European Topic Centre on Air Quality

AMBIENT AIR QUALITY, POLLUTANT DISPERSION AND TRANSPORT MODELS

by

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1 INTRODUCTION

1.1 Air pollution abatement in a European-wide context

The damages caused by air pollution in Europe are large and it is generally accepted that there is an urgent need for reduced emissions to the atmosphere (ECE-CLRTAP, WHO-Concerns for Europe's Tomorrow, EC 5th Environmental Action Programme). The damages are caused by high ambient air concentrations and depositions of many chemical components. Among the most important components are acidifying constituents (sulphur and both oxidised and reduced nitrogen compounds), photochemical components (including ozone), particulate matter and toxic compounds, such as metals, organic compounds and others. The concentrations and depositions are dependent on

- the total mass of pollutants emitted to the atmosphere and its spatial and temporal distribution
- transport and transformation processes in the atmosphere and
- deposition processes.

Assessments of emission reduction strategies must consider all three factors and the complexity of these problems call for the use of atmospheric models. Average exposure of the ecosystem to concentrations and deposition, emission scenario studies and linkage to economical aspects and cost effectiveness are all examples of areas where the models are needed.

Air pollution problems that can be handled by national legislation or by international agreements between the European countries range from urban and local to the regional and long range air pollution problems. The lifetimes of the chemical components that are largely determined by the European air pollution policy are up to a few days. Components with longer lifetimes must be considered in an intercontinental or global perspective.

The development of emission reduction strategies for acidifying components in Europe under the UN-ECE Convention and the Convention on Long Range Transboundary Air Pollution is a good example of how models can play an important role in the decision making process toward protocols on emission reductions. Regional scale models quantifying the transboundary fluxes of air pollution between the European countries and deposition to ecosystems (Barrett et al., 1995) have successfully been applied together with knowledge on ecosystem critical loads of acidity and the costs involved in emission reduction in order to find optimal solution for the reductions. This led to a renewal of the second sulphur protocol in 1994 aiming at further substantial reductions in the SO_2 emissions toward 2010. In the further work on new protocols on reduction of nitrogen emissions and emissions of Volatile Organic Compounds (VOC) the atmospheric models will have to play an even more important role due to increased complexity of the problems. Further linkage of local to regional scale and regional to global scale air pollution problems will require an intensified usage of models.

Application of models must go "hand in hand" with evaluation procedures needed to support the credibility of the model. Hence, results of carefully planned and executed international measuring programmes will be needed in the future. Furthermore, high quality input data is also needed if optimal use of the models shall be feasible. For compatibility of this data, a high level of international co-operation will be needed as well.

Reference

Barrett K., Seland X., Foss A., Mylona S., Sandnes H., Styve H. and Tarrason L. (1995), EMEP/MSC-W Report 1/95. European Transboundary Acidifying Air Pollution. Ten years calculated fields and budgets to the end of the first Sulphur Protocol.

1.2 Model development versus needs for model application

The present report aims at a documentation of the current state-of-the-art of mathematical modelling of air pollutant dispersion, transport and transformation, with emphasis on models which may be readily applied in support of environmental decision making. As a further objective, trends of ongoing work towards better and more reliable models are summarised and recommendations for further relevant research work are given. The intention is that this can facilitate subsequent activities aiming to give guidance on selection of different models to be used for air pollution regulatory and policy purposes in Europe.

Apparently, the above tasks are strongly related with identifying the needs for model application. Therefore, this report is largely based on the results of task MA3-1 (de Leeuw et al., 1995) which can be considered as a first step in the EEA Work Programme for understanding policy related needs for models in Europe.

Already in the past, model development evolved in parallel to the clarification of the potential for the practical use of models. Incidentally, the overall process of

- users adapting to the availability of new models and
- model developers becoming aware of specific needs for new model types for practical applications

is to a large extent iterative, and hence intrinsically time consuming.

The rapid growth of the public awareness concerning the need for environmental protection and for a sustainable development led in the last years to an increased political pressure towards more accurate impact assessment studies. With regard to the atmospheric environment, this implies the demand for better and more reliable models. Luckily, in the same period a revolutionary development of the hardware infrastructure took place and thus the scientific community was able to accelerate model development in the frame of large concerted international research programmes.

In the light of the above, nowadays there is an urgent need to intensify the exchange of information between model developers and potential users among environmental managers. The present report is intended to contribute towards this aim.

Reference

de Leeuw F., Berge E., Grønskei K. and Tombrou M. (1995), Review on requirements for models and model application, Report of the European Topic Centre on Air Quality to the European Environmental Agency.

1.3 Importance of model validation and evaluation

Analysing the potential for the practical use of mathematical models for air quality assessments implies investigating

- what kind of statements can be made by the aid of models (qualitative approach)
- what is the accuracy of these statements (quantitative approach).

Apparently, the former approach is easier, because it does not require more than understanding the characteristics and the range of application of a model. In addition to that, a quantification of the accuracy of model results presupposes insight into

- input data accuracy and how the latter affects the accuracy of model results
- uncertainties in model assumptions and parameterisations
- methodologies for judging to what extent model results represent reality.

As a consequence of the above, model validation (typically by the aid of available analytical solutions) should be considered as an indispensable part of the model development process, whereas an already validated model should be subject to a genuine evaluation procedure in order to ensure that potential users can assess the degree of reliability and accuracy inherent in the given model. High quality field data which are needed for evaluation purposes are, however, very rare.

1.4 Contents of the present report

The bulk of the present report is an overview of air pollution models employed (but not necessarily developed) in Europe. The presentation focuses on a summarised description of the most important existing models, their use and purposes. Particular emphasis is offered to models applicable to regulatory and policy purposes. The needs of models for the air pollution control strategies and planning, links to economical aspects and integrated assessment are discussed. Additionally, the needs for new/improved models to support decision making for the most important air pollution problems foreseen in the future are also addressed. The principal objective of this document is to facilitate subsequent activities aiming to give guidance on selection of different models to be used for air pollution regulatory and policy purposes in Europe.

2 NEEDS FOR MODELS

2.1 Policy issues related to the atmospheric environment

‘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 (Table 1).

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

The acidification is related to the emissions of sulphur dioxide, nitrogen oxides and ammonia. A combination of maps of critical loads of acidity and deposition matrices from air pollution models show that exceedances of the critical loads are found in large parts of Europe (Downing et al., 1993). Originating from emissions of nitrogen oxides and ammonia, the eutrophication of the ecosystem through excess nitrogen deposition is also a problem of growing concern

(Skeffington and Wilson, 1988). Finally, the emissions of nitrogen oxides and VOC creates high levels of near surface ozone and other toxic photochemical compounds. Critical levels of ozone according to WHO are frequently exceeded during the summer season in many parts of Europe. Also, the European ozone levels are above the critical levels for the growing season of plants in a large part of Europe (Anttila, 1993; ETC ozone exceedance report).

Well co-ordinated, long-term international actions are needed for solving regional scale air pollution problems. On the contrary, air quality at local scale, typically in urban agglomerations, may be improved with a proper abatement strategy of local character, e.g. interventions tailored to the specific situation in the area of interest. Being indispensable for optimising such abatement strategies, air pollution models may substantially support local environmental policy making.

Returning to the regional scale, at present there are clear needs to develop new protocols for the reduction of acidifying compounds created by emissions of NO_x and NH_3 and low level ozone originating from emissions of NO_x and VOC. Regional scale models will have to play an important role in the development of these protocols. Source-receptor relationships, "blame matrices" quantifying the contribution from one country to the air pollution of another country, total loads to the ecosystem, and emission scenario analysis will be important tools needed from the models. The inclusion of both the acidification problem and the surface ozone problem into the protocols will inevitably put larger demands on the capabilities of the models. Rather detailed and time consuming models will be needed to build proper control strategies based on analysis of the interactions between different air pollutants. Such simulations will have to be performed either for longer time periods or, in an attempt to reduce the computational effort, for individual representative scenarios.

Moreover, the European environment is subject to the climatic impacts of the increased concentrations of anthropogenic greenhouse gases and aerosols due to alterations they cause to the radiative balance of the earth-atmosphere system. Important issues such as assessment of available scientific information on climate change, assessment of the environmental and socio-economic impacts of climate change and formulation of appropriate response strategies have been the focal point of the Intergovernmental Panel of Climate Change (IPCC), an organisation established in 1988. In this context, the role of global scale models is essential since they can provide IPCC with the most up-to-date information on climate change (IPCC, 1995).

References

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Mapping of Critical Loads in Europe: Status Report 1993. Co-ordination Centre for Effects, National Institute of Public Health and Environmental Protection, Bilthoven, the Netherlands.

Intergovernmental Panel on Climate Change (IPCC) (1995), Radiative Forcing of Climate Change and An Evaluation of the IPCC IS92 Emission Scenarios, Cambridge University Press.

Skeffington R.A. and Wilson E.J. (1988), Excess nitrogen deposition: Issues for consideration, *Environ. Pollution* **54**, 159-184.

2.2 Instruments for air quality assessment studies

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.

Air quality monitoring may be defined as the systematic collection of information from measurements or other means to determine the levels and the time evolution of quantities relevant for air quality. Such quantities are air concentrations, fluxes of air pollutants to land or water surface and the exposure to air pollution of human beings, materials and ecosystems.

The aim of air quality monitoring is to get an estimate of the quantities required (concentrations, deposition fluxes or exposure) sufficiently representative in time and space and with the specified accuracy. Spatial scales may range from the very local scale (e.g. street level, direct surroundings of a chimney) to the global scale; time scale may range from minutes (estimation of peak concentrations) up to decades (estimation of trends).

Determining the relevant quantities requires systematic information obtained by a pre-defined information collection strategy, derived from the specified requirements. Interpretation and evaluation of the data is necessary to evaluate the required quantities and to verify that these requirements are met.

Although measurements form an important aspect of monitoring, measurements alone are rarely sufficient to arrive at the best possible description of the desired concentration or deposition space/time fields. Models are often needed to establish larger scale average exposure and depositions fields which can not easily be derived from measurements. The reason is simply that observations are made at a few locations and may therefore not be very representative of larger areas. Substantial uncertainty can be introduced if measured data are extrapolated or interpolated into large domains and models are therefore used to generate best estimates in situations where measurements are lacking or cannot be made. Models are also necessary if the relative impact of various sources (source categories, emissions from different regions or countries) or emission scenarios have to be investigated. A consistent mass budget of emission, transport and deposition can only be obtained by usage of models.

2.3 Limitations of air pollution models

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 the diagnose of 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.

2.4 Application areas of air pollution models

A wide range of different models are published in scientific papers and even a larger number of unpublished models and special model versions exists. Models can be distinguished on many grounds: e.g. the underlying physical concepts, the temporal and spatial scale, type of component. Contemporary air pollution models deal with “conventional” primary pollutants (mainly SO_2, CO, NO_x and VOC). Already at present the need is recognised to extend the models to include heavy metals and persistent organic pollutants (POPs). Modelling of visibility and particulate concentrations (PM10) are among the most important current model development trends.

There are no well defined requirements with respect to model documentation; in answer to the MA3-1 questionnaire it was mentioned that documentation should at least consist of a user manual, short technical description and the results of sensitivity and validation tests (de Leeuw et al., 1995)

In the remainder of this section, four groups of application areas are defined and their requirements are briefly discussed:

2.4.1 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. 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 disputable that this might be beyond the scope of most of the models as the models used at present are not very suitable for handling of concentration fluctuations.

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). Surprisingly, however, according to results of the MA3-1 questionnaire, in the majority of countries required model accuracy has not been specified.

According to EU Air Quality Directives, the area where threshold values are approached or exceeded has to be assessed and reported by the Member States. Both threshold values for protection of human health as for protection of ecosystem are defined for primary and secondary pollutants. Although in many situations only measuring data is used for specifying the exceedance area, models - including statistical methods for data interpolation - could significantly improve the description. No requirements are yet defined for this application type.

2.4.2 *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.

Use of atmospheric models in combination with model 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; an example of this type of *meta-models* is the source-receptor approach implemented in the RAINS model which is based on the much more complex EMEP model.

2.4.3 *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. In a series of workshops it was attempted to harmonise these on-line forecasting models. Although the workshops resulted in an exchange of views and know-how and in an on-line system of reciprocal exchange of smog information between a number of countries, no harmonisation of forecast models has been achieved.

2.4.4 *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. Hence, models of this type are not only valuable for identifying limitations and gaps in simpler policy oriented models; they could represent themselves 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.

