvement plans must be designed considering the local characteristics, both vehicle fleet and meteorological, and maximum reductions in pollutants may be obtained through different measures in different regions. If these are defined with sufficient detail in the modelling systems, the models can effectively be used as tools to aid the decision making process.

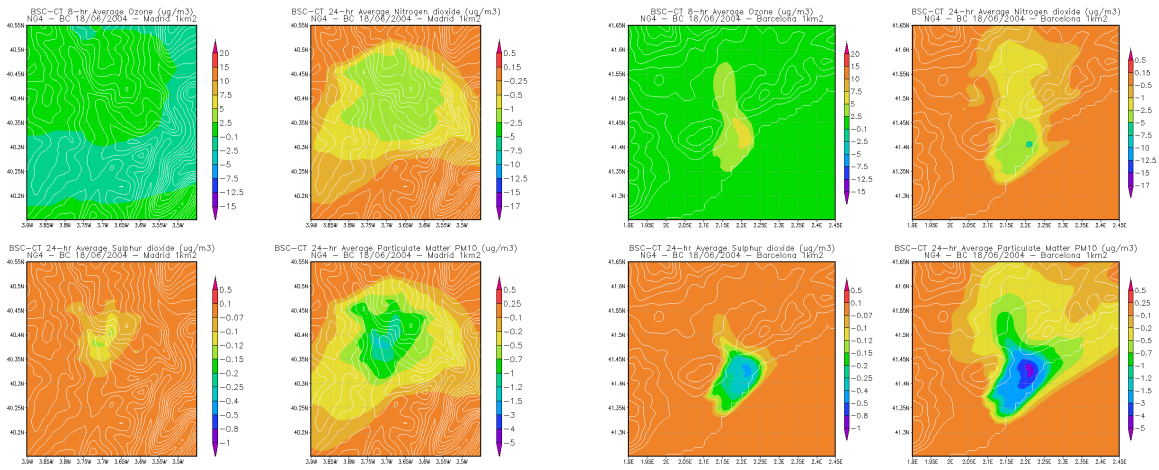

*Figure 1. Absolute changes in 8-h average concentration of O3 and 24-h average concentration of NO2, SO2 and PM10 (µg/m3) when introducing 50% of commercial light vehicles as natural gas vehicles instead of the oldest vehicles in the fleet of Barcelona (left) and Madrid (right)*

Baldasano J.M., L. P. Güereca, E. López, S. Gassó, P. Jimenez-Guerrero (2008). Development of a high-resolution (1 km x 1 km, 1 h) emission model for Spain: the High-Elective Resolution Modelling Emission System (HERMES) . Atmospheric Environment, 42 (31): 7215-7233, doi:10.1016/j.atmosenv.2008.07.026. ISSN: 1352-2310, October 2008.

Byun, D.W., Schere, K.L. (2006). Review of the governing equations, computational algorithms and other components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System, Applied Mechanics Reviews, 59(2), 51-77.

Gonçalves, M., Jiménez-Guerrero, P., Baldasano, J.M. (2009a). Emissions variation in urban areas resulting from the introduction of natural gas vehicles: application to Barcelona and Madrid Greater Areas (Spain). Science of the Total Environment 407, 3269-3281. doi:10.1016/j.scitotenv.2009.01.039.

Gonçalves, M., Jiménez-Guerrero, P., Baldasano, J.M. (2009b). High resolution modeling of the effects of alternative fuels use on urban air quality: Introduction of natural gas vehicles in Barcelona and Madrid Greater Areas (Spain). The Science of the Total Environment 407, 776-790. doi:10.1016/j.scitotenv.2008.10.017

Gonçalves, M., Jiménez-Guerrero, P., Baldasano, J.M. (2009c). Contribution of atmospheric processes affecting the dynamics of air pollution in South-Western Europe during a typical summertime photochemical episode . Atmospheric Chemistry and Physics, 9, 849-864, www.atmos-chem-phys.net/9/849/2009/. ISNN: 1680-7316, February 2009

Michalakes, J., Dudhia, J., Gill, D., Henderson, T., Klemp, J., Skamarock, W., Wang, W. (2005). The Weather Research and Forecasting Model: Software architecture and performance. Proceedings of the Eleventh ECMWF Workshop on the Use of High Performance Computing in Meteorology, Zwiefhofer, W. and Mozdzynski, G. (Eds.), World Scientific, 156-168.

### *A1.3.4 Planning study for Northern Italy using TCAM and a multi-objective decision model*

Northern Italy (Lombardy region) is an area often affected by exceedances of secondary pollutants (namely ozone, $PM_{10}$, $PM_{2.5}$, $NO_2$) due to unfavourable meteorological conditions and high anthropogenic precursor emissions. In this area nonlinearities in pollution formation and accumulation are very important and cannot be ignored when developing air quality plans.

In the framework to support the decision maker in defining sound air quality plans, a multi-objective decision model has been formalized and solved (Pisoni et al, 2009). The objectives are the secondary pollution exposure index and the cost of policy implementation. The decision variables of the optimization problem are the precursor emissions (namely VOC, $NO_X$, $NH_3$, $SO_2$ and primary PM) for the CORINAIR macro-sector. The relations between decision variables (precursor emissions reductions) and the air quality objective are described by non-linear models (Carnevale et al, 2009) described by Transport Chemical Aerosol Model (TCAM) simulations (Carnevale et al, 2008). The cost of emission reduction policies is obtained by the IIASA GAINS databases (Amann et al, 2004). The two-objective problem is coupled to an external cost evaluation module, to provide detailed information about health effects and related societal costs of the obtained optimal solutions (Pisoni et al, 2009b).

In Figure 1 (left) the solutions of the two-objective problem (Pareto boundary) are shown. The x-axis represents the cost of implementation of optimal emission reduction policies while the y-axis depicts the Air Quality Index (in this case the average $PM_{10}$ annual mean value in the domain). The policy maker can choose from these optimal solutions the most efficient policy to implemented over the domain. Figure 1 (right) shows the health effects (in months of lost life) associated to the point **A** of the Pareto boundary.

