NILU: F 4/2002

NILU: F 4/2002
REFERENCE: O-101128
DATE: FEBRUARY 2002

Dispersion models

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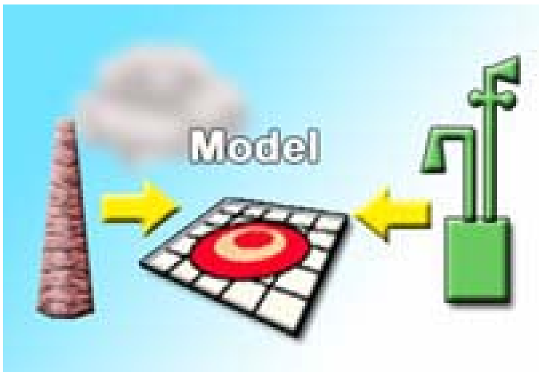
Presented at
National Training Course on
Air Quality Monitoring and Management
Lagos, Nigeria 25 - 28 February 2002



Contents

Dispersion models

1 Introduction

Atmospheric models are, broadly speaking, any mathematical procedure, which results in an estimation of ambient air quality entities (i.e. concentrations, deposition, exceedances).

In general term a distinction between process-oriented models and statistical models can be made. Process oriented models are based on the description of physical/chemical processes: starting with emissions, atmospheric advection and dispersion, chemical transformation and deposition is calculated. This type of models is able to give a description of cause-effect relations. Statistical models are valuable tools in estimating present air quality by means of interpolation and extrapolation of measuring data.

Although atmospheric models are indispensable in air quality assessment studies, their limitations should always be taken into account. Once a model has been developed, the further application of the model will be relatively cheap; however, collecting the necessary input data might be cumbersome. Models can be used for estimating past, present and future air quality, provided that information on emissions is available.

The contribution of source regions, economical sectors etc. to the ambient levels can be easily deduced from model calculations. Uncertainties in model results may be large; uncertainties are both introduced by the model concept and by the input parameters (emission data, meteorology). The model results may be representative to a limited degree. In most models an implicit spatial and temporal average is introduced which may disable a direct comparison with measurements at one location at a given moment.

Transport and dispersion models are available on all scales; from micro scale diffusion problems in street canyons to large scale intercontinental and global scale models for long-range transport problems and greenhouse gas estimates. In this presentation we will only concentrate on local scale to mesoscale models.

2 Different type of models

Wide ranges of different models have been published in scientific papers and even a larger number of unpublished models and special model versions exist. Models can be distinguished on many grounds: e.g. the underlying physical concepts, the temporal and spatial scale, and type of component. Contemporary air pollution models deal with "conventional" primary pollutants (mainly SO_2, CO, NOx and VOC).

The need is recognised to extend the models to include heavy metals and persistent organic pollutants (POPs). Also modelling secondary pollutants such as ozone is still a challenge in model development. Modelling of visibility and particulate concentrations (PM_{10}) are among the most important current model development trends.

There are no well-defined requirements with respect to model documentation. This documentation should at least consist of a user manual, short technical description and the results of sensitivity and validation tests.

2.1 Source and receptor oriented models

Numerical and statistical models are being used in air pollution studies of various content and complexity. The models can roughly be divided into two main types:

1. Source oriented models
2. Receptor models

Receptor models use measured concentrations of various air pollutants over long time periods and can by statistical analyses identify source impact and the different sources contribution to the concentration measured at specific receptor points.

The source oriented models combine information about sources (emission inventories), meteorology as well as area characteristics, topography, surface roughness etc. to estimate concentration distributions.

In the following of this report we will only discuss the **source oriented models**, as these are the only ones that adequately can be used for planning purposes. Receptor models can mainly be used for explaining measured concentrations, and is useful in such cases.

In the modern multi compartment environmental information system, i.a. the ENSIS/AirQUIS planning system, numerical air quality dispersion models (source oriented) are essential parts of the total system. These models are to be used for explanatory purposes and for planning and forecasting purposes.