References

de Leeuw F., Berge E., Grønskei K. and Tombrou M. (1995), Review on requirements for models and model application, Report of the European Topic Centre on Air Quality to the European Environmental Agency.

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3 STATE-OF-THE-ART

In this section air pollution models are reviewed separately for each scale of dispersion phenomena (global; regional-to-continental; local-to-regional; local). These scales were already introduced in conjunction with Table 1 in section 2.1. The review focuses on the availability of air pollution models for addressing the main policy issues related to the atmospheric environment. In so far, the approach followed resembles to that of previous similar attempts (van den Hout and van Dop, 1985; Szepesi, 1989; Solomon, 1995).

Apparently, it is an impossible task to make in a review proper reference of all existing models. The authors of the present report based their analysis of the state-of-the-art on those representatives of the various model categories which are most frequently found in policy-oriented air pollution studies (see also Borrell et al., 1995). The readers are encouraged to recommend the inclusion of other models by contacting the principal author of the report. In this way, the coverage will be successively improved in the course of the planned updates of the report.

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3.1 Definitions

3.1.1 Scales of atmospheric processes

Air pollution dispersion phenomena are decisively influenced by atmospheric processes which are commonly classified with regard to their spatial scale. The latter is in turn related to the characteristic time of the individual process. Orlanski (1975) recommends distinguishing the following scales:

- **Macroscale** (characteristic lengths exceeding 1,000 km); at this scale, the atmospheric flow is mainly associated with synoptic phenomena, i.e. the geographical distribution of pressure systems. Such phenomena are mainly due to large-scale inhomogeneties of the surface energy balance. Global and the majority of regional-to-continental scale dispersion phenomena are related to macroscale atmospheric processes, for which the hydrostatic approximation can be considered as valid.

- **Microscale** (characteristic lengths below 1 km); in general, air flow is very complex at this scale, as it depends strongly on the detailed surface characteristics (i.e. form of buildings, their orientation with regard to the wind direction etc.). Although thermal effects may contribute to the generation of these flows, they are mainly determined by hydrodynamic effects (e.g. flow channelling, roughness effects) which have to be described well in an appropriate simulation model. In view of the complex nature of such effects, local scale dispersion phenomena (which are to a large extent associated with microscale atmospheric processes) are mainly described with robust "simple" models in the case of practical applications, such as street canyon models etc.

***Mesoscale** (characteristic lengths between 1 and 1000 km); the flow configuration in the mesoscale is depending both on hydrodynamic effects (e.g. flow channelling, roughness effects) and inhomogeneties of the energy balance (mainly due to the spatial variation of area characteristics (e.g. land use, vegetation, water), but also as a consequence of terrain orientation and slope). From the air pollution point of view, thermal effects are the most interesting, as they are of particular importance at times of a weak synoptic forcing, i.e. bad ventilation conditions. As a minimum requirement, mesoscale meteorological models should be capable of simulating local circulation systems, as for instance sea and land breezes. Mesoscale atmospheric processes affect primarily local-to-regional scale dispersion phenomena, for which urban studies are the most important examples. The description of such phenomena requires, even for practical applications, the utilisation of fairly complex modelling tools.*

3.1.2 *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 sub-models 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 semi-empirical 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.

Table 2 summarises, for each scale of dispersion phenomena separately, which air pollution model categories have already been used for practical applications. It should be noted that identical numbers are used for the various application areas as in section 2.4:

1. regulatory purposes
2. policy support
3. public information
4. scientific research

All models mentioned in the following sections are classified into the above categories in the alphabetic list given in Appendix A1. The same list contains information on the scale of the dispersion phenomenon relevant for each model.

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		

3.1.3 Meteorological models

Meteorological models aim at understanding local, regional or global meteorological phenomena and at providing the meteorological input required by air pollution dispersion models. Numerical meteorological models can be divided into diagnostic and prognostic ones. The former do not contain time-tendency terms, as they simply interpolate and extrapolate available meteorological measurements. The latter are used to forecast the evolution of the atmospheric systems by solving the full time-dependent equations. Occasionally, prognostic meteorological models include the space-time integration of the atmospheric diffusion equation for gases and aerosols. Most prognostic models are hydrostatic. Complex terrain simulation and small-grid applications, however, require the use of more complex non-hydrostatic models.

More information on meteorological models applied in conjunction with air pollutant dispersion models is included in the following sections which deal separately with the various scales of air pollution problems.

References

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3.2 Global scale air pollution models

3.2.1 General remarks

Global-scale air pollution models study the changes in the chemical composition of the global atmosphere, focusing primarily on methane (CH_4), carbon monoxide (CO), nitrogen oxides (NO_x), non-methane hydrocarbons (NMHC), chlorofluorocarbons (CFC), hydrofluorocarbons (HFC), hydrochlorofluorocarbons (HCFC) and sulphur compounds (SO_2, aerosol particles, DMS, H_2S), together with their combined effects on the concentrations of ozone (O_3) and the oxidising capacity of the atmosphere (defined largely by the concentrations of O_3, hydroxyl (OH) and hydrogen peroxide (H_2O_2). Of vital importance are changes in the chemical composition of the troposphere (the lowest part of the atmosphere) due to their immediate effect on biological productivity and human health and their contribution to climate change. The discussion in the following concentrates, therefore, on global and hemispheric models studying primarily tropospheric changes and interactions with the overlying stratosphere.

The principal objective of global-scale air pollution models, often called Chemical/Transport Models (CTMs), is to describe and predict the evolution of the chemical composition of the atmosphere and eventually the evolution of climate in the future. The output of these models has in the last years constituted, inter alia, the basis for the activities of the Intergovernmental Panel on Climate Change (IPCC, 1995). With respect to their relationship to smaller-scale modelling, the most important function of global-scale models is to provide boundary conditions to regional models which in turn provide boundary conditions to the local/urban-scale models. In this context, while the role of global-scale modelling in the assessment of regional pollution levels is significant, their contribution to local/urban pollution modelling is rather secondary.

3.2.2 *Existing models*

CTMs of global or hemispheric scale can be one- , two- or three-dimensional (1-D, 2-D or 3-D respectively). 1-D models are oversimplified and rarely in use today, so they are disregarded in the following. 2-D models describe processes occurring with longitudinally averaged rates and concentrations, while 3-D models describe processes in all three dimensions (longitude, latitude, height).

Zonally averaged 2-D models have been used for several years to study the global/hemispheric distribution of trace gases (2-D Oslo, EMEP/MSC-E, models operating at the Universities of Bergen, Cambridge, Liège and the Max Planck and Harwell Institutes). They require less computer time and memory than 3-D models and less input data. They usually contain detailed chemical schemes and can be used to predict pollutant changes over several decades for a range of trace gas emission scenarios. Although they neglect zonal asymmetries, they prove to be useful tools for sensitivity studies and analyses. Comparison with measurements remains a major constraint in their application due to the zonal averaging employed.

3-D CTMs have been developed only recently (MOGUNTIA, IMAGES, STOCHEM, 3-D Oslo, EMEP/MSC-W, CTMK, ECHAM). They are considered the best modelling tools for the study of pollutants which are distributed very heterogeneously in time and space. Moreover, comparison of their output with measurements is more justified than in 2-D models. 3-D models use either monthly averaged wind fields to transport tracers and detailed chemistry or daily varying windfields and simplified chemistry. Today there is a trend towards including more chemical mechanisms in the latter, developing them further and coupling them with climate models. Several physical processes (cloud-processes, convective mixing, transport between the boundary layer and the free troposphere, exchange between stratosphere and troposphere) act on a sub-grid scale and are represented by parameterisations. These parameterisations should be tested carefully. Overall, there is a need for careful field observations of trace gases, laboratory investigations of chemical mechanisms and theoretical development of CTMs.

3.2.3 *Input data requirements*

Emissions. Although emissions of several atmospheric pollutants are available for Europe and North America, for the rest of the world corresponding data are very few. Moreover, on the global scale emission estimates are associated with large uncertainties for certain components such as NOx and hydrocarbons.
Air pollution models use often emission data from different sources. This makes the comparison of the performance of different models very difficult and constitutes a serious drawback in the effort to improve their formulation. Global emission assessments have been organised recently within the GEIA project

(Global Emissions Inventory Activity), recommending the use of the good quality GEIA data (Graedel et al., 1993).

Meteorological data. The meteorological information used in CTMs is either the output from General Circulation Models (GCMs) or data assimilation. The use of climatologically averaged data makes the comparison of model results with observations very difficult, so there is a trend towards using regular meteorological data from Numerical Weather Prediction (NWP) models.

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3.3 Regional-to-continental scale air pollution models

3.3.1 General remarks

Air pollution was considered as a local phenomenon until the middle of the 1960s. In the late 1960s Swedish scientists were the first to suggest a link between the large sulphur emissions in Central Europe, the high acidity of European precipitation and the harmful effects on Scandinavian freshwater ecosystems. As a result of this discovery, OECD took the initiative to a large European study of these problems in the beginning of the 1970s and after a few years the first regional scale air pollution models were set up (OECD, 1979). The models proved to be very useful tools in analysing and understanding the relations between emission transport and depositions.

The main purpose of most of the present European regional scale models is to quantify the level of SO_x, NO_x, NH_y and photooxidants (in particular O_3), the deposition of acidifying compounds to the different compartments of the ecosystem, and to understand the physical and chemical processes behind the formation, transport and deposition of these components. The list of models regional scale models given in Appendix A3 in this report are those aiming at the above mentioned environmental problems. Additionally, there is also a considerable concern regarding Heavy Metals (HM), Persistent Organic Pollutants (POP), radioactive or hazardous chemical releases, soot, particulate matter and winter smog episodes and models are under development or are in use for these purposes as well.

The most important models for HM's on the regional scale are those at the Research Centre Geesthacht in Germany (Pettersen et al., 1994), at RIVM in the Netherlands (van Jaarsveld, 1990, 1995), at DNMI in Norway (Bartnicki, 1994), at IIASA in Austria (Alcamo, et al., 1992) and at EMEP/MSC-E in Russia (Galperin, 1993). The modelling of POPs is more difficult partly because of the long life time of the different toxic compounds in the different compartments of biota. The models are still in their infancy, but a series of studies have been conducted in particular at RIVM (see van Jaarsveld and Leeuw, 1993). The importance of the oceans and the global character of the POP problem is elucidated in the model developed by Strand and Hov (1993). Model studies of winter smog episodes are found in de Leeuw and van Rheineck Leyssius (1990), while model calculations of particulate matter have been performed by van Jaarsveld (1995).

Furthermore, An important evaluation of models for long range transport of air pollution took place under the so-called ATMES-experiment (see Klug et al. (1990)) (ATMES= Atmospheric Transport Model Evaluation Study). A large number of institutions applied their regional scale air pollution models on the Chernobyl accident and the results where evaluated in the final report. Furthermore, in the European Tracer Experiment (ETEX) national emergency models and systems have been tested in real time simulations of the dispersion of a tracer released in Europe. The latest results from this exercise is described in ETEX (1995).

The basic input to the regional scale models are the meteorological data and the emission data. Winds, clouds, precipitation, surface characteristics and chemical mechanisms determine the large scale dispersion of the emitted pollutants. The final output of the models is typically average concentrations or depositions for grid-squares ranging from 50km×50 km to 150km×150 km.

3.3.2 *Existing models*

Since the 1970s, a large number of different types of models have been developed and improved. The most important European regional scale air pollution models which are currently in use are presented in tabular form in Appendix A3. The characteristics of the models are divided into: field of application, type of model, geographical domain and time periods covered, horizontal and vertical resolution, different physical and chemical formulations, input parameters such as emission data and meteorological data and finally the boundary conditions employed. By considering the fields of application we can divide the models into two main categories, namely those particularly designed for policy making and those mainly used for research purposes.

Models designed for policy purposes are often operated over long time periods (months and years) since for example acidic loads or photochemical exposure need to be assessed over long time periods. This fact partly determines the design of these models since they can not contain too detailed physical and chemical descriptions in order to be operated within realistic time-frames on today’s computers. Examples of this type of models are the DMU-model, the EMEP MSC-W Acid Rain, Photochemical and 3-D models, the EMEP/MSC-E model, the Harm model, the LOTOS model, and the TREND model. Models mainly aiming for research are the EURAD model, the IVL model, the REM3 model, the UIB model and the UK Photochemical model. The research type of models are often too complicated for long term political applications, although the difference between "policy" and "research" model is not always very clear. One should also be aware of the fact that the research type of models can be useful for policy making through verification and control of the reliability of the simpler "political" models. In the forthcoming decision making process on regional scale air pollution issues in Europe there is clearly a need for both simple and "quick answer" models that are complemented with more detailed "research" models.