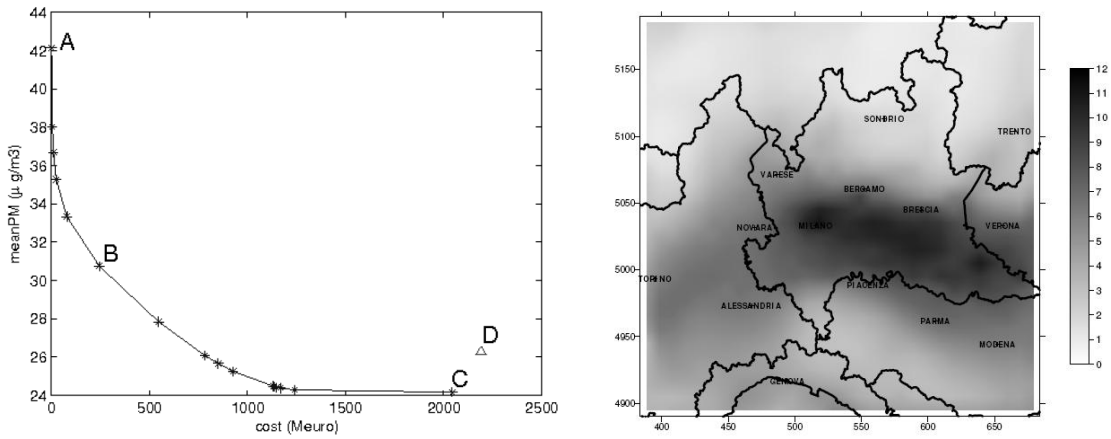


*Figure 1. Pareto boundary optimal scenarios, solutions of the two-objective problem (left) and months of lost life for the base case (right) (in Pisoni et al, 2009a, Pisoni et al, 2009b)*

The analysis of the Pareto boundary allows an assessment of the priorities of emission ablation policies supporting Environmental Authorities in reducing particulate matter exposure with minimum costs. For example, Point **B** of Pareto boundary corresponds to a policy that reduces 35% of the PM10 concentrations with only 15% of the maximum costs. The results furthermore show that the emission scenario defined by applying the Maximum Feasible Reductions (point **D**) is not a Pareto efficient solution.

Figure 2 shows the internal (due to implementation of emission reduction policies) vs external (due to morbidity and mortality) costs trends, for the optimal solutions calculated through the multi-objective approach. The costs

are per year and are computed over the whole domain. Figure 2 (left), related to internal vs morbidity (RHA-Respiratory Hospital Admissions, CVA- Cerebrovascular Hospital Admissions) costs, shows that internal costs are up to two orders of magnitude higher than morbidity costs. But looking at YOLL (years of lost life) mortality index (Figure 2, right) the external costs are higher than the internal costs, except for the extreme scenarios obtained for maximum effective reductions. This fact points out that acting on emission controls to reduce PM concentrations is greatly beneficial from a socio-economic point of view. The ratio between the external and the internal costs computed for different Pareto boundary points significantly decreases for all the indicators when Scenario O is reached. Such scenarios can be marked as optimal in terms of benefit-costs.

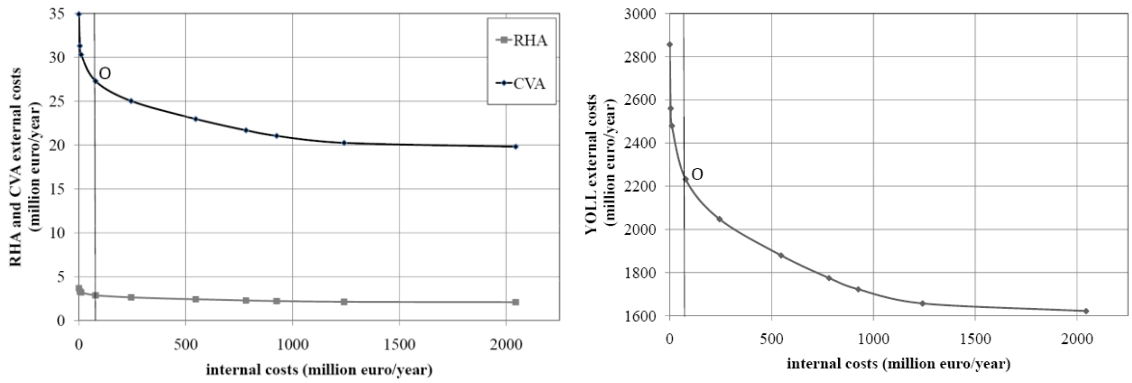


*Figure 2. Morbidity (RHA, CVA) vs internal costs (left) and mortality (YOLL) vs internal costs (right), for the optimal scenarios solutions of the two-objective problem (in Pisoni et. al, 2009b).*

M. Amann, I. Bertok, J. Cofala, F. Gyarfas, C. Heyes, Z. Klimont, W. Schopp, W. Winiwarter (2004). Clean Air For Europe (CAFE) Programme final. Tech. rep., IIASA, Laxenburg, (AU).

C. Carnevale, G. Finzi, E. Pisoni and M. Volta (2008). Modelling assessment of PM10 exposure control policies in Northern Italy, Ecological Modelling, 217, 219-229.

C. Carnevale, G. Finzi, E. Pisoni and M. Volta (2009). Neuro-fuzzy and neural network systems for air quality control, Atmospheric Environment, 43, 4811-4821.

E. Pisoni, C. Carnevale and M. Volta (2009). Multi-criteria analysis for PM10 planning, Atmospheric Environment, 43, 4833-4842.

E. Pisoni and M. Volta (2009b). Modeling Pareto Efficient PM10 control policies in Northern Italy to reduce health effects, Atmospheric Environment, 43, 3243-3248.

## *A1.3.5 Use of models in the assessment and planning of the air quality in the Netherlands*

*Large scale concentration maps*

In the Netherlands maps of the large-scale concentration are made on a yearly basis for the air pollutants for which EU regulation exists. The maps are made for past years as well as for future outlooks on a 1x1 km resolution. The maps are used in the reporting on the exceedances in the framework of the AQD and for local policy and planning. These maps are based on a combination of measurements and model calculations. The model results are calibrated with the measurements. The concentration in high emission situations are determined by adding the contribution to the concentration caused by local sources to the large-scale concentration maps. The local contribution for instance is calculated with the CAR-model (Calculation of Air Pollution from Road traffic, van den Hout en Baars, 1988) for city roads, the ISL2-model (Implementatie Standaardrekenmethode Luchtkwaliteit 2) for highways or the Clean Air Policy Tool (see below).