2.2 Models of different complexity

A variety of different models are available on the market today. Their complexity depends strongly on the type of problems, which are to be solved. Some of the parameters, which may decide how complex a dispersion model needs to be, are:

- Compound (primary, secondary)
- Source configuration
- Meteorology and climatology
- Time scale
- Spatial scale,
- Topographical features

Some models are specifically developed and applied for one application only. Very advanced models tend to only become research type models (see applications). One should note that it might be a significant step from obtaining a model to actually having an operational modelling tool even if the intention is to use this model for a specific area and a specific application.

The following examples of different types of models available are taken from the air pollution surveillance programmes. They range from simple quasi-stationary Gaussian type single source models based upon analytical solutions of the mass balance equations, to advanced numerical models, which require large computer capacity.

The different models may roughly be divided into the following categories:

- Gaussian plume models
- Numerical models
- Trajectory models (puff, segment, etc.)
- Box models
- Statistical models

The models may also be characterised according to the type of pollutant to be studied:

- Inert passive gas,
- Gases and particles influenced by physical processes (deposition, fall-out)
- Heavy gas where density may influence the transport,
- Gases subjected to chemical reactions in the atmosphere.

The description of models below is, however, strictly limited to air pollution dispersion estimates for inert passive gases and examples are given for various air quality models available. The different types of dispersion models applied to estimate the ambient impact of air pollution also reflects the different approached linked to estimating emissions from point- line and area sources.

The selection of models to be used in a specific case is dependent upon the spatial and temporal scales, complexity of source configurations and chemistry, topographical features, climate and instationarity and inhomogeneity in the meteorological conditions of the area. It is advisable to consult experts in this process.

2.3 The single source Gaussian type models

The simplest models can be used on personal computers for impact assessment. These models can estimate 1 h average concentration distributions downwind from ground level, diffusive and elevated single sources. (Sivertsen 1980, Bøhler 1987.

Gaussian type models are based on Gaussian (normal) probability distribution of the concentration (particle density) in both the vertical and horizontal direction perpendicular to the plume centreline. These models represent simple analytical solutions to the continuity equation, which require homogenous and steady state conditions. The model concept is presented below.

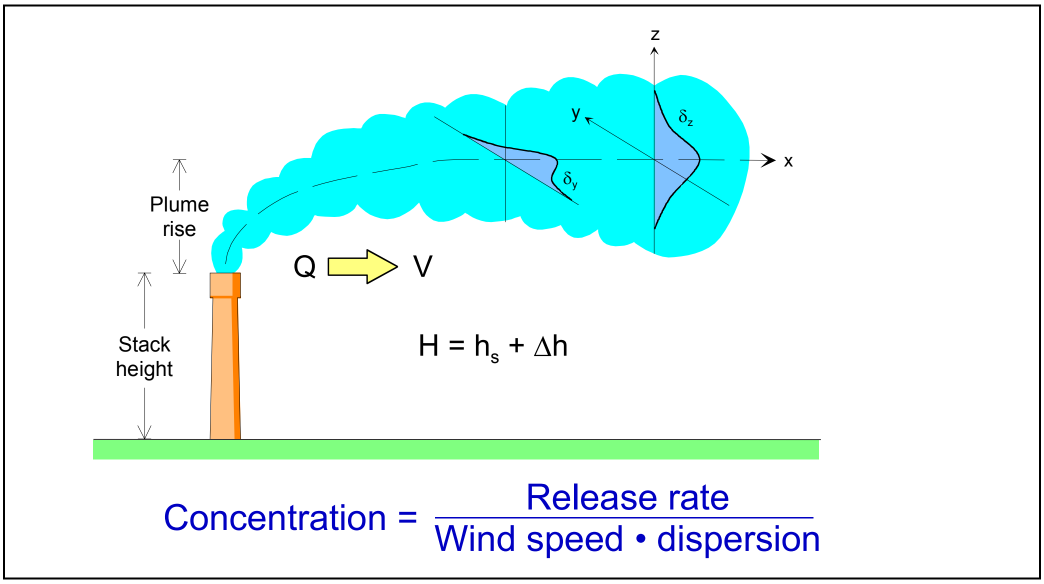


Figure 1: The concept of the Gaussian plume model.