Considering the institutions involved in the modelling as given in Appendix A3, it can be observed that universities are mostly research oriented, while the environmental or meteorological institutions are responsible for the more practical policy oriented applications.

Both Lagrangian and Eulerian dispersion models are being used in the regional-to-continental scale. In a Lagrangian framework a specific parcel of air is followed in which the concentrations of a pollutant is assumed to be homogeneously mixed. On the other hand, in an Eulerian model the chemical species are transported in a fixed grid. The main advantage of the Lagrangian approach is the simple numerical treatment of the transport term in the mass balance equation. The transport is determined by trajectories of the air flow. The main disadvantage is, however, that it is rather difficult to account for exchange processes between the air parcels and windshear and consequently three dimensional Lagrangian models are not very reliable. The numerical solution of the transport term in the Eulerian framework becomes more difficult and often requires substantial computational resources to be accurate enough compared to the Lagrangian approach. Additionally, the numerical solutions may introduce artificial non-linearities that limit the applicability of these models to source attribution procedures. However, the main advantage of the Eulerian models is the well defined three dimensional formulation which is clearly needed for the more complex air pollution problems, as foreseen on the regional scale in Europe in the next coming years.

All the models listed in Appendix A3 cover the area of interest, namely Europe, with the exception of the REM3 model which only covers Northwest Europe. The simulation period varies, however, quite a lot. The models that cover long time periods (months to years), so that calculated long term exposures can be established are the DMU model, the EMEP-models, the LOTOS model, the Harm model and the TREND model. The resolution of the policy oriented models are mostly either 150km or 50km (the LOTOS model has 0.5 deg. latitude and 1.0 deg. longitude), while the research oriented model are run with finer resolutions. The Lagrangian models are either single or two layer models while the Eulerian models employ more layers.

In general the physical and chemical schemes are more comprehensive in the research oriented models than in the policy oriented models. The most complex ones are the EURAD and the REM3 model, followed by the UIB model. Very complex air chemistry is found in the IVL model and the UK Photochemical model, but these models are not as elaborated with regard to the transport scheme and description of other physical processes. However, there are also large similarities in the modelling approaches. Either deposition velocity modelling or the resistance analogy is utilised for describing the dry deposition fluxes. Scavenging ratios are utilised in all models including wet deposition processes, with the exception of the EURAD model and the LOTOS model which include cloud chemical processes.

The EMEP, UIB and DMU models utilise emission data from the EMEP emission inventory. At MSC-W the CORINAIR data is now also used. The EMEP data are also used in combination with data from other inventories by the

EURAD model and the Harm model. Additionally, the TNO emission inventory is utilised by REM3 and the LOTOS model.

Most models employ meteorological data from a numerical weather prediction model. However, the MSC-E model and the REM3 model apply analysed meteorological observations. The Harm models utilises climatological type of data which of course limits the applicability of these models to calculate actual concentrations and depositions over certain time-periods. Finally, the boundary conditions are taken from several sources being either models of different scales, observations or climatological data.

3.3.3 Input data requirements

The most important input data needed to operate regional scale air pollution models are meteorological data, emission data, land use data, data on the orography and the air pollution concentrations at the boundaries. Among these data the meteorological and the emission data are most important and require the largest efforts of preparation. A short description of the meteorological data and the emission data is given below.

Meteorological data.
The meteorological data are derived from a so-called meteorological pre-processor. In most cases, numerical weather prediction (NWP) models are used as pre-processors. NWPs are found capable of producing reliable meteorological information on the regional scale (Gustafsson, 1993). Analysed meteorological observations are also sometimes used as seen in Appendix A3. As a general rule, the quality of the meteorological data has so far been much better than the quality of the emission data. Uncertainties in the meteorological fields of importance to regional scale air pollution are mostly found in the flow fields around complex terrain, precipitation and cloud fields and the structure of the planetary boundary layer.
The NWP model runs are initialised from advanced use of observations. Short term prediction will therefore give often the most complete description of the state of the atmosphere. For example, usage of analysed observations will result in rather uncertain estimates of the meteorological fields in remote areas, over seas and at high altitudes in the atmosphere due to lack of observations. Additionally, several important physical parameters such as surface fluxes, turbulent activity, height of the planetary boundary layer and cloud parameters are not measured regularly in the meteorological network and models are often needed to derive such quantities. It is therefore desirable that NWP-models are used as the basis for the meteorological data employed in regional scale air pollution models.

Emission data.
Clearly, together with the meteorological data the emission data are the most important input to the regional scale air pollution models. The two most

important emission inventories covering the European area are the UN-ECE/EMEP inventory (Berge et al., 1995) and the CORINAIR inventory (CORINAIR, 1995). The UN-ECE/EMEP inventory is based on the emission data that the Parties to the 1979 Geneva Convention on Long Range Transboundary Air Pollution are obliged to submit. Submissions are made of national totals, gridded data in 150 km and 50 km squares, source categories, height categories, etc. for SO_2, NO_x, NH_3, VOC, CO and CH_4. All the data are stored in the EMEP inventory. Systems for verification and quality control of the data are under development. Still a weak point with this inventory is that many parties fail to submit information on their emissions at the proper time.

The CORINAIR inventory originates from a Council Decision in 1985 on compiling a co-ordinated inventory of atmospheric emissions from the EU member states. The components presently included in the inventory are SO_2, NO_x, NH_3, VOC, CH_4, CO, CO_2 and N_2O. Detailed information on source categories, point sources etc. is included in the inventory. The emission data are reported in administrative units of each country, but the data can be transformed to grid systems applicable to models.

The European Topic Centre on Air Emissions (ETC-AEM) is taking over the responsibility of the CORINAIR emission data set. There is clearly a need for co-ordination and harmonisation of the two emission inventories in the future to avoid duplication of work, to make more emission information available to modellers and to strengthen the verification of the emission data. The latter point is rather important to the modelling community in order to make reliable estimates of the uncertainties involved in the calculated dispersion of regional scale air pollution.

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3.4 Local-to-regional scale air pollution models

3.4.1 General remarks

Air pollution was first thought to affect primarily urban areas. For this reason, the first air quality studies dealt with the situation in large cities, both in the USA and in Europe. Similarly, the first attempts towards 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 parameterization for turbulence quantities.
- Prognostic calculation of both wind fields and turbulence quantities.

The former approach, which is mainly followed in the USA, presupposes the availability of very detailed observed data which would allow an accurate wind field reconstruction (Ratto et al., 1994). This, however, is under normal circum-stances an illusion. Therefore, the latter approach, i.e. the numerical simulation of the wind and turbulence patterns in the area of interest, is nowadays widely accepted as superior.

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.

As a minimum requirement for a realistic simulation of air pollutant transport in the local-to-regional scale, a prognostic mesoscale air pollution model should include a reasonable parameterisation with regard to the dynamics of the atmospheric boundary layer (ABL). The latter depends on the turbulence characteristics which may vary with both height and time. In photochemical dispersion models it is important that the kinetics of the ongoing chemical reaction system is properly parameterised. This is being materialised by the aid of appropriate reaction mechanisms, the validity of which has to be tested against laboratory measurements.

Contrary to the macroscale, processes in the mesoscale are governed by orography and inhomogeneities in the surface energy balance. This is already implied by the fact that mesoscale processes usually extend to say twofold or threefold the extension of the 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).

Prognostic mesoscale models differ with regard to the treatment of pressure. If the characteristic horizontal length scale is less than 10 km, non-hydrostatic effects (and thus also dynamical vertical accelerations) may be neglected. In models adopting this approach, the so-called hydrostatic models, pressure can be simply obtained from the hydrostatic equation. On the contrary, in non-hydrostatic models the elliptic differential equation for pressure has to be solved. Luckily, nowadays efficient elliptic solvers are available, and so the overall computational demand of a non-hydrostatic model is not much higher than that of a hydrostatic 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 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.

Details on the overall structure of prognostic mesoscale models are given in several previous articles and books [e.g. Etling (1981), Pielke (1984), Physick (1988), Schlünzen (1994)].

3.4.2 Existing models

This section includes short descriptions of widely known air pollution models for problems in the local-to-regional scale. In addition, recent practical applications of the individual models are mentioned and, where appropriate, relevant references are given. Technical information on the models dealt with in this section is provided in Appendix A4.

MEMO (Kunz and Moussiopoulos, 1995)
This non-hydrostatic mesoscale model is a basic constituent of the EUMAC Zooming Model (EZM; Moussiopoulos, 1994 and 1995). The EZM represents one of the most widely tested European air quality model systems for urban scale applications (about 15 study cases in the last three years). MEMO solves the conservation equations for mass, momentum and several scalar quantities in terrain-influenced co-ordinates. Non-equidistant grid spacing is allowed in all directions. The numerical solution is based on second-order discretization applied on a staggered grid. Special care is taken that conservative properties are preserved within the discrete model equations. The discrete pressure equation is solved with a direct elliptic solver in conjunction with a generalised conjugate gradient method (Flassak and Moussiopoulos, 1988).
Advective terms are treated in MEMO with a monotonicity-preserving discretization scheme with only small implicit diffusion. Turbulent diffusion is described with an one-equation turbulence model. Radiative transfer in the atmosphere is calculated with an efficient scheme based on the emissivity method for long-wave radiation and an implicit multilayer method for short-wave radiation (Moussiopoulos, 1987). The surface temperature over land is computed from the surface heat budget equation. The soil temperature is calculated by solving an one-dimensional heat conduction equation for the soil. At lateral boundaries generalised radiation conditions are implemented. The current standard version of MEMO allows performing nested grid simulations.
Among other recent applications, MEMO was used in the study launched by the Greek Ministry of the Environment aiming to assess the environmental impact of constructing the New Athens Airport (Moussiopoulos et al., 1995a).

Furthermore, it was one of the models used in the “Seven-cities project” in the context of the Auto/Oil study placed by the DGXI of the European Union. Previous applications of MEMO are summarised by Moussiopoulos (1994).

RAMS (Walko and Tremback, 1991; Pielke et al., 1992).

The Regional Atmospheric Modelling System (RAMS) was developed by scientists at Colorado State University and ASTeR, Inc. for simulating and forecasting meteorological phenomena, and for depicting the results. Its major components are (i) an atmospheric model which performs the actual simulations, (ii) an isentropic analysis package which prepares initial data for the atmospheric model from observed meteorological data, and (iii) a post-processing model visualisation and analysis package which interfaces atmospheric model output with a variety of visualisation software utilities.

RAMS is a merger of a non-hydrostatic cloud model (Tripoli and Cotton, 1982) and a hydrostatic mesoscale model (Mahrer and Pielke, 1977). However, some RAMS features are summarised in the following:

- Two-way interactive nesting with any number of fine nest grids.
- Terrain influenced co-ordinate surfaces with Cartesian or polar stereographic horizontal co-ordinates.
- Cloud microphysics parameterisation at various levels of complexity.
- Various turbulence parameterisation schemes.
- Radiative transfer parameterisations through clear and cloudy atmospheres.
- Various options for upper and lateral boundary conditions.
- Various levels of complexity for surface-layer parameterisation.
- Horizontally homogenous or variable initialisation (isentropic analysis). ECMWF and NMC analysis files can also be used for initialisation.
- It is highly portable and runs in several type of computers.

HYPACT (Tremback et al., 1993)

The Hybrid Particle and Concentration Transport Package (HYPACT) is a combination of a Lagrangian particle model and an Eulerian concentration transport model. It was developed at the Colorado State University and ASTeR, Inc. The Lagrangian model attempts to deal with the subgrid-scale aspects of a pollutant release while the Eulerian model takes over when the contaminant 'cloud' becomes adequately resolved on the computational grid, thus reducing the number of particles needed and increasing the computational efficiency. With the velocity and turbulence fields simulated by RAMS, the Lagrangian model in HYPACT will advect the particles with mean and random turbulent wind components. HYPACT uses a level 2.5 turbulent closure scheme based on the prognostic turbulent kinetic energy from RAMS.

The source configurations of HYPACT are very flexible. Any number of sources may be specified anywhere in the domain and configured as a point, line, area, or volume source. The emissions from these sources can be instantaneous, intermittent, or continuous. The pollutants can be treated as gases or aerosols and a radioactive half-life or a settling velocity can be specified.

Plume rise parameterisations and a dry deposition scheme have recently been added to HYPACT.