The large-scale concentrations are calculated with the Operational Priority Substances (OPS) dispersion model (Van Jaarsveld, 2004; Van Jaarsveld and De Leeuw, 1993). The OPS model calculates annual average concentrations based on emissions and their dispersion, transport, chemical conversion and deposition. The model uses a Gaussian plume for dispersion on a local scale and a Lagrangian trajectory for long-distance transport of compounds. The large-scale concentrations contain contributions from all sources in the Netherlands and other European countries. The calculations are made on a 1x1 km resolution. The

concentration is therefore considered to be representative for averaged spatial rural and urban background concentrations.

Observations from the National Air Quality Monitoring Network (LML, 2008) are used for calibration of the calculations. About 35 observational sites are used in the calibration of the $NO_2$ concentration and about 17 sites for $PM_{10}$ concentrations. In the calibration procedure, the difference between the modelled and observed concentrations is interpolated and added to the modelled concentration. For $NO_2$, the modelled concentration was − even before calibration − very close to the observations. This is not the case for $PM_{10}$. The available quantified direct anthropogenic emissions and the secondary inorganic aerosols account for only about half of the observed concentrations (Matthijsen and Visser, 2006). The other half is from emissions of sea salt, wind blown dust, hemispheric transport, elementary carbon, organic compounds and metal oxides (Buijsman et al., 2005). The contributions from these sources are accounted for in the calibration.

Spatial distributions, which show concentrations for years into the future, use emissions from the scenarios and long-term (1990–1999) average meteorology. Projected $PM1_{10}$ concentrations for future years are corrected by the same value as the difference found between modelled and observed $PM1_{10}$ concentrations over the most recent four years.

*Clean Air Policy Tool*

With a view to improving air quality and meeting air quality limit values quickly, and at the same time allowing for new spatial development projects, a new Air Quality law came into operation in The Netherlands. The core of the National Plan is a cooperation programme between central government and the provincial and municipal authorities. To support the process of identifying areas where air quality problems remain unabated and identifying the policy actions to be taken by the various authorities, Goudappel Coffeng have developed a software application called the “Clean Air Policy Tool (CAPT-NL)” (in Dutch “Saneringstool”). This application has also an English version: http://www.saneringstool.nl/saneringstool_ENG.html .

The Clean Air Policy Tool maps the air quality along the entire Dutch road network and other possible hot spots (e.g. intensive livestock breeding). The software tool assists users in finding possible $NO_2$ and $PM_{10}$ exceedances as well as which specific policy measures are foreseen. Air quality calculations for the main road network use the VLW model (Vermeulen, 2009). Those for the secondary road network are based on the CAR model. The Clean Air Policy Tool provides a forecast for the years 2011, 2015 and 2020.

The Clean Air Policy Tool was a major building block for the derogation proposal of the Dutch government. This proposal was ratified by DG Environment in April 2009. The final result of the Clean Air Policy Tool is the situation before and after local policy measures. In total for more than 6000 road segments policy measures are foreseen. Most popular policy measure is to include emissions restrictions for buses in the regional public transport concessions. A second popular policy measure is the implementation of an environmental freight transport zone.

Buijsman, E., Beck, J.P., van Bree, L., Cassee, F.R., Koelemeijer, R.B.A., Matthijsen, J., Thomas, R., Wieringa, K., 2005. Particulate matter: a closer look, MNP report 500037011, Netherlands Environmental Assessment Agency, ISBN 9069601338, Bilthoven, The Netherlands.

Hout KP van den, Baars HP. 1988. "Development of two models for the dispersion of pollution from road traffic: the TNO traffic-model and the CAR-model". TNO Report R88/120 (in Dutch).

LML, 2008. Dutch National air quality monitoring network National Institute of Public Health and the Environment, Bilthoven, Netherlands, Bilthoven, The Netherlands, http://www.lml.rivm.nl.

Matthijsen, J., Visser, H., 2006. PM10 in the Netherlands, Methods, concentrations and uncertianties, MNP report 500093005, Netherlands Environmental Assessment Agency, Bilthoven, The Netherlands.

Van Jaarsveld, J.A., 2004. The Operational Priority Substances model, RIVM report no. 500045001, National Institute of Public Health and the Environment, Bilthoven. The Netherlands, http://www.mnp.nl.ops.

Van Jaarsveld, J.A., De Leeuw, F.A.A.M., 1993. An operational atmospheric transport model for priority substances, Environmental Software 8, 93-100.

Vermeulen, A.T., 2009. VLW versie 2.70: Korte beschrijving van meest recente versie van het verkeersmodel VLW. ECN-E--06-050 (In Dutch).

### *A1.3.6 Action plan for reduction of ground-level ozone in air quality management areas in Croatia*

A preliminary assessment of air quality made in Croatia, based on available measurement, emission data and EMEP model results for the period 2004-2006 (Vidic, 2007), indicated that ozone constitutes a continuous and persistent environmental problem, partly due to a geographical position, but mostly due to a distribution of strong regional/European sources of $NO_x$ and VOC emissions. The assessment showed that AOT40 values for vegetation and crops, as well as values of SOMO35 are heavily exceeded over the whole territory of Croatia with peaks in coastal regions. Even though number of days with exceedances of 8-hr maximum concentrations is within the limits for most sites, the average values of ozone concentrations are high over a long periods of time covering vegetation periods for crops and vegetation (spring-summer-autumn).

In order to further explore ozone conditions and options for the reduction of its precursors, a comprehensive modelling study has been conducted in 2009-2010 (Action plan for reduction of ground-level ozone in air quality management areas, Vidič et al. 2010). A regional air pollution modelling system (EMEP4HR) has been developed in order to apply the Unified EMEP model at finer resolutions (i.e. national scales and finer time scales). For this purpose, high resolution (10-km grid) emission inventory for Croatia was developed (e.g. Jeričević et al. 2007; Prtenjak et al. 2009). Outside Croatian domain, 50-km resolution emissions were interpolated to 10-km grid (Fig. 1). The EMEP4HR model was implemented as a support to the Croatian authorities to meet requirements of EU legislation on air quality and in particular to:

- Assess the spatial distribution of ozone, $NO_x$ and VOC concentrations
- Calculate exceedances above the threshold value
- Calculate health related SOMO35 indicator
- Calculate AOT40 for forests and crops
- Compare measured and modelled concentrations,
- Assess the ability of the modelling system to reproduce ambient air quality conditions for all criteria pollutants
- Simulate results of different emission reduction options.