Gaussian type dispersion models are the most commonly applied models in practical use to day. The equation for calculating the concentration (***C***) at ground level, assuming total reflection of the plume at the surface, can be written:

$$C = Q\left[\exp\left(-H^2 / 2\sigma_z^2\right)\cdot\left(-y^2 / 2\sigma_y^2\right)\right] / \left(\pi\sigma_y\sigma_z \cdot u\right)$$

where ***Q*** = release rate (µg/s)
H = effective plume height
σ = dispersion parameters (m)

The co-ordinate y refers to horizontal direction perpendicular to the plume axis, and z is the height above the ground. The ground is assumed to be flat and uniform.

The parameters σ_y and σ_z are the standard deviations of the concentration distribution in y and z directions, respectively. The parameters are usually referred to as the diffusion parameters. The values σ_y and σ_z are functions of the turbulent state of the atmosphere, which again is a function of the mechanical induced turbulence (wind shear, wind profile) and the convective turbulence (temperature profile).

An example of a Gaussian type dispersion model that has been widely used for estimation of impact from single sources and industries is the US-EPA model ISCST2. The Pasquill stability classes are required as input. Equations that approximately fit the Pasquill-Gifford curves are used to calculate the dispersion parameters in rural mode. In case of urban mode, the dispersion parameters are determined with the expressions of Briggs as reported by Gifford, and which represent a best fit to urban vertical diffusion data reported by McElroy and Pooler. Concentrations are calculated for a time series of meteorological data. The yearly average, the n largest concentrations and a time series of concentrations for several times can be reported by ISCST2. (For further reading see: Hanna et.al 1982)

2.3.1 Multiple source Gaussian models

One step up represents the short-term model for estimating 1 h average concentration distributions for emissions from a number of sources in a specified area (grid). The sources may by point sources or area sources. Area sources may be simulated by a number of points or with initial spread inside the area. The multiple source Gaussian type models have been used for estimating long term impact in urban areas or short and long term impact around industrial complexes. This type of models usually estimates short term or long term integrated concentrations in a gridded co-ordinate system.

Two different type of such models have been developed at NILU; CONDEP for monthly, seasonal and annual average concentration distribution estimates (Bøhler 1987) and KILDER which is a flexible emission inventory linked to multiple source Gaussian type dispersion models for line, area and point sources. (Gram and Bøhler 1992).

To match the specific problem the user will specify the grid system used by the models and the area considered. The resolution, grid spacing and total area can easily be modified and changed depending upon the specific needs.

These models need as input data some background information on;

- Source characteristics and emission data,
- Area characteristics (surface roughness, topography etc.),
- Measurement data (measurement type, heights etc.),
- Meteorological data (wind, stability, mixing height, temperatures etc.),
- Dispersion coefficients (type to be used and parameters),
- Dry and wet removal coefficients,
- Location of receptor points (distances or grid specifications).

All the NILU models have been well documented and are being used for planning purposes and for impact assessments both nationally and internationally.

2.3.2 US EPA Climatological Dispersion Model (CDM)

The CMD model determines long-term (seasonal or annual) concentrations of non-reactive pollutants in rural or urban settings using average emission rates from point and area sources and a joint frequency distribution of wind direction, wind speed, and stability.

The Gaussian plume hypothesis forms the basis for the calculations similar to the NILU KILDER model mentioned above. Computations can be made for up to 200 point sources and 2500 area sources at an unlimited number of receptor locations.

CDM2 is an enhanced version of CDM and includes the following options: 16 or 36 wind-direction sectors; stack-tip downwash; and gradual (transitional) plume rise. The user has a choice of seven dispersion parameter schemes. Optional output includes point and area concentration rises and histograms of pollutant concentration by stability class. CDM 2.0 is a preferred model for regulatory applications in simple urban terrain. Input files have to be provided in ASCII format.

