ATMOSPHERIC AIR POLLUTION EMISSIONS

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Abstract: Air pollution modelling serves to relate air quality to emissions in a quantitative sense, and provides a better basis for describing areas of exceedance in the entire zone. It also provides additional essential information for the management of the air quality in the zone, as required under the FWD.
All three methods or tools provide information with inherent uncertainty. By uncertainty we mean a quantitative measure of the most likely possible deviation of the value from the "true" value. See the text box below which defines some relevant concepts in this context.
Measurements — apart from sampling and analysis errors - may introduce major uncertainties if stations are not representative, meaning that air quality in the surroundings differs substantially from air quality at the station, or that concentrations vary appreciably in time while the measurements have only limited time coverage.
Emission inventories can be incomplete or may be based on inaccurate or inappropriate emission factors or activity figures.

Keywords: atmospheric, emission, models, air, pollution emissions, e.g. source categories.

1. INTRODUCTION

Unlike previous EC legislation on air quality the FWD envisages the use of tools other than measurement to provide the full picture needed to underpin successful air quality management.

Three main assessment methods or tools can be used singly or in combination for preliminary air quality assessment:: air emission inventories, air pollution modelling, preliminary air quality measurements.

Preliminary air quality measurements (preliminary in the sense that these measurements do not serve to demonstrate compliance with Article 6 of the FWD) are used to explore air quality, particularly at those places where exceedances are to be expected, and/or emission information is inadequate [2].

Air emissions inventories provide comprehensive information on sources and their emissions and emission fluxes in the entire zone. This enables a first estimate of areas at risk of exceeding limit and target values.

Models may produce uncertain results either due to uncertainty in input such as meteorological quantities or emission data, or because of improper description or calculation of atmospheric processes and the resulting concentrations.

These assessment uncertainties can be reduced if information from all three methods is available. In order to judge the overall uncertainty in the assessment result, it is necessary to quantify and document uncertainties for each of the assessment methods.

As the FWD and Daughter Directives are implemented, the air quality is expected to change over the years for a variety of reasons. These include changes in human activity patterns (city growth, traffic increase, industrial production), technological developments (penetration of three-way catalyst, industrial abatement technology, etc.), and air quality management. Therefore, it is important to re-assess air quality on a regular basis, or if specific reasons suggest that this should be done.

1.1. AIR POLLUTION - LEGISLATION IN EU

A substantial body of Community legislation has been adopted by the Council and the European Parliament in relation to ambient air quality. This is summarised below and links provided to the relevant documents [21] .

Council Directive 96/62/EC on ambient air quality assessment and management is commonly referred to as the Air Quality Framework Directive. It describes the basic principles as to how air quality should be assessed and managed in the Member States. It lists the pollutants for which air quality standards and objectives will be developed and specified in legislation.

Council Directive 1999/30/EC_relating to limit values for sulphur dioxide, nitrogen dioxide and oxides of nitrogen, particulate matter and lead in ambient air. The directive was is the so-called "First Daughter Directive". The directive describes the numerical limits and thresholds required to assess and manage air quality for the pollutants mentioned. It addresses both PM10 and PM2.5 but only establishes monitoring requirements for fine particles.

Directive 2000/69/EC of the European Parlament and of the Council relating to limit values for benzene and carbon monoxide in ambient air. This was the Second Daughter Directive and established the numerical criteria relating to the assessment and management of benzene and carbon monoxide in air.

Directive 2002/3/EC_of the European Parlament and of the Council relating to ozone in ambient air. This was the Third Daughter Directive and established target values and long term objectives for the concentration of ozone in air. Ozone is a secondary pollutant formed in the atmosphere by the chemical reaction of hydrocarbons and nitrogen oxides ion the presence of sunlight. As such the directive also describes certain monitoring requirements relating to volatile organic compounds and nitrogen oxides in air.

Directive 2004/107/EC of the European Parliament and of the Council relating to arsenic, cadmium, mercury, nickel and polycyclic aromatic hydrocarbons in ambient air. This is the Fourth Daughter Directive and completes the list of pollutants initially described in the Framework Directive. Target values for all pollutants except mercury are defined for the listed substances, though for PAHs, the target is defined in terms of concentration of benzo(a)pyrene which is used as a marker substance for PAHs generally. Only monitoring requirements are specified for mercury.

Council Directive 85/203/EEC on air quality standards for nitrogen dioxide. The air quality limits in this directive remain in force until such time as those in the First Daughter Directive become legally binding on the Member States.

Council Decision 97/101/EC_establishing a reciprocal exchange of information and data from networks and individual stations measuring ambient air pollution within the Member States. This "EoI Decision" describes the procedures for the dissemination of air quality monitoring information by the Member States to the Commission and to the public.