MERCURE (Elkhalfi and Carissimo, 1993)
This non-hydrostatic model, which was developed at Electricité de France, uses the inelastic approximation, and solves the relevant conservation equations on a staggered Arakawa-B grid. A fractional time step technique is applied, in which the advection, diffusion, pressure and continuity are solved separately. The advection step consists in a semi-lagrangian scheme. The diffusion step uses an implicit scheme with a splitting in the 3 directions. In the pressure continuity step, the Poisson equation is solved by a conjugate gradient method. The topography is taken into account by using a terrain-influenced co-ordinate system. The wave reflections on lateral and upper boundaries can be minimised by a viscous damping layer.
MERCURE includes two parameterisations of turbulent diffusion. In the first one, the exchange coefficients are diagnosed according to formulation of Louis (1982). In the second one, they are calculated by solving the conservation equations for turbulent kinetic energy and its dissipation rate (E-ε closure). The radiative effects are parameterised with mono-band schemes and can include absorption and short wave diffusion by clouds and aerosols. The surface temperature is computed with the force-restore method, and the surface humidity is calculated with a two-layers model.
The MERCURE model has been tested on boundary layer data (diurnal evolution during the Wangara experiment), and on orographic problems (Elkhalfi and Carissimo, 1993) by comparison with analytic solutions and with data from the Pyrénées experiment (PYREX). It has also been applied to simulate the land-sea breeze cycle in the framework of the APSIS project (Carissimo et al., 1995).

TVM (Schayes et al, 1995; Thunis, 1995)
The TVM model (Topographic Vorticity Model) is a non-hydrostatic Boussinesq and inelastic atmospheric model written in a terrain-influenced co-ordinate system. It solves prognostic equations for the two horizontal vorticity components, temperature, and specific humidity as well as for Turbulent Kinetic Energy (TKE) required by the 1.5 turbulence closure. TVM includes a third order advection scheme and allows for irregular grid spacing in all spatial directions. It was applied mainly for sea-breezes circulation in complex terrain configurations: applications in this respect include the study of (1) the Fos (near Marseille) campaign (Bornstein et al, 1995), (2) the Athens peninsula circulation (Thunis et al, 1993), (3) the New York City urban influence on wind patterns etc. Other type of applications include dynamically forced circulation, e.g. mountain waves and/or mountain windstorms (Thunis, 1995). TVM is built in a modular way, and includes more or less 60 routines.

UDM-FMI (Nordlund et al., 1995)
The urban dispersion modelling system UDM-FMI includes a Gaussian multiple source plume dispersion model and a meteorological pre-processing model, based on the Monin-Obukhov type boundary layer scaling. The dispersion model includes a treatment for point, line, area and volume sources. It allows for the influence of a finite mixing height, plume rise, down-wash phenomena and chemical transformation and deposition. The model estimates hourly time series of the concentrations of sulphur dioxide, nitrogen oxides and carbon monoxide. It also computes statistical parameters from the time series, which can be compared to air quality guidelines.

DISPERSION (Omstedt, 1988)
The model system, which has been developed at SMHI, brings together the results of recent research on dispersion modelling in a code which runs on a personal computer in Microsoft Windows or on a workstation. The first version of the model is described by Omstedt (1988). An updated dispersion model, based on the Danish OML-model (see section 3.5), is used for point sources, including effects of plume rise, plume penetration, buildings etc. For line sources dispersion parameters are related to basic boundary layer parameters in a continuous way. A street canyon dispersion model is used, which includes a chemical scheme for nitrogen oxides. The model includes also a source register system and a flexible emission module for traffic sources. Emission factors are calculated as a function of traffic volumes, driving pattern, cold start effects, mean vehicle speed, air temperature etc., for ten different vehicle types, (Egebäck et al., 1991). The meteorological inputs can be generated in a flexible way from either routine meteorological data, meteorological mast data or weather prediction model data. A user-friendly Desktop Mapping software is integrated into the model which enables e.g. calculations of population exposure.

MARS (Moussiopoulos et al., 1995b).
This Eulerian photochemical dispersion model is extremely versatile in the sense that the user may select the level of complexity with regard to

- the numerical algorithm used,
- the vertical discretization and
- the chemical mechanism embedded.

Hence, the computational effort may be easily adapted to the type of application (i.e. “research” or policy type).
If highest accuracy is required, a fully implicit self adaptive method is used, i.e. an implicit algorithm characterised by a variable time step and a variable order. In addition, the coupled description of the combined effects of vertical diffusive transport and chemical transformation of pollutants is possible (Moussiopoulos, 1987). By this approach the feasible error caused by splitting the operators associated with vertical diffusion and chemistry can be avoided (Graf and Moussiopoulos, 1991). Turbulent diffusion is described by the aid of an one-equation turbulence model with a suitable algebraic parameterisation for the mixing length.

Topography is properly considered by using terrain-influenced co-ordinates. Flux conservation is ensured by adopting a staggered grid. In addition to the standard fully 3-D version, a three-layer version of MARS exists, which may be efficiently used on workstation platforms.
MARS may be used in conjunction with any chemical reaction mechanism. In several recent model applications the EMEP MSC-W reaction mechanism has been used in the version approved by the LACTOZ Steering Group (Wirtz et al., 1994).
In conjunction with MEMO, MARS is being increasingly used in the last years for air quality studies, primarily for urban agglomerations. Examples for recent applications are the "Ozone project" in the context of the Auto/Oil study placed by the DGXI of the European Union and the "Heilbronn Ozone Experiment". In the latter application, nested grid simulations were performed with MEMO and MARS for the situation prevailing during the experiment in order to analyse the detailed meteorological and air pollutant measurements carried out during this period and in an attempt to draw conclusions with regard to the effectiveness of the emission reduction interventions (Moussiopoulos et al., 1995c). Previous applications of MARS are summarised by Moussiopoulos (1994).

CIT (McRae et al.,1982; McRae and Seinfeld, 1983, Russell et al., 1988)
As one of the most reputed photochemical dispersion models from the U.S., CIT has not only been applied for several North American airsheds (e.g., Harley and Cass (1994) discuss an estimation of the emissions and the formation of the organic air pollutants in Los Angeles), but also for European situations. Giovanoni et al. (1994), for instance, investigated the formation of ozone in the Swiss Alps. Usually, the meteorological data needed to run the CIT model are being diagnostically derived from measurements.
The model characteristics of the CIT model are as follows:

- calculation of advection using the Galerkin FEM-method
- chemical transformation described with the LCC mechanism (Lurmann et al. 1987)
- chemical reaction system solved by applying a semi-implicit procedure following Young and Boris (1977)
- application of operator splitting, the integration of each single operator being performed in fractional steps.

CALGRID (Yamartino et al., 1992).
Some of the basic features of this widely used photochemical model for urban scales are:

- A horizontal advection scheme that prohibits negative concentrations and exhibits little numerical diffusion.
- A full resistance-based model for computation of dry deposition rates as a function of geophysical parameters, meteorological conditions and pollutants characteristics.

- A modern photochemical scheme, based on the SAPRC mechanisms (Carter, 1990). The main advantage of the implementation of the SAPRC chemical mechanism is that can be upgraded, relatively easily, without any major changes of the rest of the code.
- Excellent documentation (Yamartino et al., 1989).
- Three options for the vertical layer structure.
- Many options for the level of complexity and detail for such input data as the emission inventory, the initial and boundary conditions.
- A wide variety of output options.

UAM (Ames et al., 1985; Chico and Lester, 1992)
The Urban Airshed Model (UAM) is a Eulerian model which calculates the concentrations of both inert and chemically reactive pollutants by solving the advection/diffusion equation using the method of fractional steps. At each integration time step, typically in the order of five minutes, the terms in the equation that represent the different atmospheric processes (e.g. chemistry or diffusion) are solved separately in several steps using the most efficient numerical integration technique for the given process. First the advection/ diffusion operator is treated, sequentially in the x- and y-directions; subsequently, emissions are injected and vertical advection/diffusion is solved; finally, chemical transformations are described by the aid of the CBM.
The UAM employs finite differencing numerical techniques for the solution of the advection/diffusion equation. The region to be simulated is divided into a three dimensional grid covering the region of interest. Horizontal grid cells are rectangular and equidistant. Vertical layer thicknesses are defined by the user based on the diffusion break, the top of the region, the number of layers below and above the diffusion break, and the minimum layer thickness. The diffusion break usually corresponds to the base of an inversion layer, either an unstable convective layer during the day (i.e. the mixing height) or a shallow mechanically mixed layer at night. The region top is usually defined at or slightly above the maximum daily diffusion break.

EPISODE (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.

The model runs of the UNIX 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) being finalised at NILU, which includes an operative emissions model, and data (measured and calculated) presentation tools.

EKMA-OZIPM4. The U.S. EPA **E**mpirical **K**inetic **M**odelling **A**pproach**,** **Oz**one **I**sopleths **P**lotting Package (Version **4**), is a parameterised chemical mechanism, in which ozone isopleths are generated as a function of initial volatile organic compounds and NO_x concentrations using the Carbon Bond 4 reaction Mechanism (Whitten and Gery (1985). In the EKMA methodology, a chemical reaction mechanism for photochemical smog is used to predict the maximum ozone concentration achieved over a fixed time of irradiation, as a function of initial precursor concentrations(VOC and NO_x). The maximum ozone concentrations corresponding to each set of initial concentrations are then represented as isopleths, from which control requirements are obtained graphically by assuming that the reductions in initial concentrations needed to lower the maximum ozone concentration from one isopleth to another, are linearly related to the emissions of each precursor. The chemical reaction mechanism is integrated from early morning to calculate the evolution of species concentrations in a hypothetical air parcel that starts from the city centre and is advected by the wind. The air parcel may increase in size due to changes in the mixing height and acquire additional pollutants from both fresh source emissions and entrainment of aged pollutants from aloft.

DRAIS (Tangermann-Dlugi and Fiedler, 1983; Nester et al.,1987)
With the non-hydrostatic model KAMM as meteorological pre-processor (Dorwarth, 1986; Adrian and Fiedler, 1991, Adrian, 1994), this model was used in the framework of the TULLA-project. Vogel (1991) investigated the distribution of the reactive pollutants downwind of the city of Heilbronn. A further application was the study of the influence of the biogenic emissions to the ozone concentration in the Upper Rhein valley. The model characteristics are as follows:

- Advection calculation using a flux-corrected transport scheme with small numerical diffusion (Hugelmann, 1988; Sweby, 1984)
- Chemical transformation described with the RADM (Stockwell, 1986) or RADM2 reaction mechanisms (Stockwell et al., 1990)
- Chemical equation system solved on the basis of the qssa-procedure (Hesstvedt et al., 1978) extended by Chang et al. (1987),
- Application of operator splitting, the integration of each single operator being performed in fractional steps.

MATCH (Persson et al., 1994)
MATCH is a 3-dimensional Eulerian atmospheric dispersion model integrated with a sub-gridscale model for large point sources. Emissions can be specified both as area and point sources and with a high temporal resolution. The model

includes, for the time being, chemistry for the 10 most important compounds for oxidised sulphur and oxidised and reduced nitrogen. Measured concentration of background O_3 are used as input to the model and a local adjustment of the O_3 concentration due to local NO- and NO_2-concentrations and solar radiation is done. The sink mechanisms for each compound are specified as a function of surface characteristics and meteorological conditions.

3.4.3 *Input data requirements*

Several types of data sets are required as input to prognostic mesoscale air pollution models:

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.

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).

As already mentioned, in most cases the above requirements cannot be fulfilled.
If the wind and turbulence fields are calculated prognostically, mainly radiosonde observations are required. It is sufficient to have records from one station once a day, although it is much better to have information from several stations several times in the course of the day. In particular, data on height, pressure, temperature, relative humidity, wind speed and direction are necessary. As an alternative, meteorological input data may be derived from previous analyses, e.g. from the European Centre of Medium Weather Forecast (ECMWF). In the case of prognostic models data from surface observations are usually not needed at input.

Emission data.
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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3.5 Local scale air pollution models

3.5.1 General remarks

From the late 1950's onwards atmospheric dispersion models based on Gaussian distribution and Pasquill-Gifford classes have been used for regulatory purpose in Europe.

In the last 20 years, increasing understanding of both the structure of the boundary layer and dispersion science have lead to development of a new generation of dispersion models based on boundary layer parameterisation. The meteorological input to these models is based on new methodologies where the vertical profiles of velocity, temperature and turbulence are dependent on the height of the boundary layer and a Monin-Obukhov length scale determined by the temperature, the friction velocity and the heat flux.