The CDM model is based on discrete stability classes, while more updated models such as the Danish OML model is based on boundary layer scaling. The OML is thus more flexible.

2.3.3 Urban Background Models combined with Gaussian source models

Modern Gaussian plume model are often based on boundary layer scaling instead of relying on Pasquill stability classification. A Danish developed OML model may be applied for distances up to about 20 km from the source in non-complex terrain. The sources are industrial stacks, and possibly also area sources. Detailed analysis can be performed for the contribution of industrial sources to air pollution levels (Løfstrøm and Olesen, 1988).

The OML may be combined with the urban background model, UBM, which is a simple urban dispersion model that can predict the spatial distribution of pollutants in a grid over the city. For the selected pilot areas a grid size of 1x1 km^2 may be suitable. All sources within a grid are treated as area sources. The model takes into account the interaction with the regional background and handles simple photochemistry between NO, NO_2 and O_3 to be able to predict NO_2 concentration. The UBM model can calculate concentration levels of the following pollutants provided that regional background levels and emission data is available: NO_2, SO_2, lead, particles (PM_{10}) and benzene.

2.3.4 The US EPA AIRMOD model

The AERMOD is actually a modelling system with three separate components: AERMOD (AERMIC Dispersion Model), AERMAP (AERMOD Terrain Pre-processor), and AERMET (AERMOD Meteorological Pre-processor).

Special features of AERMOD (US EPA 1998a) include its ability to treat the vertical in-homogeneity of the planetary boundary layer special treatment of surface releases, irregularly shaped area sources, a three plume model for the convective boundary layer, limitation of vertical mixing in the stable boundary layer, and fixing the reflecting surface at the stack base. A treatment of dispersion in the presence of intermediate and complex terrain is used that improves on that currently in use in the US EPA industrial models (ISCST) (US EPA 1992) and other models, yet without the complexity of the Complex Terrain Dispersion Model-Plus (CTDMPLUS).

To the extent practicable, the structure of the input or the control file for AERMOD is the same as that for the ISCST3 (US EPA 1993) . At this time, the

AERMOD contains the same algorithms for building downwash as those found in the ISCST3 model.

The AERMET (US EPA 1998 b) is the meteorological pre-processor for the AERMOD. Input data can come from hourly cloud cover observations, surface meteorological observations and twice-a-day upper air soundings. Output includes surface meteorological observations and parameters and vertical profiles of several atmospheric parameters.

The AERMAP (US EPA 1998c) is a terrain pre-processor designed to simplify and standardize the input of terrain data for the AERMOD. Input data include receptor terrain elevation data. The terrain data may be in the form of digital terrain data that is available from the U.S. Geological Survey. Output includes, for each receptor, location and height scale, which are elevations used for the computation of airflow around hills.

2.3.5 Traffic models

Small-scale models are also available for estimating the air pollution load from traffic in street canyons and along roads. A commercially available model, ROADAIR (Larssen and Torp, 1993), estimates emissions, concentrations and exposure along the road system based upon traffic data. These input data may originate from traffic models or from traffic density data and on-line traffic counting.

The ROADAIR model calculates:

- Emissions of CO, NO_x and CO_2 from the traffic on each road link,
- Concentrations of CO, NO_2 and PM_{10} at chosen distance from the road curb for each road link,
- Road dust deposition (g/m^2 month) along each road link,
- Population exposure to CO, NO_2 and PM_{10} ,
- Nuisance from air pollution experienced by persons in their residence.

The road network model CONTILINK, developed by Norwegian Institute for Air Research (NILU), calculates emissions from a defined set of line sources. For each hour total concentrations of CO, NOx and PM10 are calculated at specific receptor points as a result of emission from the line sources based on hourly stationary meteorological conditions using Gaussian dispersion parameters. The modules used in the model are similar to ROADAIR.

The Danish OSPM model is a street canyon model, which is widely recognised and used. A street canyon is a street with continuous buildings of several storeys tall buildings at both sides of the street. However, the model can be used for streets with irregular buildings or even buildings on one side only but it is best suited for regular street-canyon configurations. The model should not be used for crossings or for locations far away from the traffic lanes.