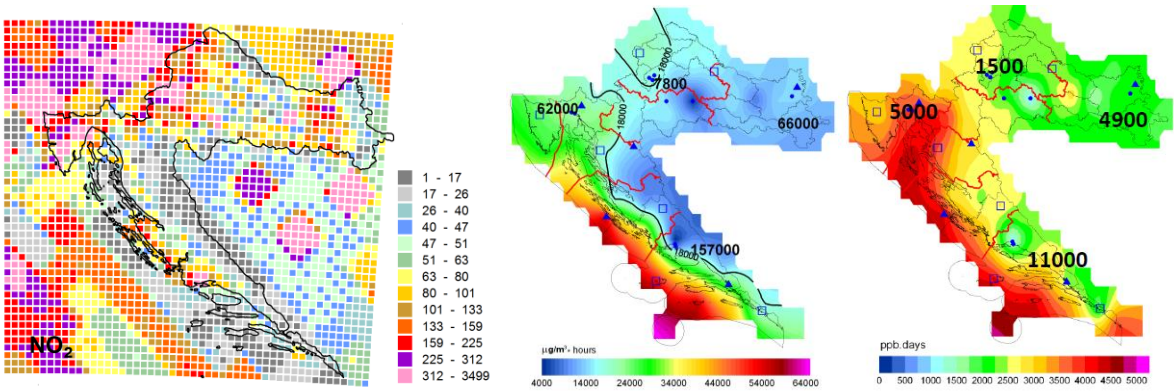


*Figure 1. The gridded emissions of $NO_2$ (t/year) used in the EMEP4HR model at 10 km x 10 km horizontal resolution (left), AOT40 for forests in µg/m³.hours (middle) and SOMO35 in ppb.days (right). Numbers represent values obtained from measurements.*

Calculations were carried out for four different emission reduction scenarios: base model run with all emissions included, model run without Croatian emissions, run with the scenario of 30% $NO_x$ reduction from all Croatian emission sources and activity sectors and model run with the scenario of 30% $NO_x$ reduction from emission sources in energy and industrial sectors. The model results were compared to the corresponding measurements of ozone and a good agreement was found in most cases.

Since ambient levels of $O_3$ and $NO_2$ are strongly coupled the response to reductions in the emissions of $NO_x$ is highly non-linear. Model results show that even with high reduction measures of $NO_2$ introduced locally, only small improvements in ozone reduction are achieved. Nevertheless, the effectiveness of reduction options in areas with $NO_x$/VOC limitations has been identified. Overall results of the study show that reduction of ozone concentrations based only on national emission reduction measures is insufficient and that ozone can be regulated only through internationally harmonized emission reduction policy.

Jeričević, A., Kraljević, L., Vidič, S., and Tarrasón, L.: Project description: High resolution environmental modelling and evaluation programme for Croatia (EMEP4HR), available at http: //geofizika-journal.gfz.hr/vol24.htm, Geofizika, 24 (2), 137–143, 2007.

Vidič, S and Benković V., 2007.: 'Preliminary assessment of air quality in Croatia', pp 49, MHSC.

Vidič, S, Kraljević, L. and Benković V., 2007.: 'Action plan for reduction of ground-level ozone in air quality management areas in Croatia', pp 57, MHSC.

## A1.4 Examples for air quality forecasting and short term action plans

### *A1.4.1 Forecast models for determining the risk of exceedance of alert thresholds and the development of short term action plans in Portugal*

Air quality forecasting is a challenging scientific problem, which has recently undergone considerable pressure in many urbanised and industrialised countries due to the increasing awareness of the effect on health and environment of pollutants emissions into the atmosphere. For the operational forecast of air quality over mainland Portugal, the MM5-CHIMERE numerical modelling system was adopted. The forecasting system is designed to deliver values in the early morning (D+0) for the same and the next 2 days. Meteorological forecasts are obtained at day D+0 using the MM5 mesoscale meteorological model forced by the AVN/NCEP global forecasts. Processed meteorological variables are then provided to the chemistry-transport model, as well as the emissions. This forecasting system began real-time application in 2005, regarding gaseous pollutants, and in 2006 was extended for aerosols. During these two years it has been tested and validated against monitoring data. Concerning the chemical model evaluation, the comparison between air quality index observed and predicted at background stations shows an agreement of 60% and a success of detecting alarms higher than 50% (but with several false alarms) for both $O_3$ and $PM_{10}$. There is no obvious trend for model performance decreasing with the lead time. This validated forecast system was then launched for public dissemination beginning in 2007 through web page (www.prevqualar.org/mapanacionalprevzonas.do) and media. Strategic emission reduction (short term plans) measures are planned in order to react to bad air quality forecast and to estimate the risk of alert threshold exceedance.

This operational service was developed under a protocol with the Environmental Protection Agency of Portugal.

### *A1.4.2 Operational Air Quality Forecasting Systems for Italy and Rome Metropolitan Area*

Following increasing interest from the scientific community, the new European Air Quality Directive and the needs of policy makers, a national scale forecast system named 'QualeAria' has been built for Italy starting from the background experience of the EU 5th Framework Programme project FUMAPEX (Baklanov et al., 2007; Finardi et al., 2008) and within the international cooperation promoted by COST ES0602 Action (http://www.chemicalweather.eu).

The modelling system is designed following a framework similar to that adopted for the MINNI project (Zanini et al., 2005), implementing the same modelling system and computational domain extension: a) the operational horizontal resolution is 12 km; b) the meteorological downscaling is produced by RAMS model driven by NCEP forecast; c) Italian (ISPRA2005) and European (EMEP) inventories are used to produce emissions; d) prognostic boundary conditions for gas species are provided on a daily basis by MATCH-MPIC global chemical weather forecast (http://www.mpch-mainz.mpg.de/~lawrence/forecasts.html ), e) the FARM model provides the predictions of transport and chemical transformations for gaseous and particulate pollutants, using SAPRC90 gas-phase mechanism and aero3 particulate module.

The forecasting system produces every day 48 hour predictions of different species concentrations (CO, SO2, NO2, Ozone, PM10, PM2.5). Hourly plots and daily statistics are available on the system web site (http://www.aria-net.eu/QualeAria ). One of the main aims of regional and national scale air quality forecast systems is to provide proper boundary conditions for urban or local scale forecast that can provide a relevant support to air quality management and health protection over the areas more affected by pollution events. In this context, QualeAria is used to provide boundary conditions to the air quality forecasting system for Rome and its surrounding region (Figure 1), that has been developed in cooperation with the Environmental Protection Agency of Lazio Region (ARPA-Lazio) and put on operation since spring 2008 and its results can be considered reliable from late summer 2008.