Commission Decision 2004/461/EC laying down a questionnaire for annual reporting on ambient air quality assessment under Council Directives 96/62/EC and 1999/30/EC and under Directives 2000/69/EC and 2002/3/EC of the European Parliament and of the Council. This decision specifies the format and content of Member States' Annual Report on ambient air quality in their territories.

Laboratory researches emphasized that lignin as a result its separation from sulphate residual solution threw precipitation in acid hydride medium, is a product with important specific functional properties, with a large utilization and good efficaciousness in electrotechnics, metallurgy industry and wood industrialization.
According with this situation our target in this situation study is to realize products with original technologies in laboratory conditions, lignin representing filling material, with binders from synthetic resins of polycondensation, to confer the products of erect reliableness. With this end in view, the researches realize they straightened in next directions: obtain of blends of fount for the metallurgical industry, the procurement of plate’s fiber wooden.

2. MATERIALS AND METHODS

“Traditional’ air pollution problems are the local scale ones, i.e. those occurring in the surroundings of isolated sources. More recently, environmental policy is to a large extent confronted with global scale problems (global warming, ozone depletion). Other important policy issues related to the atmospheric environment are acidification, eutrophication, photo-oxidant formation, urban air pollution and the problem of air toxics [7].

In air pollution assessments information on all parts of the cause-effect chain have to be collected. Not only a physical/chemical description of ambient air has to be presented in such a way that it can be compared with effect threshold values, but also the relation between this effect quantity and the atmospheric emissions from sources (e.g. source categories, countries, regions, economical sectors) should be quantified. Only when all three elements, (threshold or critical values, ambient parameters and emissions) are available, can an optimal abatement strategy be developed. Three types of instruments are used in assessment studies: emission inventories, atmospheric dispersion and transport models and air quality measuring programmes.

Table 1: Policy issues related to the atmospheric environment and corresponding scale(s) of dispersion phenomena.

Policy issue	Scale of dispersion phenomenon			
	Global	Regional-to-continental	Local-to-regional	Local
Climate change	X			
Ozone depletion	X	X		
Tropospheric ozone		X		
Tropospheric change		X		
Acidification		X		
Nutrification		X		
Summer smog		X	X	
Winter smog		X	X	
Air toxics		X	X	X
Urban air quality			X	
Industrial pollutants			X	X
Nuclear emergencies		X	X	X
Chemical emergencies		X	X	X

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.

3. RESULTS AND DISCUSSIONS

3.1. Regulatory purposes

In nearly all European countries models are presently in use for 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 highways. 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 [15].

3.2. Policy support

As discussed above, in air quality assessment studies models play an important role next to emission inventories and measuring programmes. Frequently for policy support also the effect of abatement measures has to be forecasted by the models; this may require that the model also gives reliable results under pollution conditions which differ strongly from the present situation.

3.3. Public information

In public information the role of models is expected to grow. Requirements for models for public information parallel to a large extent those for policy support as far as it concerns assessment studies. For on-line information to the public on air quality and the possible occurrence of smog episodes, air quality forecasting models are needed

3.4. Scientific research

Among the major objectives for research type models is 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 to be not suitable for practical applications: their requirement on Computational effort was too high for application in the above three fields. Thanks to the tremendous hardware development, however, the situation is rapidly changing in favour of complex research type models.

3.5. Air pollution model types

Models describing the dispersion and transport of air pollutants in the atmosphere can be distinguished on many grounds, for example: on the spatial scale (global; regional-to-continental; local-to- regional; local), on the temporal scale (episodic models, (statistical) long-term models), on the treatment of the transport equations (Eulerian, Lagrangian models), on the treatment of various processes (chemistry, wet and dry deposition), on the complexity of the approach.

Following Zannetti (1993), the following model categories can be distinguished:

Plume-rise models. In most cases, pollutants injected into ambient air possess a higher temperature than the surrounding air. Most industrial pollutants, moreover, are emitted from smokestacks or chimneys and therefore possess an initial vertical momentum. Both factors (thermal buoyancy and vertical momentum) contribute to increasing the average height of the plume above that of the smokestack. Plume-rise models calculate the vertical displacement and general behaviour of the plume in this initial dispersion phase. Both semi-empirical and advanced plume-rise formulations are available.

Gaussian models. The Gaussian plume model is the most common air pollution model. It is based on the assumption that the plume concentration, at each downwind distance, has independent Gaussian distributions both in the horizontal and in the vertical. Almost all the models recommended by the U.S. Environmental Protection Agency (EPA) are Gaussian. Gaussian models have been modified to incorporate special dispersion cases. A simplified version of the Gaussian model, the Gaussian climatological model, can be used to calculate long-term averages (e.g. annual values).

Semi-empirical models. This category consists of several types of models which were developed mainly for practical applications. In spite of considerable conceptual differences within the category, all these models are characterised by drastic simplifications and a high degree of empirical parameterisations. Among the members of this model category are box models and various kinds of parametric models.