The model takes into account the re-circulation of air in the street canyon and also simple photochemistry between NO, NO_2 and O_3 to predict NO_2 concentrations. The model is a combined Gaussian plume model (direct contribution from traffic) and a box model (re-circulation contribution). The model takes into account the interaction with the urban background air. Hourly concentrations of all calculated pollutants or/and statistical parameters as average values and percentiles. The application of the Danish OSPM model is for simulation of air pollution from traffic in urban streets, air quality assessment, regulatory purposes and compliance checking, scenarios for policy support, public information, and scientific research e.g. for human exposure assessment to traffic air pollution.

2.3.6 Numerical models

On a spatial scale from about 1 to 100 km there are several types of numerical models available; both Lagrangian type and Eulerian type models. The Lagrangian type models follow puffs of air pollutants estimating in each puff the turbulent diffusion, chemical reactions and deposition processes. The turbulence description and the diffusion processes may be treated in different ways.

One example is the INPUFF model (Knudsen and Hellevik, 1992), which is based upon Gaussian concentration distributions in the puff. This model also includes chemical and physical reactions and processes. Another model of this type is the Danish operational puff diffusion model RIMPUFF (Mikkelsen et al., 1987). This model was developed by Risø National Laboratory to provide risk and safety assessment in connection with e.g. nuclear installations.

2.3.7 The EPISODE model

One example of a Eulerian type numerical dispersion model is the EPISODE model developed by Grønskei et al. (1993). The EPISODE model is a mass-consistent, 3-layer (in the vertical) model solving the basic transport-diffusion equations. Based upon spatially distributed and time dependent input data of emissions, wind and turbulence, the model gives time-dependent concentrations in any receptor point within the modelling area.

Area-distributed sources (domestic, small industry, etc.) are treated within a grid system of typically 0.5-1 km. Superimposed on this, road traffic and point sources are treated in separate sub-grid models (Gaussian line-source dispersion of traffic emissions, and puff-trajectory model for point sources). Winter-type NO-NO_2-O_3 chemistry is included, and summer type photochemistry calculation schemes are being introduced into the model.

When the size of the puffs reaches the horizontal and vertical grid size the transport and dispersion is treated as a numerical box model. The mass of pollutants is then added to the average value for that grid element. The model can thus treat point sources, area/volume sources and line sources. The wind field used as input to the model may be homogeneous or inhomogeneous for each time step dependent upon the meteorological input data available.

The model runs on a Windows NT platform, and has been used for simulation of nitrogen oxides and ozone, and SPM ($PM_{2.5}$) in Oslo (Larssen et al., 1994). Presently, the model is being included in an integrated air quality information system (AIRQUIS), which includes an operative emission inventory model, air quality measurements (measured and calculated) and statistical and graphical presentation tools.

2.3.8 Mesoscale models

The numerically simulating air pollutant transport and transformation were made in the local-to-regional scale, which, broadly speaking corresponds to the mesoscale. In this context, it has been recognised for a long time that urban scale problems can only be treated successfully by the aid of mesoscale air pollution models where either a large enough domain is considered or accurate boundary conditions are established. The former is in conflict with the limited hardware resources - an aspect of paramount importance for practical applications. For the latter, models with nesting capabilities are required - and those have only recently become available.

For a longer period of time, it was considered as impossible to apply mesoscale air pollution models for policy purposes. In fact, all models, which are currently available for practical applications, emerged from research activities covering broad fields of atmospheric physics and chemistry as well as advanced numerical techniques for the solution of partial differential equations.

Mesoscale air pollution models require at input considerable meteorological information. In the last years, two different approaches were followed in this respect:

- Diagnostic wind field calculation, in conjunction with an empirical parameterisation for turbulence quantities.
- Prognostic calculation of both wind fields and turbulence quantities.