The modelling system resembles that previously realized for Turin (Baklanov et al., 2007; Finardi et al., 2008), and its predictions are published on the ARPA-Lazio web site (http://www.arpalazio.net/main/aria/previsioni/index.php ). A preliminary evaluation has been devoted to verifying the ability of the AQ forecast to reproduce the observed concentration of major pollutants (Finardi et al., 2009). Currently the forecasting system has been shown to work satisfactorily for $NO_2$, but shortcomings in regard to the long range transport of PM are evident in the forecasts. In this regard the enhancement of boundary conditions and the inclusion of Sahara dust forecasts (http://www.bsc.es/projects/earthscience/DREAM ) are among the priorities for further forecasting system development. A near-real-time air quality analysis system implementing air pollution data assimilation is presently under development to integrate Rome city air quality analysis tools and to allow a better initialization of the air quality forecast.

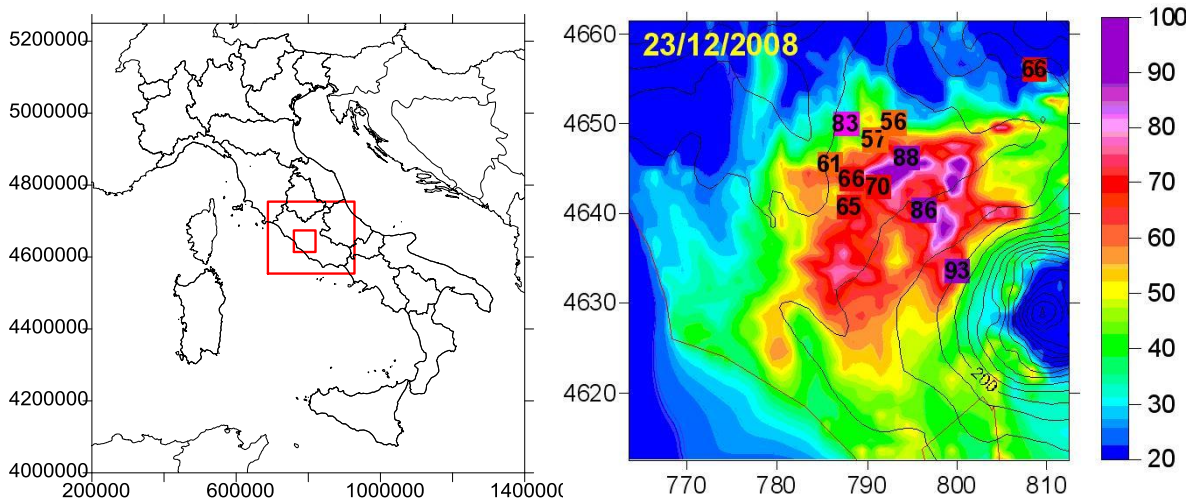


*Figure 1. Lazio regional (4 km resolution) and Rome metropolitan (1 km resolution) computational domains (left) and PM10 daily average concentration predicted on the inner domain for 23/12/2008.*

Zanini G., Pignatelli T., Monforti F., Vialetto G., Vitali L., Brusasca G., Calori G., Finardi S., Radice P., Silibello C. (2005) The MINNI Project: An Integrated Assessment Modeling System For Policy Making. In Zerger, A. and Argent, R.M. (eds) MODSIM 2005 International Congress on Modelling and Simulation. Modelling and Simulation Society of Australia and New Zealand, December 2005, pp. 2005-2011. ISBN: 0-9758400-2-9.

Baklanov A., Hänninen O., Slørdal L. H., Kukkonen J., Bjergene N., Fay B., Finardi S., Hoe S. C., Jantunen M., Karppinen A., Rasmussen A., Skouloudis A., Sokhi R. S., Sørensen J. H., (2007) Integrated systems for forecasting urban meteorology, air pollution and population exposure. Atmos. Chem. Phys., 7, 855–874, 2007.

Finardi S., De Maria R., D'Allura A., Cascone C., Calori G., Lollobrigida F., (2008) A Deterministic Air Quality Forecasting System For Torino Urban Area, Italy. Environmental Modelling and Software, 23, 344-355.

Finardi S., D'Allura A., Maddalena M., Morelli M., Bolignano A. Sozzi R. (2009) An Air Quality Forecast System For Rome Metropolitan Area: First Evaluation And Identification Of Critical Issues. Proceedings of 7th International Conference on Air Quality - Science and Application (Air Quality 2009), Istanbul, 24-27 March 2009.

### *A1.4.3 Operational system of mineral dust transport to Southern Europe, Northern Africa and Middle East.*

The operational forecasting system is based in the DREAM regional dust model (Nickovic et al., 2001) which is embedded on-line into the NCEP/Eta atmospheric model. The current model version BSC-DREAM8b (www.bsc.es/projects/earthscience/DREAM/) , described in detail by Pérez et al. (2006a,b), includes a high resolution size distribution within the 0.1–10 mm radius range according to Tegen and Lacis (1996), source distribution derived from D'Almeida (1987) and dust radiative feedbacks. BSC-DREAM8b predicts the atmospheric life cycle of the mineral dust and relies on an enhanced high resolution USGS (1 km) vegetation dataset. The model is initialized with 24-hourly (at 12UTC) updated NCEP (National Center for Environmental Prediction) 0.5º x 0.5º forecast data and the initial state of dust concentration in the model is defined by the 24-hour forecast from the previous-day model run. For BSC-DREAM8b the horizontal (1/3º) and vertical (24 z-levels) resolution is kept. The latitudinal forecast domain covers 15ºN to 60ºN, the longitudinal 25ºW to 50ºE. This operational system has been implemented and supported by the Earth Sciences Department of the Barcelona Supercomputing Center (BSC-CNS).

Qualitative and quantitative verification studies performed so far for DREAM (e.g. Balis et al., 2006; Pérez et al., 2006a; Jiménez-Guerrero et al., 2008) using data from observation networks such as the European Lidar Network EARLINET, the AERONET/PHOTONS sun photometer network, satellite and ground level PM levels (EMEP) outline the good skills of the model concerning both the horizontal and vertical extent of the dust plume in the geographic region of application. Moreover the model has been validated and tested against measurements at source regions for SAMUM (Haustein et al., 2009) and BODEX campaigns (Todd et al., 2008).