Eulerian models. The transport of inert air pollutants may be conveniently simulated by the aid of models which solve numerically the atmospheric diffusion equation, i.e. the equation for conservation of mass of the pollutant (Eulerian approach). Such models are usually embedded in prognostic meteorological models. Advanced Eulerian models include refined submodels for the description of turbulence (e.g. second-order closure models and large-eddy simulation models)

Lagrangian models. As an alternative to Eulerian models, the Lagrangian approach consists in describing fluid elements that follow the instantaneous flow. They include all models in which plumes are broken up into elements such as segments, puffs, or particles. Lagrangian models use a certain number of fictitious particles to simulate the dynamics of a selected physical parameter. Particle motion can be produced by both deterministic velocities and semi-random pseudo-velocities generated using Monte Carlo techniques.

Hence, transport caused by both the average wind and the turbulent terms due to wind fluctuations is taken into account.

Chemical modules. Several air pollution models include modules for the calculation of chemical transformation. The complexity of these modules ranges from those including a simple, first-order reaction (e.g., transformation of sulphur dioxide into sulphates) to those describing complex photochemical reactions. Several reaction schemes have been proposed for simulating the dynamics of interacting chemical species. These schemes have been implemented into both Lagrangian and Eulerian photochemical models. In Eulerian photochemical models, a three-dimensional grid is superimposed to cover the entire computational domain, and all chemical reactions are simulated in each cell at each time step. In the Langrangian photochemical models a single cell (or a column of cells or a wall of cells) is advected according to the main wind in a way that allows the injection of the emission encountered along the cell trajectory.

Receptor models. In contrast to dispersion models (which compute the contribution of a source to a receptor in effect as the product of the emission rate multiplied by a dispersion coefficient), receptor models start with observed concentrations at a receptor and seek to apportion the observed concentrations at a sampling point among several source types. This is done based on the known chemical composition of source and receptor materials.

Receptor models are based on mass-balance equations and are intrinsically statistical in the sense that they do not include a deterministic relationship between emissions and concentrations. However, mixed dispersion-receptor modelling methodologies have been developed and are very promising.

Stochastic models. Stochastic models are based on statistical or semiempirical techniques to analyse trends, periodicities, and interrelationships of air quality and atmospheric measurements and to forecast the evolution of pollution episodes. Several techniques are used to achieve this goal, e.g., frequency distribution analysis, time series analysis, Box-Jenkins and other models, spectral analysis, etc. Stochastic models are intrinsically limited because they do not establish cause-effect relationships. However, statistical models are very useful in situations such as real-time short-term forecasting, where the information available from measured trends in concentration is generally more relevant (for immediate forecasting purposes) than that obtained from deterministic analyses.

3.6. Input data requirements

Geographic data. They include the orography (i.e., elevations above the sea level) and the land use, if possible in various files for the different seasons of the year. The land use is usually distinguished into pre-selected categories, including at least arid, agricultural, forested, semi-urban and urban areas. It is important to have precise information on the land-water distribution for each grid cell. Although the models require all these data in gridded format, it is preferable to have access to data organised in a Geographical Information System
Soil parameters. For each land use type, a variety of quantities has to be known, including optical properties (albedo, emissivity) and thermophysical parameters (density, heat capacity, thermal conductivity). Moreover, the soil wetness has to be known.

Table 2. Application areas of various air pollution model categories depending on the scale of the dispersion phenomenon (1: regulatory purposes; 2: policy support; 3: public information; 4: scientific research).

Scale of atmospheric process	Microscale	Mesoscale	Macroscale	
Scale of dispersion phenomenon	Local	Local-to-regional	Regional-to-continental	Global
Model type				
Plume-rise	1,2,4			
Gaussian	1,2,4	1,2		
Semi-empirical	1,2,3,4	1,2,4		
Eulerian	1,2,4	2,3,4	2,4	2,4
Lagrangian	4	4	2,4	
Chemical	(1,2,)4	2,3,4	2,4	2,4
Receptor		2,4		
Stochastic		2,4		

Meteorological data In case that a diagnostic wind model is applied, observed data are required, which should be: representative for the whole area of interest; sufficient to characterise the three- dimensional wind field (i.e., vertical information is necessary for at least some of the measuring locations).

4. CONCLUSIONS

Like in the case of geographic data, models require emission data in gridded format, although it is preferable to have access to data organised in a Geographical Information System. Usually, data are necessary in hourly intervals. It is a clear advantage to have separate data files for each source category, as this is a prerequisite for considering the impact of various emission intervention scenarios. For point sources, all data needed to estimate the effective height have to be known as well. In some cases it might prove helpful to have emission data for a coarser grid around the area of interest in order to derive reliable lateral boundary conditions.

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