In view of the above, a mesoscale air pollution model usually represents a model system consisting of

- A wind model (either a diagnostic or a prognostic one) and
- A dispersion model.

Both Eulerian and Lagrangian model types are being employed in case of inert (non reactive) pollutants. A Eulerian dispersion model is easily embedded in a prognostic wind model, the combination being frequently termed “prognostic mesoscale air pollution model”. Eulerian dispersion models predominate in the case of reactive pollutants, typically ozone and its precursors. Here it is usual practice to apply the wind model first and the (photochemical) dispersion model subsequently.

Mesoscale processes usually extend to say twofold or threefold the extension of the atmospheric boundary layer (ABL). In prognostic mesoscale models the large scale (temporal and spatial) distribution of all problem variables is assumed to be known and is used to define initial and boundary conditions. Major aim of these models is to describe how the problem variables are affected by mesoscale influences (e.g. those associated with orography and inhomogeneities in the surface energy balance).

In most of the contemporary prognostic mesoscale models a transformation to terrain-influenced co-ordinates is performed to avoid difficulties in the formulation of the boundary conditions at surface. In some models a pressure co-ordinate is used in the vertical direction. Individual mesoscale models differ also with regard to

- The structure of the computational domain (dimensionality, grid definition),
- The utilised parameterisations,
- The method of initialisation,
- The imposed boundary conditions and
- The applied numerical techniques

2.4 The operational dispersion model

Operational dispersion models contain the type of input data that has been described earlier in this chapter:

- Emission data,
- Meteorology (wind, turbulence, temperature),
- Chemical reaction mechanisms,
- Deposition mechanisms.

The input to these models may come from a monitoring programme or be taken from historical data records or pre-estimated variables. The figure below indicates the procedures of an operational model.

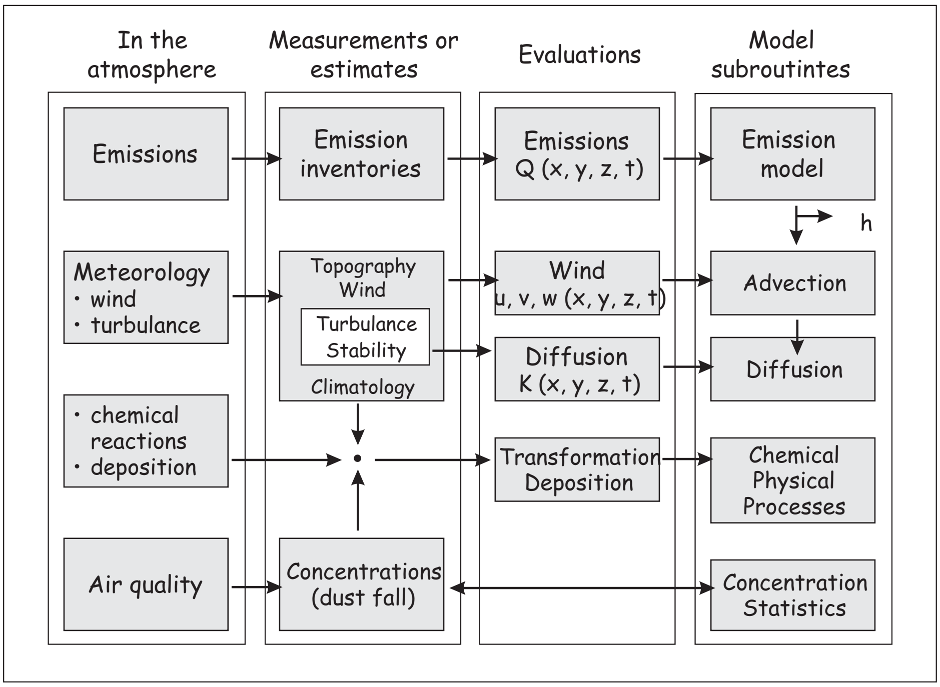


Figure 2: The procedure of an operational dispersion model used in practical applications.

A dispersion model is often more useful than a measurement programme. At least together with measured air quality data the model is superior compared to the single point measurement data only.