The increased use of practical operational models for regulatory and planning purposes require the models to give more reliable and accurate results. The air quality guidelines in different countries are becoming increasingly stringent and detailed. This underlines the needs for verified models which replies the needs with regard to air quality management.

3.5.2 *Existing models*

In connection to the workshop in Mol on "Operational Short-Range Atmospheric Dispersion Models for Environmental Impact Assessment in Europe", arranged by the ad-hoc group for Harmonisation of models in Europe, a model validation exercise was conducted. Prior to the workshop, a Model Validation Kit was distributed to a number of research groups. The Model Validation Kit is a collection of three experimental data sets (Kincaid, Gladsaxe and Lillestrøm) and software for model evaluation.

VITO, Belgium have also carried out a comparison exercise of six Gaussian dispersion models used for regulatory purposes in Europe. This exercise was carried out by using one year of meteorological data from the meteorological tower in Mol and three release heights (30 m, 80 m and 150 m).

In the following, short descriptions are given for the models used in the two comparison exercises.

IFMD. The Belgian Immission Frequency Distribution Model, IFDM, uses the Bultynck-Malet stability classification scheme which distinguishes 7 classes. The dispersion parameters that correspond to each stability class are based on the analysis of wind fluctuations. IFDM does not consider the consequences of a limited mixing height. Computations are made using a time series of hourly meteorological data. The routinely reported output parameters are the yearly averages, and a series of hourly and daily concentrations for each receptor point.

PLUIMPLUS. In the Netherlands the "National Lange Termijn Frequentie Model" was developed as a consensus between industry, administrators, and scientists. PLUIMPLUS is one of the commercially available PC-implementations of this model. Stability classes for this model have to be determined with the KNMI-system, which is based on cloud cover, wind speed, time of the day and season, and which is very similar to Pasquill's system. The concentration is Gaussian distributed in vertical direction, and uniformly distributed over a 30 degree sector in horizontal direction. The meteorological data are in the form of a joint frequency table of stability class, wind speed (3 classes), and wind direction (12 sectors). PLUIMPLUS calculates yearly averages and uses empirical relationships to estimate percentiles of hourly and daily averages.

ISCST2. The US-EPA model ISCST2 is used in several European countries for regulatory purposes. 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.

AUSTAL86. The German technical instructions on air quality control, TA-Luft, are translated into a programme system: AUSTAL86. The stability classification scheme is described in TA-Luft and is based on wind speed and cloud cover during day or night periods. The corresponding dispersion parameters depend upon the effective source height. The meteorological input data are in the form of a joint frequency table of stability class, wind speed (9 classes) and wind direction (36 sectors). The model generates yearly averages and 98 percentiles of hourly averages. The receptor grid can no be chosen as it is determined as a function of the source configuration.

OML. Characteristic for this Danish model (developed at NERI) is that it does not use stability classes, but instead describes dispersion processes in terms of basic scaling parameters, such as friction velocity, Monin-Obukhov length, and the convective velocity scale. Before being used by the model, meteorological measurements must be pre-processed. OML also requires meteorology on an hourly basis, and returns yearly averages, the n largest hourly averaged concentrations, and the 99-percentiles of hourly concentrations for each month.

UK-ADMS. Developed at the UK Met office, this model comprises a number of modules, each representing either a physical process of dispersion of gases or data input and output. Similar to the OML model, UK-ADMS describes dispersion processes in terms of atmospheric basic scaling parameters. The plume rise is calculated by integrating a set of equations linking the fluxes of mass, heat and emitted material. Entrainment of ambient air and partial penetration of inversion layer is included. The output from the model is similar to the OML model.

HPDM. The **H**ybrid **P**lume **D**ispersion **M**odel, developed by Sigma Research Corporation (USA) operates similar to OML. HPDM can either use measured or pre-processed meteorological data. The output is percentiles and average values for the period considered.

INPUFF. The US-EPA developed model INPUFF is a puff trajectory model using three dispersion algorithms, Pasquill-Gifford scheme or on site scheme and conjunction between these. The on site scheme are using meteorological measurements calculating dispersion parameters. The plume rise used is the methods of Briggs. The output from the model is similar to HPDM in selected receptor points.

In the remainder of this section, further local scale models are presented:

CTDMPLUS. The US-EPA **C**omplex **T**errain **D**ispersion **M**odel **Pl**us Algorithms for **U**nstable **S**ituations (Perry et al. 1989), is a multiple point-source Gaussian plume dispersion model for use in all stability conditions for complex terrain applications. Its use of meteorological input and terrain information is different than current EPA models; considerable detail for both types of input data is required and is supplied by pre-processors specifically designed for CTDMPLUS.

CTDMPLUS requires the parameterisation of individual hill shapes using the terrain pre-processor and the association of each model receptor with a particular hill. A central feature of the model is its use of a critical dividing-streamline height (H_C) to separate the flow in the vicinity of a hill into two separate layers (over the top of the hill and in a horizontal plane around the hill), according to the kinetic energy of the flow. However, although multiple terrain features are modelled by CTDMPLUS, the plumes impinging on a downwind hill are assumed to be influenced by upwind features only in the effects found in the on-site meteorological measurements.

The model does not use stability classes, but instead describes dispersion processes in terms of basic scaling parameters, such as friction velocity, Monin-Obukhov length, and the convective velocity scale. Thus, hourly profiles of the wind and temperature measurements are used by the CTDMPLUS meteorological pre-processor in order to compute plume rise, plume penetration, convective scaling parameters, the value of H_C, and the Froud number above H_C. For the unstable conditions the model relies on a probability density function description of the vertical velocities to estimate the vertical distribution of pollutant concentration. In stable and neutral conditions the profiles of turbulence data are used to compute plume dispersion parameters at plume height.

The model calculates on an hourly basis the plume trajectory deformation by each hill. The computed concentration at each receptor is then derived from the receptor position on the hill and the resultant plume position and shape.

SCALTURB (Gryning et al., 1987)

The Norwegian Institute for Air Research (NILU) has developed an operational dispersion model based on boundary layer parameterisation and dispersion regimes. The input to the model is fundamental meteorological parameters which are pre-processed in a meteorological pre-processor to obtain boundary layer parameters such as Monin-Obukhov length, friction velocity and mixing height. The atmospheric boundary layer is divided into scaling regimes, for which models for dispersion in the vertical is given. The models give crosswind integrated concentration. The lateral distribution is always assumed to be Gaussian, while generally the vertical concentration profile is proposed to be other than Gaussian. The model input is hourly meteorological data and the output is from one hour to yearly averages and percentiles of hourly averages.

CAR. For monitoring of air quality at street level in the Netherlands the CAR model (**C**alculation of **A**ir pollution from **R**oad traffic) has been developed (Eerens et al., 1993). CAR is a simple parameterised and easy-to-use model which runs on a PC. In the Netherlands, the model supports provincial and municipal authorities in the implementation of air quality decrees under the Air Pollution Act. CAR predicts yearly averaged concentrations and 98-percentile values of components emitted by traffic such as NO_2, CO, lead and benzene. By analysis of measured concentrations in streets and an extensive programme of wind tunnel experiments the relation between emissions and concentrations was investigated for a large number of configurations which differs with respect to dimensions, distances and shapes of streets, its buildings and trees. Based on these studies, parameters with the largest influence on the concentrations were selected. After the development the model has been evaluated by means of an intensive measuring programme in different traffic situations and street configurations. At present there is a yearly calibration of model parameters based on the measurements of 13 urban monitoring stations.

CARSMOG. A recent extension of the CAR model is the CARSMOG model (den Tonkelaar and Wildschut, 1993, den Tonkelaar 1995) which on-line calculates hourly concentrations of traffic related pollutants for standard streets in all major Dutch cities. CARSMOG calculates concentrations in 'standard' streets using a normalised annual averaged street contribution, the distribution of traffic emissions over the hours of the day, days of the week and month of the year and the fluctuating traffic pattern obtained from a comparison between measured and modelled street concentrations for operational street stations. The CARSMOG system enables authorities to carry out an on-line (real-time) and continuous inspection of air quality in cities.

OSPM (Berkowicz et al., 1985)
As a support to the standard monitoring activities and in order to provide tools for evaluation of abatement strategies a new air pollution dispersion model - the Operational Street Pollution Model (OSPM) - has been developed at the National Environmental Research Institute (NERI), Denmark. The model includes a simplified description of flow and dispersion conditions in streets. Concentrations of exhaust gases are calculated using a combination of a plume model for the direct contribution and a box model for the recirculating part of the pollutants in the street. In spite of the simplifications, the model is able to

properly simulate the dependence of air pollution levels on meteorological conditions, such as wind speed and wind direction. OSPM includes also a chemical sub-model which is used to calculate the conversion of NO to NO_2. Using actual meteorological observations and estimations of emissions the model provides hourly values of concentrations at prescribed receptor points in the street.

CAR-FMI (Härkönen et al., 1994).
Finnish Meteorological Institute (FMI) has developed a model for predicting dispersion of pollution from a road, for use in regulatory context. The model includes an emission model, treatment of the meteorological time series, a dispersion model, statistical analysis of the computed time series of concentrations and a graphical Windows-based user interface. The model has been named CAR-FMI, i.e., Contaminants in the Air from a Road. The model is based on a partly analytic solution of the Gaussian diffusion equation for a finite line source by Luhar and Patil (1989), and it allows for any wind direction with respect to the road. The chemical transformation is modelled by using the so-called discrete parcel method, and it includes the basic reactions of nitrogen oxides, oxygen and ozone. The relevant meteorological parameters are evaluated using stability data produced by a meteorological pre-processing model.

ROADAIR (Larssen and Torp, 1993; Torp et al., 1994).
The ROADAIR model has been developed as a combination of *the Nordic Car Exhaust Model* which was developed in 1980-84 to enable the calculation of air pollution problems in street canyons, the EPA HIWAY model for calculation of roadside air pollution in country and a method providing emission factors for different vehicles. The principle was to estimate the maximum short-term concentrations of CO and NO_2, taking account of the rush-hour traffic conditions, the canyon geometry and the worst-case dispersion conditions. From the first version 1.5 till the present version 3.1, the model has been developed to take into account non-canyon streets/roads, suspended particles, and the exposure of residents near the road network, based upon a building register. The version 3.1 is now to be used as a regulatory model in Norway, to determine in which areas/places abatement measures are necessary according to the law. The model calculates emissions and maximum short-term concentrations of CO, NO_2 and PM at given distances from each junction in a defined road network, defined via a road and traffic data input register.

CONTILINK (Larssen et al., 1993).
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, NO_x and PM_{10} 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.

3.5.3 *Input data requirements*

Emissions. These simple models for regulatory use need standard physical data for the stacks, such as stack height and diameter, exit gas velocity and temperature and emission rates. The emission rates can be a fixed value or time dependant.
The traffic models need as input standard description of the road network, such as number of cars per day, number of lines, average driving velocity, steepness of the road and description of the surroundings, (open area, scattered buildings, street canyon).

Meteorology. Some of the models are screening type models, which use default meteorology as input, describing a critical meteorological situation. Other models use a set of meteorological situations as input, described in wind and stability classes.
The new generation of models use pre-processed meteorological data based on similarity theory for the atmospheric surface layer. The required measurements include parameters such as profiles of wind and temperature, cloud cover or net radiation in addition to surface roughness.

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4 QUALITY ASSURANCE OF AIR POLLUTION MODELS

The quality of an air pollution model can be judged in terms of

- model consistency (i.e., the way in which 'reality' is reflected in the simulation results) and
- model accuracy, which can be estimated in the course of an appropriate model evaluation procedure.

Apparently, quality criteria for air pollution models have to focus on well-documented descriptions of the model itself and of the procedure used for model evaluation.

4.1 Model documentation

The availability of models for the analysis of air pollutant transport and transformation at various scales can easily lead to misinterpretations of their results or even to the misuse of these models. One of the means to improve this situation is to provide better model descriptions. Rather than being an aim in itself, an attempt towards better model documentation should primarily aim at better stimulating the use of models and model results (Noordijk, 1992).

At present air pollution models at all scales are documented through publications in scientific journals or technical reports. The level of documentation is mostly on describing the mathematical and numerical methods used formulating the model, together with descriptions of the parameterisations employed and the choices of parameters and constants. The quality and detail of information may vary considerably and the documentation on how to use the modelling system is often limited. There are clearly needs to strengthen the model documentation including descriptions of the model input and output, the model formulation and the procedure for using the model, area of application, how it has been evaluated and the expected accuracy in the modelled quantities. Ideally, a model manual describing the above items should follow each model. Still, much remains before the models have reached this level of detailed documentation.