BSC-DREAM8b is one of the forecast models included in the Sand and Dust Storm Warning Advisory and Assessment System (SDS-WAS; www.bsc.es/sds-was) project promoted by the WMO. The SDS-WAS mission is to enhance the ability of countries to deliver timely and quality sand and dust storm forecasts, observations, information and knowledge to users through an international partnership of research and operational communities.

Balis, D., Amiridis, V., Kazadzis, S., Papayannis, A., Tsaknakis, G., Tzortzakis, S., Kalivitis, N., Vrekoussis, M., Kanakidou, M., Mihalopoulos, N., Chourdakis, G., Nickovic, S., Perez, C., Baldasano, J. M. and Drakakis, M. "Optical characteristics of desert dust over the East Mediterranean during summer: a case study", Ann. Geophys., 24, 807–821, 2006.

Haustein, K., Pérez, C., Baldasano, J. M., Müller, D., Tesche, M., Schladitz, A., Esselborn, M., Weinzierl, B., Kandler, K. and Hoyningen-Huene, W. v. "Regional dust model performance during SAMUM 2006", J. Geophys. Res. Lett., 36, L03812,doi:10.1029/2008GL036463, 2009.

Jiménez-Guerrero, P., Pérez, C., Jorba, O. and Baldasano, J. M. "Contribution of Saharan dust in an integrated air quality system and its on-line assessment", J. Geophys. Res. Lett., 35(3), 2008.

Nickovic, S., Kallos, G., Papadopoulos, A. and Kakaliagou, O. "A model for prediction of desert dust cycle in the atmosphere", J. Geophys. Res., 106(D16), 18113-18130, doi: 10.1029/2000JD900794, 2001.

Pérez, C., Nickovic, S., Baldasano, J. M., Sicard, M., Rocadenbosch, F. and Cachorro, V. E. "A long Saharan dust event over the western Mediterranean: Lidar, Sun photometer observations, and regional dust modeling", J, Geophys. Res., 111(D15214), doi:10.1029/2005JD006579, 2006a.

Pérez, C., Nickovic, S., Pejanovic, G., Baldasano, J. M. and Ozsoy, E. "Interactive dust-radiation modeling: A step to improve weather forecasts", J, Geophys. Res., 11(D16206), doi:10.1029/2005JD006717, 2006b.

Todd, M. C. "Quantifying uncertainty in estimates of mineral dust flux: An intercomparison of model performance over the Bodélé Depression, northern Chad", J. Geophys. Res, 113, 2008.

### *A1.4.4 CALIOPE: An operational air quality forecasting system for Spain*

The CALIOPE air quality forecasting tool based on the WRF/HERMES-EMEP/CMAQ/BSC-DREAM8b modelling system has been developed by the Earth Sciences Department of the Barcelona Supercomputing Center (Baldasano et al., 2008a) to provide a better understanding of the dynamics of atmospheric pollutants and to allow early communication when air quality thresholds are exceeded. The mesoscale meteorological model (WRF) and the chemical transport model (CMAQ) run at the high resolution of 4 km for the Iberian Peninsula and 12 km for Europe. Also in cooperation with CIEMAT the CHIMERE model is used for the assessment. The HERMES-EMEP emission model has been specifically developed as a high-resolution (1 x 1 $km^2$, 1 hr) for Spain (Baldasano et al., 2008b). The dust production from the North African continent is simulated by the BSC-

DREAM8b model which uses an improved 8-bin aerosol description at a resolution of 0.3º (see Perez et al., 2006 a,b). The simulation of such a high-resolution model system has been made possible by its implementation on the MareNostrum supercomputer. The group operationally provides 2-day Spanish and European air quality forecasts at surface level and assessment services to end-users who take advantage of this high spatial and temporal resolution of the air quality modelling system.

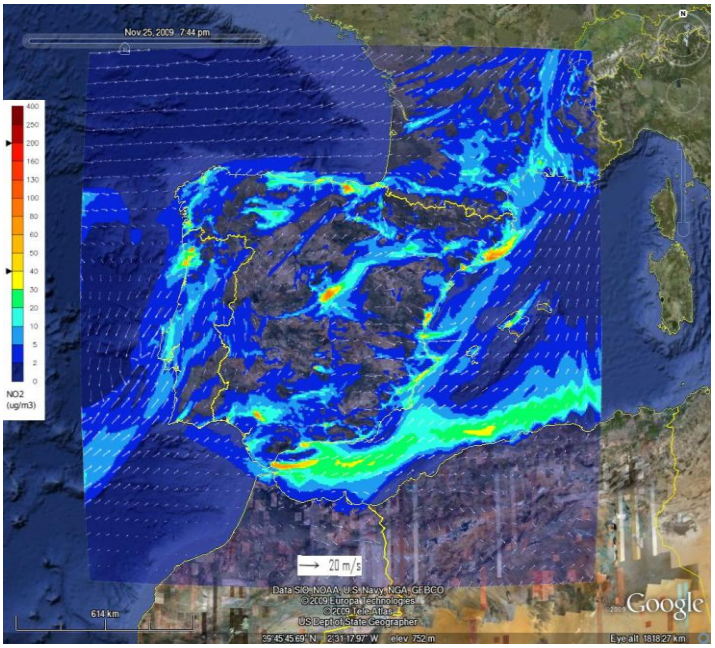


*Figure 1. Simulated 2-day forecast of NO2 surface concentrations over the Iberian Peninsula at a resolution of 4 x 4 km2, 1 hr. Day of simulation: Nov. 25th, 2009.*

This forecasting service (http://www.bsc.es/caliope) offers state-of-the-art predictions of gas pollutants ($O_3$, $NO_2$, $SO_2$, CO) and particulate matter ($PM_{2.5}$ and $PM_{10}$). The qualitative and quantitative evaluation of the model was performed for a reference year (2004) using data from ground-based measurement networks (EMEP, CSIC, Spanish air quality network provided by CEAM). As a further step, an operational evaluation system was designed to provide quasi-online evaluation products for the 24h and 48h forecasts of the Spanish domain. For this purpose, more than 130 air quality stations, 6 ozone sondes and the OMI retrieval information are introduced to the system on a daily basis. A web-based visualization system allows a straightforward access to all the evaluation products.