The type of model to be utilised for a specific application will be dependent upon several factors such as:
- Accuracy
- Available computer capacity
- Economic resources
- Source types (chemical compounds)
- Point source/area source
- Continuous or puff-release
- Terrain (type, complexity, surface)
- Scale (time and space)
- Averaging time for estimated concentrations

A model produces a complete picture of the concentration distribution for an area. A source-oriented model can calculate the contribution, and evaluate the importance, of each source to the total picture. Models can also be used to evaluate the representativity of measured data.

For further information on the use of models Hanna et al. (1982) give a good overview of the topic. One important issue when using dispersion models is to obtain adequate meteorological input data. Meteorological pre-processors have been developed during the last few years to handle this problem. (Paumier et al., 1985 and Bøhler et al., 1995). These pre-processors can estimate meteorological dispersion and the basic meteorological variables of interest for diffusion modelling based upon the current concepts regarding the structure of an idealised boundary layer. (Gryning et al., 1987). Methods are also provided for estimating the vertical profiles of wind velocity, temperature and the variances of the vertical and lateral wind velocity fluctuations.

3 Different model applications

Air quality dispersion models have been and are being used for several purposes. Some of the most important areas in which models are of greatest importance are in:

1. Existing and future single source impact evaluations
2. Siting of large single sources relative to sensitive areas
3. Stack height evaluation to avoid adverse impacts
4. Estimate the effect of cleaning device
5. Evaluate impact of accidental releases
6. Deposition problems
7. Odour problems
8. Photochemical oxidants
9. Estimate of impact from remote sources
10. Area and land use planning purposes
11. Traffic planning and impact of traffic

12. Planning of measurement programs
13. Analysis of measurement data
14. Trend analysis
15. Forecast of episodes

Four typical examples in a slightly wider framework are applications for:
- Regulatory purposes
- Policy support
- Public information and
- Scientific research

3.1 Regulatory purposes

Model results are used in issuing emission permits (usually for single sources) or for environmental impact studies related to, for example, industrial plants and new roads. In general terms, models in this application area have to provide spatial distribution of high episodic concentrations and of long-term averaged concentrations for comparison with air quality guidelines.

A wide range of pollutants is modelled (e.g. SO_2 , NO_2 , suspended particles, but also toxic substances like heavy metals and organics). In some situations the desired model output should include information on odorous components. It is indisputable that this might be beyond the scope of most of the models since the models used at present are not very suitable for handling concentration fluctuations in a proper manner.
In the framework of a European ad hoc initiative on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes standardised methods e.g. tools for model evaluation: reference data set, software and protocols for model evaluation are being developed (Olesen and Mikkelsen, 1992).

3.2 Policy support

The effect of abatement measures has to be forecasted by the models. This may require that the model also give reliable results under pollution conditions, which differ strongly from the present situation.

Use of atmospheric models in combination with models for other compartments (e.g. soil, water but also emission modules) in order to obtain a more integrated approach is becoming more and more important. For practical reasons this might imply that more simplified models without losing essential information has to be developed.

3.3 Public information

Requirements for models for public information are increasing. Demands have also been increasing when it comes to the use of air pollution models as policy support and as part of the assessment studies. This has also lead to a need for on-line information to the public using dispersion models both for estimating impact areas (exposure to the population) and for forecasting air pollution into the next 24 or 48 hour.

Occurrence of smog episodes will have to be forecasted with an improved accuracy in the future. The role of models in public information is still expected to grow.

3.4 Scientific research

Among the major objectives for research type models are the description of dynamic effects and the simulation of complex chemical processes involving air pollutants. Until very recently, this type of models proved in most cases not to be suitable for practical applications: their requirement on computational effort was too high for application in the above three fields. Thanks to the tremendous computer hardware development, however, the situation is rapidly changing in favour of complex research type models. Hence, models of this type are not only valuable for identifying limitations and gaps in simpler policy oriented models; they could represent the proper policy supporting models in the near future. For this reason, research type models are also discussed, at least partially, in the present report.

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