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Dispersion modelling and use of meteorological data

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Dispersion modelling and use of meteorological data

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.

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Wide ranges of different models have been published in scientific papers and even a larger number of unpublished models and special model versions exist.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 SO₂, CO, NO_x and VOC).

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. The NILU developed AirQUIS planning system, uses numerical air quality dispersion models.

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

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 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 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 The US EPA AIRMOD model

The AERMOD is actually a modelling system with three separate components: AERMOD (AERMIC Dispersion Model), AERMAP (AERMOD Terrain Preprocessor), 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).

2.3.4 Traffic models

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.

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/m² month) along each road link,
- Population exposure to CO, NO₂ and PM₁₀,
- Nuisance from air pollution experienced by persons in their residence.

2.3.5 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.

2.3.6 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 massconsistent, 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-NO₂-O₃ chemistry is included, and summer type photochemistry calculation schemes are being introduced into the model.

2.3.7 Mesoscale models

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.

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 coordinate 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. Figure 2 indicates the procedures of an operational model.

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



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

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.

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

4 Meteorological data

As part of the air pollution monitoring programmes Automatic Weather Stations (AWS) is currently being installed at selected sites in the urban areas normally together with one of the automatic air quality monitoring stations. Meteorological "surface data" such as winds, temperatures, stability, radiation, turbulence and precipitation are being transferred to a central computer via radio communication, telephone or satellite together with air quality data.

Continuous measurement of meteorology should include sensors for the most important parameters such as:

- 1. Wind speeds,
- 2. wind directions,
- 3. relative humidity,
- 4. temperatures or vertical temperature gradients,
- 5. net radiation,
- 6. wind fluctuations or turbulence,
- 7. precipitation and
- 8. atmospheric pressure.

Meteorological data will for instance be needed as input to the air pollution planning tool (such as the AirQUIS database), both for interpretation of air quality data and for modelling purposes.

4.1 Wind

Local wind and temperature patterns play a significant role on the dilution of air pollution. The transport of pollutants emitted into the atmosphere is a function of the local (average) wind direction. The dilution of pollution is mainly a function of wind speed and turbulence. This wind is again influenced by:

- Topography, which channels the wind and modify the local wind directions,
- Vegetation and buildings, which influence on the surface friction and reduce wind speed at the surface,
- Net radiation and radiation balance, which influence on the atmospheric stability, and thus on the vertical wind profile,
- Local and mesoscale sources of heating and cooling setting up thermally driven local winds.

All these factors interact to change the dispersal conditions of the atmosphere.

4.2 Turbulence

The atmosphere can disperse gases and particulate matter rapidly because it is turbulent. Turbulent flow can be defined as having the ability to disperse embedded gases and particles at a rapid rate. Turbulence is the primary process by which momentum, heat, and moisture are transported into the atmosphere from the surface of the earth and then mixed in time and space.

Turbulence can be visualised as consisting of irregular swirls of motion called eddies. Usually turbulence consists of many different size eddies superimposed on each other. Thus, a continuous hierarchy exists from the largest down to the smallest eddies, with molecular diffusion occupying the bottom of the scale.

The effect of eddy motion is very important in diluting concentrations of pollutants. An air parcel that is displaced from one level in the atmosphere to another can carry both momentum and thermal energy with it. Obviously it will also carry the pollution emitted into the air parcel. Hence, the turbulent motions in both the horizontal and vertical directions will diffuse smoke and pollution.

The effect of different eddy sizes on a plume is shown in the Figure below.



Figure3: (a) Plume dispersing in a field of small eddies in a stable atmosphere (inversion). The plume will move in a relatively straight line, with gradual increase of its cross section.
(b) Plume dispersing in a field of well defined large eddies (near neutral atmospheric conditions). Turbulent eddies with typical size less than the plume dimension will disperse the plume effectively.
(c) Plume dispersing in a field of large and various sized eddies. This is

atypical daytime situation with unstable atmospheric conditions. The dispersed plumes will both grow and meander as it moves downwind.

Atmospheric turbulence depends in general on the magnitude of three factors: mechanical effects or the roughness of the ground, horizontal and vertical wind shear, and thermal instability. These factors are described separately in the following chapters.

4.3 Meteorological data from forecast models

In areas where meteorological data are not being measured in situ, data may be generated from numerical weather forecast models. Numerical forecast models have been developed to estimate the wind fields, which have been used as input to the AirQUIS air pollution dispersion modelling system to estimate concentration distributions for the next 24 and 48 hours.

The wind field has been estimated based on the European HIRLAM50 numerical weather prediction model. The wind patterns predicted by HIRLAM50 is then compared to locally observed winds and turbulence, so that future predictions of weather patterns can be used to estimate the local wind- and turbulence patterns and thus the air pollution concentrations in the receptor points where statistical relationships have been established.

The results from the HIRLAM 50 model with 50 km or 10-km resolution have also been used as input to a mesoscale model, MM5, to produce a more detailed wind field. The development of the MM5 model is a continuation of a development that started at NCAR in the seventies. The PSU/NCAR mesoscale model is a limited-area, hydrostatic or non-hydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale and regional-scale atmospheric circulation (Anthes and Warner, 1978).

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Clean Air for Asia Training Programme				
For urban areas:				
	Multiple source Gaussian Models			
	Input data requirements;			
۲	 source characteristics and emission data, area characteristics (surface roughness, topography etc.), 			
	 measurement data (measurement type, heights etc.), meteorological data (wind, stability, mixing height. 			
NILU	temperatures etc.),			
	 dispersion coefficients (type to be used and parameters), dry and wet removal coefficients 			
	 Incation of receptor points (distances or grid specifications). 			
	ESEI The Deserver of Sec			













£	Clean Air for Asia Training Programme
	The Emission Model
	in AirQUIS
2	Input from the Industry module distributed in points
NILU	Input from the Traffic module calculations distributed
	Input from area sources Temperature correction Temperature correction
	ESEI Tax Alexandre State











































