PUBLICATIONS

5. MODELLING

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5. Modelling

5.1 Introduction

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

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

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

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

5.2 Selection and application of models

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

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

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

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

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

Although atmospheric models are a basic tool in air quality assessment studies their limitations

should always be taken into account. Thus, before attempting to select or apply a model one should have in mind that uncertainties in model results may be large, introduced either by the model concept and/or by the input parameters. In particular:

- There is no one model capable of properly addressing all conceivable situations even for a broad category such as point sources.
- Meteorological as well as topographical complexities of the area, which are usually associated with potential exceedance of air quality standards, are rarely responsive to a single mathematical treatment; case-by-case analysis and judgement are frequently required.
- Consistency in the selection and application of models, input data and air quality data is very important. It is useless to calculate an air quality field with a spatial resolution that is much higher than that of the emission field.
- It is necessary to get balance in the detail and accuracy of the data involved: emissions inventory, meteorological data, and air quality data. Availability of appropriate data should be investigated before applying any model. A model that requires detailed, precise input data should not be used when such data are not available.
- The representativeness of model results may be limited; in most models a spatial and temporal averaging is introduced which may complicate a direct comparison with measurements at a given location and time.
- The involvement of specialists is necessary whenever the more sophisticated models are used or the area of interest has complicated meteorological or topographic features.

Particularly for first screening purposes, or in case of limited input information, the use of simple models may be appropriate. A description of such simple air pollution models for calculating the concentrations from different sources in an urban environment is provided in Annex 5.1. If initial screening leads to the conclusion that levels may be of the order of the limit values, more sophisticated models should be selected.

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

1 Define the pollutant, and the output quantity to be modelled (concentration fields, or (spatial maximum) concentrations in streets or near point sources, usually for concentration statistics, for instance annual average, 98 percentile of hourly values ...)

2 Define the time resolution needed (the averaging time for the concentration)

3 Define the "model output area" for which the model calculations should be made (usually a zone or agglomeration) and the spatial resolution needed.

4 Define the accuracy in the output quantity that is required

5 Determine the model area (this may extend considerably beyond the output area, particularly in case of pollutants with long range transport!)

6 Investigate the availability of emission data (in the model area)

7 Investigate the availability meteorological and topographical data (in the model area)

8 Investigate available air quality data (in the model output area)

9 Check available computer resources

10 Select models that are suitable for the pollutant (taking into account its chemistry and deposition), for the relevant output quantity, with the appropriate resolution in space and time, within the required accuracy, and for the area under consideration (taking into account its topography and meteorological characteristics)

11 Consider the computer requirements of the model(s); if these surpass available computer resources, reconsider model choice.

12 Reconsider the requirements on emission and meteorological data of the model(s) selected and, if necessary, collect more detailed input data (or reconsider the model choice)

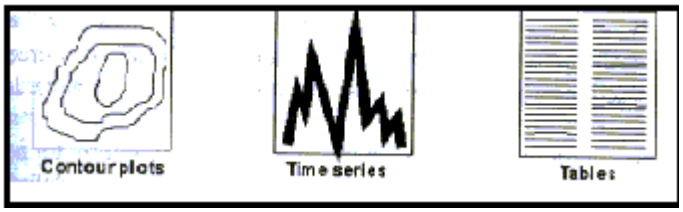
13 Prepare input data

14 Run the model

15 Compare results to available air quality data and critically evaluate. If necessary, rerun model (This will involve specialists guidance). Annex 5.2 lists model evaluation parameters (Grønskei *et al.*, 1997) that are recommended for comparing model results and air quality data.

16 Map output; here various forms of output can be made, for example

Contour plots appropriate for presenting the concentration fields and the spatial maxima. Time series appropriate for calculating the exceedances, annual average, 99.7 percentiles.
Tables appropriate for presenting the concentration statistics.



17 Assess uncertainty.

5.3 Application to four pollutants

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

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

		NO_X and NH_3 in a large area to be taken into account.	
Nitrogen dioxide and nitrogen oxides	■ 1h average concentration exceedances < 8 hours a year (equivalent to 99.9 percentile) example: (Valkonen et al., 1996) ■ annual average NO_2 conc. ■ annual average NO_X ($NO+NO_2$)	■ area or line sources for road traffic ■ elevated sources for power generation ■ Exceedances may be primarily expected in streets or in districts with heavy traffic, or close to industrial sources of NO_X.	■ Microscale (urban roadways) The models may be the same with the ones for SO_2 with the addition of a simple atmospheric chemistry scheme for NO_2 transformation ■ sub-mesoscale (area sources) UDM-FMI (Kukkonen et al., 1996), ADMS-Urban (Carruthers et al., 1995), OZIPM4/EKMA (Jeffries and Sexton, 1987) ■ Elevated point sources In mesoscale, the models may be the same with the ones for SO_2, with the addition of a simple atmospheric chemistry scheme for NO_2 transformation and deposition: ■ UDM-FMI (Kukkonen et al., 1996), or more comprehensive photochemical models: UAM (Chico and Lester, 1992), CALGRID (Yamertino et al, 1992), CIT (Russel et al., 1988), EZM (Moussiopoulos, 1995)
Lead	annual average conc. of Pb	■ road traffic, (diminishing source due to penetration of lead-free gasoline). Possible exceedances to be expected in streets with busy traffic in countries where leaded gasoline is still in use. ■ point sources of metal industries where exceedances are expected due to major emissions both from chimneys and from ore heaps.	■ Microscale (urban roadways) As for SO_2 ■ sub-mesoscale (area sources) As for SO_2 ■ Elevated point sources ■ Stock piles

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

5.4 Uncertainty of model results

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

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

predictions:

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

Annex 5.3 provides information on model uncertainty related to meteorology.

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

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

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

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

Bias evaluation	Ratio of the difference between the mean predicted concentration and the mean observed concentration to the mean observed concentration
Error analysis	The root mean square of the difference between predicted and observed concentrations

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

Annex 5.1 provides formulae for some of these methods.

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

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

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