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4.2 Model evaluation

The way to evaluate air pollution models seems to be straightforward: Model predictions are compared against appropriate measurements and identified deviations are statistically analysed to allow quantifying the model uncertainties. In spite of the simplicity of this method, there are considerable difficulties both in properly defining the evaluation procedure and in interpreting its results:

- Different evaluation procedures should be applied to the various model categories. By other words, the experimental data set needed to evaluate the models as well as the evaluation software should be tailored to the specific application.
- Deviations between model results and observations may be caused by a variety of reasons: Shortcomings in model assumptions and parameterisations, errors and inaccuracies in input data (in particular emission data and meteorological data), uncertainties related to the stochastic nature of atmospheric processes, uncertainties in observations, uncertainties in the representativeness of both observed and modelled data etc.

4.2.1 Local scale

Valuable experience with regard to model evaluation has been already collected in the case of simple models: A series of workshops was organised by the Steering Committee on "Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes", one of the objectives being to test evaluation procedures for single source short-range atmospheric dispersion models (Olesen and Mikkelsen, 1992). Several steps have been taken during the past few years with regard to models assuming homogeneous terrain and inert pollutants. Specifically, a "Model Validation Kit[1]" was created as the basis for the work on model evaluation. Being a collection of three experimental data sets and suitable software, this "Model Validation Kit" was meant to serve as a common frame of reference. Very recently, this kit was used for a common evaluation exercise involving five models (Kretzschmar et al., 1994). A lot of useful information emerged from this exercise, including

- the identification of strengths and weaknesses of models,
- the clarification of problems with model evaluation procedures and
- the need for continued model evaluation.

4.2.2 Local-to-regional scale

Only preliminary activities towards model evaluation have taken place in the case of local-to-regional air pollution models. The main reason for this is that most so far field campaigns in this scale focused mainly on meteorology, the primary aim being to describe complex atmospheric transport phenomena. As an example, the main objective of the recent TRACT campaign was to investigate the orography influence on the dispersion characteristics (Zimmermann, 1995). Air pollutant concentration measurements taken in such campaigns are not

[1] which might better have been termed "Model Evaluation Kit"

sufficient for a conclusive description of the governing transport and transformation mechanisms. The latter have occasionally been analysed in the frame of small scale experimental activities which were carried out to study partial aspects of the photooxidant problem in Europe.

As an example for an attempt towards model evaluation, the APSIS activity was performed with the objective to check the capabilities of contemporary models to describe wind flow and ozone formation in an urban area (Moussiopoulos, 1993). Although APSIS was rather a demonstration exercise than an in-depth evaluation project, its findings lead to the following conclusions:

- Contemporary prognostic mesoscale models are capable of reproducing most of the wind field features which significantly affect air pollutant concentrations in complex airsheds like Athens.
- Statistical analyses of deviations between model results and presently available measured data may lead to useful assessments of the wind model performance (Kunz and Moussiopoulos, 1995).
- Available experimental data sets are hardly sufficient for a conclusive evaluation of photochemical dispersion models.

The consequence from the latter conclusion is that detailed field campaigns are needed in order to build a comprehensive experimental database for the conclusive evaluation of present and future air pollution models at the local-to-regional scale. Such campaigns should primarily aim to check the model accuracy with regard to budgets for all major compounds. In addition, the experimental evidence should allow representing the interaction between anthropogenic and natural emissions.

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4.2.3 *Regional-to-continental scale*

The EMEP database (Schaug et al., 1994) has so far been the most frequently employed source for evaluation of European scale models. The EMEP database consists of a few tenths to nearly hundred stations (varying from one chemical component to another) throughout Europe. The data are collected at the national level, while they are stored and controlled at the EMEP database. An disadvantage of the EMEP database is that only surface measurements are available. Large amounts of additional observations exist on the national level, but the data are often difficult to access and the quality is so inhomogeneous that it may be difficult to employ.

Clearly, there is a need to harmonise and to collect and systematise the large amount of observations on the national level in order to make more data available for model evaluation. Additionally, considerable efforts should be devoted to establish the quality and the representativeness of the measurements in cases where this is uncertain. In this respect, significant advances were achieved in the frame of EUROTRAC's subproject TOR (Cvitaš and Kley, 1994). The three dimensional models should to a larger extent be analysed by usage of height dependent data, and there is a large need for such data on the European scale. Measuring campaigns with a high spatial coverage of atmospheric data is until now missing in Europe. The establishment of a data base from such a campaign would be of large importance to the evaluation of a large number of air pollution models in Europe.

It is worth mentioning that useful experience with the statistical evaluation of regional-to-continental scale models was gained in the frame of the ATMES experiment (Klug et al., 1990).

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4.2.4 *Global scale*

On the global scale, the measurements available are those obtained in the different continents either as part of international programmes or just as national data. The abundance of data is largest in Europe and North America and there is a large need for high quality measurements in other parts of the world. A measurement network co-ordinated by the Global Atmospheric Watch (GAW) programme of the World Meteorological Organisation (WMO), was established in 1989 (Mohnen, 1995) and it will increase the number of observations throughout the world. The main objective of GAW is to investigate the changing chemical composition of the atmosphere (greenhouse gases including ozone, acidifying pollutants, toxicity of precipitation, aerosols and solar radiation) on the basis of monitoring data collected at about 30 global and over 100 regional stations. Quality assurance and quality control of the monitoring data is paid large attention and constitutes an essential part of the GAW structure.

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4.3 Status of model documentation and evaluation

An assessment of the status of documentation and evaluation of available air pollution models cannot be performed without an in-depth review of each individual model. Such a tremendous effort would be beyond the scope of the present report. As a first approach, therefore, the experiences and opinions of the contributors to this report on the current status of model documentation and evaluation are summarised in Table 3. The appraisal is performed collectively for all models relevant to address the policy issues introduced in Table 1 (section 2.1), although in some cases considerable variations exist among the various models in question.

Table 3: Estimated current status of model documentation and evaluation for various policy issues related to the atmospheric environment (see text)

Policy issue	Status of documentation	Status of evaluation
Climate change	2	3
Ozone depletion	2	3
Tropospheric ozone	2	4
Tropospheric change	2	4
Acidification	2	2
Nutrification	3	3
Summer smog	2	2
Winter smog	3	3
Air toxics	3	4
Urban air quality	2	3
Industrial pollutants	2	2
Nuclear emergencies	2	3
Chemical emergencies	2	4

The grades from 1 to 5 have the following meaning:

Documentation

1. Complete documentation available, ranging from the scientific description down to users manuals with details on the machine code. Obviously, a grade that is hard to obtain.
2. Rather good scientific documentation and less complete users manuals.
3. Worse scientific documentation as compared to grade 2.
4. Generally, incomplete or messy documentation.
5. No documentation at all.

Evaluation

1. Hard to achieve because of either still pending work on evaluation, or minor limitations in the measurements available (quality, representativeness, coverage etc.), or both.
2. Extensive and good model evaluation has been performed, but still uncertainties because of major limitations in the measured data.
3. Considerable uncertainties because of both lack of measurements and an inadequate evaluation procedure.
4. Only first attempts towards evaluation.
5. No evaluation at all.

5 TRENDS IN AIR POLLUTION MODELLING

5.1 Model development

5.1.1 Global scale

In view of the need to assess the environmental and socio-economic impacts of atmospheric and climate change in order to formulate appropriate response strategies, the dominant trend in global air pollution modelling is inevitably directed towards improvement and further development of 3-D chemical transport models as well as coupling them together with climate models. A series of important issues needs still to be addressed such as better simulation of sub-grid processes, convective transport and wet deposition of aerosols, better quantification of oxidant and heterogeneous mechanisms, high quality measurements of ultra-violet radiation, larger computer capacity to handle all processes that are believed to be important. This requires a better understanding of the atmospheric chemistry by a combination of careful field observation, laboratory investigation and theoretical modelling. Access to good quality emission data (global emission inventories) and meteorological information is necessary to build trust in the output of the models. Access to high quality global monitoring data sets on synoptic and even smaller scales is also needed in order to evaluate the performance of these models.

5.1.2 Regional-to-continental scale

Today's Long Range Transport Air Pollution Models (henceforth LRTAP-models) are well advanced in many aspects both in their ability to simulate complicated physical and chemical processes accurately and to be useful tools for decision makers. However, there are also clear needs for further development of the models as described in the following.

The policy oriented models should be developed further to account fully for the three-dimensional structure of the dispersion of pollutants. Such developments have so far partly been limited by insufficient computer capacity, but the present progress in Massive Parallel Computing is promising and will probably solve these problem in a few years. More resources should be devoted to include the chemically important clouds into the LRTAP-models, and in the case of Eulerian models, source attribution techniques must be developed. Linkage of acid rain chemistry and photochemistry in rather comprehensive LRTAP-models is needed to account for both the acidification and the tropospheric ozone problem in future multi-pollutant protocols.

As more and more complicated policy oriented models are developed, the needs for stronger links between policy supporting programmes and scientific programmes are growing. Parts or sub-modules of policy oriented models could preferably be developed in close co-operation with Universities. For the support of environmental decisions less complex models should be developed by simplifying those parts of the complex models that are not very sensitive to the results.

Further improvements of the LRTAP-models should especially be sought for:

- Determination of mixing heights
- Vertical convective transport mechanisms
- Chemical mechanism emphasising cloud and aerosol chemistry
- Improvement of numerical techniques
- Reprogramming for Massive Parallel Computers

5.1.3 Local-to-regional scale

The so far experience with air pollution models in the local-to-regional scale confirms the importance of taking into account larger scale processes by the aid of appropriate nesting techniques. In view of several concerted international research activities towards improving the nesting capabilities of individual models or model systems, a significant progress can be expected for the next future with regard to the potential of numerically simulating processes extending over several scales.

Another trend for refining mesoscale air pollution models is the adoption of nudging[2] as an option to ensure that model results adapt to observed data. This option could be of particular importance especially in situations where the air pollution model is driven directly by the aid of analysed data, as for example ECMWF data.

Along the same lines, another subject of current research and development is the method of linking prognostic mesoscale models to three-dimensional microscale models. This linking would allow taking proper account of prevailing mesoscale conditions when describing transport phenomena which occur in street canyons or while air flows around obstacles.

From the point of view of parameterising physical processes, further model development currently concentrates on an improved treatment of turbulent transport. Thanks to the continuing hardware development and the additional chances arising from the possibility to parallelize existing codes, several new approaches could be materialised in models devised for the practical application. Examples are non-local closure techniques or even large eddy simulation.

[2] inclusion of extra terms in the model equations guaranteeing that the model results gradually converge to analysed data from observations.

Last not least, there is an obvious trend towards a more realistic description of chemical transformation processes in mesoscale air pollution models. Apart from the gradual refinement of individual chemical mechanisms embedded in the models, the attempt is made in present to properly describe the interrelation of homogeneous and heterogeneous chemical processes. As an example, photochemical reactions appear to be considerably affected by the presence of aerosols, and therefore an adequate description of the physico-chemical behaviour of aerosols could be proved to be a prerequisite for reliable simulations of ozone formation in dusty atmospheres.

5.1.4 Local scale

The model evaluation exercise mentioned in section 3.5 showed that significant differences exist between the results of the models. While part of the differences can be attributed to the use of different stability classification schemes and associated dispersion parameters, other elements such as discretisation of the meteorological data, the wind profile, and the particular software implementation might also be responsible for some of the differences found.

The improvement of computer capacity and skills make it possible to develop new operational and practical regulatory models which are more complex and describe the physics of the atmosphere better. Future initiatives should be focused on:

- Standard of meteorological input data
- Harmonisation of meteorological pre-processors
- Scientific basis for next generation of operational models
- Procedures for model evaluation
- Establish databases for model evaluations

Requirements concerning model capabilities depend on the environmental problem in question and the regulatory needs. The decision makers may need calculation of quantities such as:

- Long term average concentration
- Frequency distributions
- Maximum concentrations

The use of operational models for planning purposes is important and the modelling system should therefore be user friendly and give the answers needed for air quality management.

5.2 Effects on humans and ecosystems

The critical level or load is defined as the concentration or deposition of a pollutant in the atmosphere above which direct adverse effects on receptors, such as plants, ecosystems or materials may occur. In practice, the approach has been to assign a critical value to a given receptor, and to compare this critical value with actual or estimated (modelled) values. The components of major concern on the regional to continental scale in Europe has so far been the near surface ozone concentrations and the accumulated deposition of acidifying sulphur compounds and acidifying and nutrifying nitrogen compounds.