This project is being funded by the Spanish Ministry of Environment (441/2006/3-12.1, A357/2007/2-12.1, 157/PC08/3-12.0) and will provide a service for air quality forecasting with a high spatial resolution for the Iberian Peninsula, Balearic and Canary islands nesting in urban areas with high resolution.

Baldasano J. M., P. Jiménez-Guerrero, O. Jorba, C. Pérez, E. López, P. Güereca, F. Martin, M. García-Vivanco, I. Palomino, X. Querol, M. Pandolfi, M.J. Sanz and J.J. Diéguez: CALIOPE: An operational air quality forecasting system for the Iberian Peninsula, Balearic Islands and Canary Islands - First annual evaluation and ongoing developments. Adv. Sci. and Res., 2: 89-98, 2008a.

Baldasano J.M., L. P. Güereca, E. López, S. Gassó, P. Jimenez-Guerrero: Development of a high-resolution (1 km x 1 km, 1 h) emission model for Spain: the High-Elective Resolution Modelling Emission System (HERMES). Atm. Environ., 42 (31): 7215-7233, 2008b.

Pérez, C., Nickovic, S., Baldasano, J. M., Sicard, M., Rocadenbosch, F. and Cachorro, V. E. "A long Saharan dust event over the western Mediterranean: Lidar, Sun photometer observations, and regional dust modeling", J, Geophys. Res., 111(D15214), doi:10.1029/2005JD006579, 2006a.

Pérez, C., Nickovic, S., Pejanovic, G., Baldasano, J. M. and Ozsoy, E. "Interactive dust-radiation modeling: A step to improve weather forecasts", J, Geophys. Res., 11(D16206), doi:10.1029/2005JD006717, 2006b.

## A1.5 Examples of model quality assurance protocols

### *A1.5.1 Review of the Unified EMEP model*

In 2003 the Unified EMEP model was reviewed and evaluated. This was carried out through peer review, validation exercises and model formulation inter-comparison. Results, discussions and conclusions were addressed in a final workshop. The aim of the review was stated clearly in the workshop report.

> *"The objective of the workshop was to peer review the performance of the unified EMEP model. The review considered the ability of the EMEP model to provide concentration and deposition data to facilitate the evaluation of the effects of air quality on ecosystems, support the assessment of health effects by providing regional concentrations of health-relevant pollutants, determine trends in regional air concentration and deposition data over Europe, and establish the response of regional air quality to emission changes for use in the development of emission reduction strategies (source-receptor calculations)."*

The review was accomplished through the following mechanisms:

> *"The review and the evaluation of the model were based on three elements: examination of the processes and meteorological parameterizations, chemical mechanisms and the sources of model input data; evaluation of the model performance against daily observations of key model species and fluxes for the period 1980 – 2000; and a consideration of the source-receptor relationships for sulphur, nitrogen, ozone and particulate matter < 2.5 mm and < 10 mm (*$PM_{2.5}$ *and* $PM_{10}$*)."*

Though no quantitative quality indicator was specified to evaluate the model, the peer review process provided an assessment of whether or not the model satisfactorily addressed the application for which it was intended. The assessment related the model performance to other models as well as to the validation exercise. For the most part the model was found to be performing satisfactorily but a number of weaknesses in the model were highlighted and recommendations for improvements were given.

TASK FORCE ON MEASUREMENTS AND MODELLING REVIEW OF THE UNIFIED EMEP MODEL: United Nations, Economic and Social Council report: EB.AIR/GE.1/2004/6. http://www.unece.org/env/documents/2004/eb/ge1/eb.air.ge.1.2004.6.e.pdf

### *A1.5.2 Model validation exercise for micro-scale meteorological models, COST 732*

Several documents were produced during the COST732 action. One of these documents provided general guidance on model evaluation protocols (Britter and Schatzmann, 2007) whilst another (COST732, 2009), which is still under completion, provides an example of the implementation of these protocols in a validation exercise. This second document reflects the implementation of the recommended evaluation protocols. The following aspects were covered in that excercise.

1. *Validation objective:* The general validation objective was defined as being "to acquire a general insight into the state of art in model performance"
2. *Validation metrics (quality indicator) and quality acceptance criteria (quality objectives):* The following metrics and their quality objectives were used for both velocity fields and concentrations. There were no stringent criteria applied in this study but the following values, taken from VDI (2005) and Hanna et al. (2004), were used as a guide.
    a. Hit rate (q); $q < 0.66$
    b. Factor of two of observations (FAC2); $FAC2 > 0.5$
    c. Fractional bias (FB); $|FB| < 0.3$
    d. Geometric mean bias (MG); $0.7 < MG < 1.3$
    e. Normalised mean square error (NMSE); $NMSE < 4$
    f. Geometric variance (VG); $VG < 1.6$
3. *Model verification:* A methodology for assessing the numerical error estimation was applied to the participating models using the Richardson Extrapolation (RE).
4. *Database and data description:* The database was provided and documented.

5. *Validation tools:* A common excel based tool was provided for the validation exercise containing both quantitative metrics as well as visualisation for exploratory analysis.
6. *Results and discussions:* As a result of the exercise a number of points were discussed concerning fitness for purpose of the models and the metrics, the methodology in general, implementation of the exercise and the usefulness of the datasets.
7. *Conclusions:* In accordance with the validation objective conclusions concerning the state of the art in model performance were drawn.

Britter R. and Schatzmann M. (eds), 2007: Model evaluation guidance and protocol document, COST Action 732: Quality assurance and improvement of micro-scale meteorological models, 27p. (http://www.mi.uni-hamburg.de/fileadmin/files/forschung/techmet/cost/cost_732/pdf/GUIDANCE_AND_PROTOCOL_DOCUMENT_1-5-2007_www.pdf)

COST 732 (2009) Model Evaluation Case Studies: Approach and Results. Draft Version, May 2009 (119 pages, 4.3 MB). Available from http://www.mi.uni-hamburg.de/Official-Documents.5849.0.html

Hanna, S. R., Hansen, O. R. & Dharmavaram, S. (2004): FLACS CFD air quality model performance evaluation with Kit Fox, MUST, Prairie Grass, and EMU observations. Atmospheric Environment, Vol. 38, 4675-4687.

VDI (2005). Environmental meteorology – Prognostic microscale windfield models – Evaluation for flow around buildings and obstacles. VDI guideline 3783, Part 9. Beuth Verlag, Berlin.