Critical levels of ozone have been derived on the European scale (Anttila, 1993, EMEP, 1995) and models have been applied to calculate the exceedances above the critical levels. Based on experience in agriculture and plant sciences it has been found that the response to ozone is cumulative and therefore depends on the length of the exposure period. A simple criterion for exposure is the AOT (ozone exposure accumulated over threshold), and at present a cut-off of 40 ppb has been chosen (AOT40). In other words the critical level for crops is expressed as the sum of hourly concentrations above 40 ppb during the growing season. Examples of calculated AOT40 is found for example in Simpson (1994).

A critical load is defined as the "highest deposition of a compound that will not cause chemical changes leading to long-term harmful effects on ecosystem structure and function (Downing et al., 1995). The models are then utilised to calculate the exceedances to the critical loads in model grid-elements in order to get a quantitative picture of the damage to the ecosystem (Barrett et al., 1995). The critical load of acidity has so far been applied quite extensively for sulphur throughout the process of defining the latest sulphur protocol for long range transboundary fluxes of sulphur. The usage of critical levels and loads in combination with model calculations is expected to be of increasing importance to the forthcoming processes of deriving new NO_x and VOC protocols.

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5.3 New concepts

Air quality is only one part of an environmental aspect to be accounted for in planning and decision processes. In this respect an air quality model has to include flexible procedures to identify sensitive parameters and to clarify their functional relationships with emissions and adverse effects of pollution.

Methods have been developed to compare the costs of measures to improve air quality with the costs of adverse effects of pollution. Abatement strategies are then based on integrated assessment models accounting for several adverse effects caused by the same groups of sources.

From a mathematical point of view, selection of optimal abatement strategies have been discussed by several authors, e.g. by Gustavson et al. (1974). From a practical point of view, the application of models were included in larger systems considerations when air quality policies were implemented in urban and local areas, i.e. in Germany (Fortak, 1974) and in USA (Slater, 1974).

Simple proportionality models between emissions and adverse effects have been used in national economic models to clarify air aspects of planning and management (Morris and Slater, 1974).

In order to substantiate the functional relationships on different spatial scales effects of emission conditions have to be taken into account, i.e. stack height, spatial and temporal vacation in emission intensity.

Environmental costs of alternative scenarios depend on the sum of adverse effects of a number of local pollution problems and on the scale of variability in ecosystem sensitivity regarding

- health effects
- environmental degradation
- forestry practice
- corrosion

Effects quantified in economic terms may be insufficient as cost-exposure relationships are poorly defined, and in Europe ambient air quality standards are accepted as a political decision on the air quality constraint on activities causing pollution emissions.

For most pollutants adverse effects increase gradually with ambient air concentration and a limit value may be formulated somewhat arbitrarily. However, it makes the assessment studies easier to perform. It is expected that in the future, when the cost-exposure curves are better defines the models may be modified accordingly.

Within the UN Economic Commission for Europe (ECE) working groups on developing elements in comprehensive models of pollution have been established, i.e. working groups on effects, on strategies and on technology.

The task force for integrated assessment modelling co-ordinate work for the group on strategies. Several models have been applied to clarify the improvement of air quality as a result of alternative scenarios on emission reductions in Europe. An example is the Rains model (Alcamo et al., 1990). The calculation procedure in Rains consist of several model elements, i.e.

- emission model
- atmospheric transport
- acidification/deposition

The effect of different emission scenarios on acidification of soil and water have been clarified including the costs to avoid "Critical loads of acidification" in different areas.

Uncertainty analysis of the probabilistic accident consequence codes has been performed under contracts by DGXII Radiation Protection Research and DGXI-A-I Radiation Protection as a joint study of CEC and USNRC.

A package of programs have been developed for calculating probabilistically the health effects, economic costs and effects of countermeasures following accidents in nuclear industries (Cook et al., 1994).

The dispersion module includes a combination of the Gaussian puff model including trajectory calculation on local and large scale. These techniques could be applied in other applications of dispersion models as well in particular considering a number of industrial activities.

Studies to clarify the economic effect of pollution deteriorating materials have been developed for many years in particular in England and in the Nordic countries. The identification and assessment of material damage by air pollution include data on dose-response and the effect on "service life" as well as the building register on a regional and urban scale (Ecotec, 1986; Kucera et al., 1993).

As the computer capacity has increased tremendously in the last decade, it is possible to account for more details in data on emissions and effects. In some countries the next generation air quality modelling system is under development (Hansen et al., 1995). In other countries emission data have been collected and environmental models improve the basis for decisions considering sustainable development, in particular on a regional scale (Pulles, 1995; Borrell et al., 1995). On urban and local scales air pollution models as flexible tools to integrate scientific results in environmental policy have been developed (Moussiopoulos, 1995; Bøhler, 1995). These tools may also help communication between groups of specialists, specialists and decision authorities as well as information to the public.

New software and hardware techniques simplify communication. However, when interpretations of results are not filtered by the specialists, specification of the errors and uncertainties in calculated results have to be communicated as well.

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6 SUMMARY AND CONCLUSIONS

The main purpose of this report was to review existing air pollution models for all scales of dispersion phenomena focusing on model availability for addressing the main policy issues related to the atmospheric environment. As, inevitably, a large number of models could not be considered in the review, readers are encouraged to recommend the inclusion of other models in the next edition of the report.

It is generally accepted that air pollution models are important tools not only for assessing emission reduction strategies, but also for estimating exposures and for investigating economical aspects of air pollution. Moreover, there is a trend towards an increased role of air pollution models in the decision making process. As a matter of fact, models are already available for most of the applications where they might be of use, while at the same time the status of model documentation is considered to be satisfactory. Yet, the majority of environmental managers appears not to be fully aware of the capabilities of existing models. Moreover, model accuracy seems not being an important issue among environmental managers, not even in countries where models are being excessively used for regulatory purposes.

Future model refinements should be compatible with the needs of model users. Correspondingly, a continuous contact and exchange of information between environmental managers and model communities should be established and maintained. Among the major objectives of such a contact is to identify the needs for specific activities aiming at a further improvement of model documentation and a better assessment of model accuracy. Only with such activities it will be possible to improve the status of model evaluation, which seems to be unsatisfactory at present.

The trend towards more accurate air pollution models forces to abandoning the conventional rigid separation of atmospheric processes into individual scales. Multi-scale approaches will be indispensable in the future, and nesting techniques are necessary in order that models which were developed for individual scales be properly combined to describe processes extending over several scales.

As model evaluation is impossible without appropriate experimental data, there is an obvious need for

- co-ordinating experimental campaigns at proper locations in Europe,
- creating adequate experimental databases on primary pollutants (including particulate matter) and photochemical air pollution over complex terrain, and
- conducting in-depth model evaluation activities.

APPENDIX

A1 Classification of air pollution models

Model name	Scale of dispersion phenomenon	Model category	Chemistry
2-D OSLO	global	2D-Eulerian	yes
3-D OSLO	global	3D-Eulerian	yes
AUSTAL 86	local	Gaussian	no
CALGRID	local-to-regional	3D-Eulerian	yes
Cambridge model	global	2D-Eulerian	yes
CAR	local	Semi-empirical	no
CAR-FMI	local	Gaussian	yes
CIT	local-to-regional	3D-Eulerian	yes
CONTILINK	local	Gaussian	no
CTDMPLUS	local	Gaussian	no
CTMK	global	3D-Eulerian	yes
DISPERSION	local-to-regional	Semi-empirical	no
DMU	regional-to-continental	2D-Eulerian	yes
DRAIS	local-to-regional	3D-Eulerian	yes
ECHAM	global	3D-Eulerian	yes
EKMA/OZIPM4	local-to-regional	Chemical	yes
EMEP/MSC-E	global	2D-Eulerian	yes
EMEP/MSC-E/ acid deposition	regional-to-continental	2 layer Eulerian	yes
EMEP/MSC-W	global	3D-Eulerian	yes
EMEP/MSC-W/ photochemistry	regional-to-continental	2D-Lagrangian	yes
EMEP/MSC-W/ acid rain	regional-to-continental	2D-Lagrangian	yes
EMEP/MSC-W/ sulphur	regional-to-continental	3D-Eulerian	yes
EPISODE	local-to-regional	3 layer Eulerian	yes
EURAD	regional-to-continental	3D-Eulerian	yes
HARM	regional-to-continental	2-D Lagrangian	yes
HARWELL	global	2D-Eulerian	yes
HPDM	local	Gaussian	no
HYPACT	local-to-regional	3D-Eulerian	no
IFDM	local	Gaussian	no
IMAGES	global	3D-Eulerian	yes
INPUFF	local	Gaussian	no
ISCST 2	local	Gaussian	no
IVL	regional-to-continental	2 layer Lagrangian	yes

A1 Continued

Model name	Scale of dispersion phenomenon	Model category	Chemistry
Liège model	global	2D-Eulerian	yes
LOTOS	regional-to-continental	3D-Eulerian	yes
Mainz model	global	2D-Eulerian	yes
MARS	local-to-regional	3D-Eulerian	yes
MATCH	local-to-regional	3D-Eulerian	yes
MEMO	local-to-regional	3D-Eulerian	no
MERCURE	local-to-regional	3D-Eulerian	no
MOGUNTIA	global	3D-Eulerian	yes
OML	local	Gaussian	no
OSPM	local		no
PLUIMPLUS	local	Gaussian	no
RAMS	local-to-regional	3D-Eulerian	no
REM3	regional-to-continental	3D-Eulerian	yes
ROADAIR	local	Gaussian	yes
SCALTURB	local	Gaussian	no
STOCHEM	global	3D-Lagrangian	yes
TREND	regional-to-continental	Statistical	yes
TVM	local-to-regional	3D-Eulerian	no
UAM	local-to-regional	3D-Eulerian	yes
UDM-FMI	local-to-regional	3D-Eulerian	no
UiB	regional-to-continental	2D-Eulerian	yes
UiB model	global	2D-Eulerian	yes
UK photochemical model	regional-to-continental	2 layer Lagrangian	yes
UK-ADMS	local	Gaussian	no

A2 Global scale models

Model	2-D Oslo	Harwell model
Institution	University of Oslo	Harwell Laboratory
Application	Research/policy making	Research
Type of model	2-D Eulerian	2-D Eulerian
Domain	Global	Global
Simulation period	Monthly, Annual	Monthly, Annual
Horizontal resolution	Zonally averaged with 10^0 meridional resolution	24 equally spaced grid squares in sine (latitude) co-ordinates
Vertical resolution	0.5 km below 3.25 km and 1.0 km above up to 16.25 km	Varying between 10 and 30 grid squares up to 24 km
Transport scheme	Smolarkiewicz scheme	Gear's method/combined chemistry and transport
Dry deposition	Deposition velocities	Deposition velocities
Wet deposition	Heterogeneous scavenging. of soluble species by rain and sticking on aerosols	Scavenging ratios
Chemistry	Gas phase chemistry, 49 species, ca 100 reactions	56 chemical species, 91 thermal reactions, 27 photolytic processes, 7 reactions on NO_3 night-time chemistry
Emissions	NOx, SO_2, CO, NMHC from EPA, CH_4 calculated by the model	NOx, N_2O, H_2, CO, CH_4, NMHC from various sources
Meteorology	Monthly and/or seasonal means based on observations, GCM models or combination	Atmospheric circulation derived from a GCM, fields of the stream function and diffusion tensor for each month of the year - Analysed observations
Boundary conditions	Model derived climatological data	Zero
Reference	Isaksen and Hov (1987), Fuglestvedt et al. (1994)	Hough (1991)

A2 Continued

Model	UIB model	Cambridge model
Institution	University of Bergen	University of Cambridge
Application	Research	Research
Type of model	2-D Eulerian	2-D Eulerian
Domain	Global	Global
Simulation period	Monthly, Annual	Monthly, Annual
Horizontal resolution	75 equally spaced latitude points from pole to pole	Zonally averaged with 9.47^0 meridional resolution
Vertical resolution	33 equally spaced pressure levels from 1000 to 10 hPa	Half a pressure scale height (~3.5 km) up to 60 km
Transport scheme	Bott scheme	Zonal mean circulation and eddy transport
Dry deposition	Deposition velocities	Deposition velocities depending on the surface type
Wet deposition	Scavenging ratios	Scavenging ratios
Chemistry	44 chemical species, 126 chemical reactions	6 chemical families (Ox, HOx, NOx, ClOy, BrOy, CHxOy), ca 200 reactions
Emissions	NOx, CO and the most important HCs	CH_4, CO, NOx from various sources
Meteorology	GFDL general circulation/tracer model	Mean circulation based on forcing by latent and radiative heating and eddy transport processes
Boundary conditions	Observations	
Reference	Strand and Hov (1993; 1994)	Law and Pyle (1993a;b)