# Annex 2: Quality indicators for meteorological and air quality model evaluation

Adapted from COST 728 (Schluenzen and Sokhi, 2008)

*$P_i$ denotes predicted values, $O_i$ denotes observed values, N - number of values considered*

| 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 | $\sigma_o = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(O_i - \overline{O}\right)^2}$ | | ✓ | ✓ |
| Standard deviation of modelled results | $\sigma_P = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(P_i - \overline{P}\right)^2}$ | Same as $\sigma_o$ | ✓ | ✓ |
| 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 | $STDE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left[\left(P_i - \overline{P}\right) - \left(O_i - \overline{O}\right)\right]^2}$ | 0.0 | ✓ | ✓ |
| Fractional Bias | $FB = \frac{\left(\overline{P} - \overline{O}\right)}{0.5\left(\overline{P} + \overline{O}\right)}$ | 0.0 | | ✓ |

| Parameter | Formula | Ideal value | Meteorology | Air quality |
|---|---|---|---|---|
| Geometric mean bias | $MG = \exp\left(\frac{1}{N}\sum_{i=1}^{N}\ln P_i - \frac{1}{N}\sum_{i=1}^{N}\ln O_i\right)$ | 1.0 | | ✓ |
| Geometric variance | $VG = \exp\left(\left(\frac{1}{N}\sum_{i=1}^{N}\ln P_i - \frac{1}{N}\sum_{i=1}^{N}\ln O_i\right)^2\right)$ | 1.0 | | ✓ |
| Skill variance | $SKVAR = \frac{\sigma_P}{\sigma_O}$ | 1.0 | ✓ | ✓ |
| Root mean square error | $RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2} = \sqrt{BIAS^2 + STDE^2}$ | 0.0 | ✓ | ✓ |
| Normalised mean square error | $NMSE = \frac{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2}{\overline{P}\,\overline{O}}$ | 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 | $FAC2 = \frac{1}{N}\sum_{i=1}^{N} n_i$ <br> $n_i = \begin{cases} 1 \text{ for } 0.5 \le \left\lvert\frac{P_i}{O_i}\right\rvert \\ 0 \text{ else} \end{cases}$ | 1.0 | | ✓ |
| Hit rate | $H_c = \frac{1}{N}\sum_{i=1}^{N} n_i$ <br> $n_i = \begin{cases} 1 \text{ for } \frac{E_i}{\lvert O_i\rvert} \le A \text{ or } \lvert E_i\rvert \le DA \\ 0 \text{ else} \end{cases}$ <br> A – desired relative accuracy <br> DA minimum desired absolute accuracy | 1.0 | ✓ <br> For the DA for temperature, dewpoint , wind and pressure, see the Table bellow | ✓ |
| Index of agreement | $IOA = 1 - \frac{\sum_{i=1}^{N}(P_i - O_i)^2}{\sum_{i=1}^{N}\left[\lvert P_i - \overline{P}\rvert + \lvert O_i - \overline{O}\rvert\right]^2}$ | 1.0 | | ✓ |

| Parameter | Formula | Ideal value | Meteorology | Air quality |
|---|---|---|---|---|
| Unpaired peak concentration accuracy | $A_u = \frac{P_{max} - O_{max}}{O_{max}}$ <br> $P_{max}$ , $O_{max}$ are unpaired maxima (no timing/spacing considered) | 0.0 | | ✓ |
| Spatially-paired peak concentration accuracy | $A_s = \frac{P_{max,x} - O_{max,x}}{O_{max,x}}$ <br> $P_{max,x}$ , $O_{max,x}$ are maxima paired in space (but not in time) | 0.0 | | ✓ |
| Hit ratio | $HR = \frac{a+d}{a+b}$ with <br> a: forecast event yes, observed event yes <br> b: forecast event yes, observed event no, <br> c: <br> d: forecast event no, observed event no | 1.0 | ✓ | |
| False alarm ratio | $FAR = \frac{b}{a+b}$ | 0.0 | ✓ | |
| Direction weighted wind error | $DIST = \frac{1}{N}\sum_{i=1}^{N}\sqrt{\left(\left(u_{pi} - u_{oi}\right)^2 + \left(v_{pi} - v_{oi}\right)^2\right)}$ | 0.0 | ✓ | |
| Probability of Detection | $POD = \frac{a}{a+c}$ | 1.0 | ✓ | |
| Gross error | $GE = \frac{1}{N}\sum_{i}^{N}\lvert P_i - O_i \rvert$ | | ✓ | |

## Desired Accuracy (DA)

(see Schluenzen and Sokhi, 2008 for more details)

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

## Benchmarks for meteorological meso-scale model evaluation

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

| 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 |

EPA Draft 2009. Reassessment of the Interagency Workgroup on Air Quality Modeling (IWAQM) Phase 2 Summary Report: Revisions to Phase 2 Recommendations

Tesche, T.W., D.E. McNally, and C. Tremback, 2002. Operational Evaluation of the MM5 Meteorological Model Over the Continental United States: Protocol for Annual and Episodic Evaluation. Prepared for US EPA by Alpine Geophysics, LLC, Ft. Wright, KY, and ATMET, Inc., Boulder, CO. http://www.epa.gov/scram001/reports/tesche_2002_evaluation_protocol.pdf

Emery, C., E. Tai, and G. Yarwood, 2001: "Enhanced Meteorological Modeling and Performance Evaluation for Two Texas Ozone Episodes", report to the Texas Natural Resources Conservation Commission, prepared by ENVIRON, International Corp, Novato, CA.

*Table A2.1. Glossary of terms used in quality assurance and model verification*

| Concept | Meaning |
|---|---|
| | |
| **Benchmarking** | A standardized 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;<br>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.<br>Benchmarking provides modellers with an external reference and best 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.<br>Adapted from: Vlăsceanu, L., Grünberg, L., and Pârlea, D., 2004, Quality Assurance and Accreditation: A Glossary of Basic Terms and Definitions (Bucharest, UNESCO-CEPES) Papers on Higher Education, ISBN 92-9069-178-6. http://www.cepes.ro/publications/pdf/Glossary_2nd.pdf |
| **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 that it has been designed for |
| **Model Inter-comparison** | 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, giving 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 USA EPA (2009) for the quantitative and qualitative methods used to assess the degree to which a model corresponds to reality (model validation). The term is preferred by US EPA, as opposed to 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 to characterise 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 USA EPA (2002) as an element in quality assurance plan 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 USA 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 models ability to react to changes in important input parameters such as emissions or meteorology in a satisfactory way. |