A2 Continued

Model	Liège model	Mainz model
Institution	University of Liège	Max Planck Institute for Chemistry
Application	Research	Research
Type of model	2-D Eulerian	2-D Eulerian
Domain	Global (from 85^0 S to 85^0 N)	Global
Simulation period	Monthly, Annual	Monthly, Annual
Horizontal resolution	Zonally averaged with 5^0 meridional resolution	Zonally averaged with 10^0 meridional resolution
Vertical resolution	1 km from 0 up to 85 km	11 layers up to 100 hPa (0.6 km up to 3.5 km and 2 km up to 24.2 km)
Transport scheme	Zonal mean circulation and eddy transport	Zonal mean circulation and eddy transport
Dry deposition	Deposition velocities depending on the surface type and the time of the year for some types	Deposition velocities
Wet deposition	Hough (1991) parameterisation	Scavenging ratios
Chemistry	ca 60 chemical species, 130 chemical/photochemical reactions	51 chemical species
Emissions	NOx, N_2O, H_2, CO, CH_4 from various sources	NOx, CO, CH_4, NMHC from various sources
Meteorology	Interactively calculated dynamical fields	Output from the GFDL General Circulation Transport model
Boundary conditions	Estimates, observations or zero	Observations, stratospheric model output, estimates
Reference	Hauglustaine et al. (1994)	Kanakidou et al. (1991)

A2 Continued

Model	EMEP/MSC-E	EMEP/MSC-W
Institution	Russian Hydrometeorological Centre	DNMI (The Norwegian Meteorological Institute, Oslo, Norway)
Application	Research	Research
Type of model	2-D Eulerian	3-D Eulerian
Domain	Northern Hemisphere (north of 20^0 N)	Northern Hemisphere (north of 20^0 N)
Simulation period	Monthly, Annual (1991- 1994)	Monthly, Annual (1988)
Horizontal resolution	150 km	150 km
Vertical resolution	1 layer up to 700 hPa	10 isentropic levels up to 100 hPa
Transport scheme	Pekar scheme	Smolarkiewicz scheme
Dry deposition	Dry deposition velocities depending on the surface type, temperature and precipitation amounts	Resistance analogy, dependence on stability, surface type, latitude and time of the year
Wet deposition	Scavenging ratios	Scavenging ratios, 3-D description of precipitation
Chemistry	Linear chemistry, 11 species, 12 chemical reactions based on ozone creation potential	DMS, SO_2, SO_4=, linear chemistry
Emissions	Anthropogenic SO_2, NOx, NH_3 from EMEP, EPA totals, distribution at MSC-E	Oceanic DMS, anthropogenic SO_2, SO_4^{2-}, NAPAP, EMEP and various sources
Meteorology	6-h prognoses from the Russian Hydrometeorological Centre	6-h ECMWF analyses
Boundary conditions	Model calculations or zero	Surface values or zero
Reference	Sofiev et al. (1995)	Tarrasón and Iversen (1995)

A2 Continued

Model	STOCHEM	MOGUNTIA
Institution	UK Met Office	Stockholm University (sulphur module), Max Planck Institute, University of Wageningen (photo-chemical modules)
Application	Research/policy making	Research/ policy making
Type of model	3-D Lagrangian	3-D Eulerian
Domain	Global	Global
Simulation period	Monthly, Annual (mid 1994 - mid 1995)	Monthly, Annual
Horizontal resolution	1.25^0 Long. x 0.833^0 Lat.	10^0 longitude x 10^0 latitude
Vertical resolution	9 vertical levels	10 layers between the surface and 100 hPa
Transport scheme	Lagrangian	Zonal mean circulation and eddy transport based on 3-D wind fields
Dry deposition	Deposition velocities depending on the surface type	Deposition velocities depending on the surface type
Wet deposition	Radioactive decay (first order removal)	Scavenging ratios, heterogeneous processes in clouds and on aerosol particles
Chemistry	50 species, 16 photolytic reactions, 90 chemical reactions	Variable number of components and reactions depending on the application
Emissions	NOx, H_2, CO, CH_4, NMHC, HCHO, CH_3CHO from the GEIA network	SOx, NOx, CO, CH_4, the most important NMHC from various sources
Meteorology	6-h analyses from the NWP model at the UK Met. Office	Climatological data
Boundary conditions	Reflection	
Reference	Collins et al. (1995)	Langner and Rodhe (1991), Lelieveld and van Dorland (1995), Kanakidou et al. (1992), Zimmermann (1988)

A2 Continued

Model	IMAGES	3-D Oslo
Institution	BISA (Belgian Institute for Space Aeronomy, Brussels) NCAR (National Centre for Atmospheric Research, Boulder, Colorado)	University of Oslo
Application	Research/policy making	Research/ policy making
Type of model	3-D Eulerian	3-D Eulerian
Domain	Global	Global
Simulation period	Monthly, Annual	Monthly, Annual
Horizontal resolution	5^0 longitude x 5^0 latitude	10^0 longitude x 8^0 latitude
Vertical resolution	25 sigma levels up to 50 hPa	9 levels along sigma co-ordinates from the surface to 10 hPa
Transport scheme	Semi-Lagrangian scheme	Method of conservation of second order moments, mass flux convection
Dry deposition	Deposition velocities depending on the surface type	Deposition velocities
Wet deposition	Scavenging coefficients	Heterogeneous scavenging of soluble species by rain and sticking on aerosols
Chemistry	41 chemical species, 125 chemical reactions and 26 photodissociations	49 components, 85 thermal reactions, 16 photolytic reactions
Emissions	NOx, CO, CH_4, NMHC from OECD, UN statistics and various sources	NOx, CO, CH_4, NMHC emission rates from various sources
Meteorology	Analysed climatological data from ECMWF	Output from the NASA-GISS GCM model
Boundary conditions	Observations	Climatological data
Reference	Müller and Brasseur (1995)	Berntsen and Isaksen (1994), Berntsen et al. (in press)

A2 Continued

Model	CTMK	Chemistry/Climate Model ECHAM
Institution	KNMI (Royal Netherlands Meteorological Institute)	Wageningen University
Application	Research/policy making	Research
Type of model	3-D Eulerian	3-D Eulerian
Domain	Global (regional zoom option)	Global
Simulation period	Monthly, Annual	Monthly, Annual
Horizontal resolution	Variable (10^0 long x 8^0 lat., 5^0 long x 4^0 lat. or 2.5^0 long. x 2.5^0 lat.)	5.6^0 x 5.6^0
Vertical resolution	15 sigma levels up to 5 hPa (new version with 18 eta levels in preparation)	19 layers in hybrid sigma-p- co-ordinate system up to 10 hPa
Transport scheme	Slopes scheme of Russel and Lerner or 2nd order moments scheme of Prather for advection Tiedtke convection scheme	Semi-lagrangian advection scheme, Tiedtke convection scheme
Dry deposition	Prescribed (land/sea) deposition velocities	Deposition velocities depending on turbulence, surface cover and vegetation activity
Wet deposition	Climatological precipitation data	ECHAM parameterisation schemes
Chemistry	13 components, 25 reactions (MOGUNTIA photoch. scheme)	Roelofs and Lelieveld parameterisation
Emissions	NOx from the AERONOX project (and optionally CO and CH_4)	NOx, CO, CH_4, SO_2 and DMS from various sources
Meteorology	6-h ECMWF analyses	GCM - ECHAM based on ECMWF analyses
Boundary conditions	O_3 at 50 hPa and NOx source in upper layer (optionally CO and CH_4 prescribed at surface)	Model calculations
Reference	Velders et al. (1994)	Roelofs and Lelieveld (1995)

A3 Regional/continental scale models

Model	DMU-model	EMEP/MSC-W/ Acid Rain
Institution	National Environmental Research Institute of Denmark (DMU)	DNMI
Application	Research, Danish Policy making	Decision making/UN-ECE, National Policy making in Norway, Research
Type of model	Eulerian 2-D	2-D Lagrangian
Domain	Europe	Europe
Simulation period	Annual	Annually (1985-1993)
Horizontal resolution	50 km	150 km and 50 km
Vertical resolution	1 layer	1 layer, PBL height
Transport scheme	Pseudo-spectral	2-D trajectories
Dry deposition	Deposition velocities applied to PBL concentrations	Resistance analogy approach with land use data
Wet deposition	Scavenging ratios	Scavenging coefficients
Chemistry	Explicit, 35 species, 70 reactions	Acid rain linear chemistry with 10 sulphur and nitrogen components
Emissions	EMEP 150 km for SOx, NOx and VOC. Asman inventory for NH_3	EMEP official submitted area sources (150km and 50km) SOx, NOx and NH_3. Also CORINAIR90 for 50km
Meteorology	European Centre for Medium Range Forecasting (ECMWF)	NWP-model of the Norwegian Met. Inst. with 50 km resolution
Boundary conditions	Background values	Global/Hemispheric models and observations
Reference	Zlatev (1995)	Barrett et al. (1995)

A3 Continued

Model	EMEP/MSC-W/ Photochemistry	EMEP/MSC-W/ sulphur
Institution	DNMI	DNMI
Application	Decision making/UN-ECE, National Policy making in Norway, Research	Research, Decision making/UN-ECE in the future
Type of model	2-D Lagrangian	3-D Eulerian
Domain	Europe	Europe
Simulation period	6 months periods(1985, 1989, 1990)	Monthly, Annual (1992)
Horizontal resolution	150 km	50 km
Vertical resolution	1 layer, PBL height	20 layers, terrain following sigma system
Transport scheme	2-D trajectories	Bott-scheme
Dry deposition	Deposition velocity, input modified as a function of stability and time of the year	Deposition velocity, input modified as a function of stability and time of the year
Wet deposition	Scavenging coefficients	Scavenging coefficients
Chemistry	Explicit gas-phase only, 66 species, 140 reactions	Two sulphur components, linear chemistry
Emissions	EMEP official submitted area sources (150km and 50km) SOx, NOx, VOC and CO. Also CORINAIR90 for 50km	EMEP official submitted area sources (50km) and CORINAIR90 for SOx
Meteorology	NWP-model of the Norwegian Met. Inst. with 50 km resolution	NWP-model of the Norwegian Met. Inst. with 50 km resolution
Boundary conditions	Global/Hemispheric models and observations	Hemispheric model
Reference	Simpson (1993)	Jakobsen et al. (1995)

A3 Continued

Model	EMEP/MSC-E Acid Deposition	HARM-model
Institution	Russian Hydrometeorological Centre	UK Met. Office, University of Edinburgh, University of Hull
Application	Research, National decision making in Russia	Research, UK National Policies
Type of model	Two layer Eulerian	Lagrangian
Domain	Europe and Asian part of Russia	Europe
Simulation period	Annual	Annual
Horizontal resolution	150 km	20 km
Vertical resolution	2 layers	1 layer (fixed)
Transport scheme	Quasi-Lagrangian, particle in cell	Trajectories
Dry deposition	Deposition velocity, input modified as a function of vertical stability	Deposition velocity applied to the PBL-concentrations
Wet deposition	Scavenging coefficients	Scavenging coefficients/Constant drizzle
Chemistry	Acid rain linear chemistry with 11 sulphur and nitrogen components including one reaction for ozone	9 components, coupled sulphur and nitrogen
Emissions	EMEP official submitted area sources (150km) SOx, NOx, NH_3 and VOC	150 km SOx, NOx and NH_3 from EMEP, 10 km from NETCEN
Meteorology	Analysis of meteorological observations	Climatological data
Boundary conditions	Hemispheric model	Climatological data or zero
Reference	MSC-E (1993)	Derwent et al. (1988), Metcalfe et al. (1995)

A3 Continued

Model	LOTOS	TREND-model
Institution	TNO	RIVM
Application	Decision making, Research	Policy making, Research
Type of model	3-D Eulerian	Climatological/Statistical
Domain	Europe	Europe
Simulation period	Episodic/Annual	Monthly, Annual
Horizontal resolution	0.5 degree. latitude 1.0 degree. longitude	Analytical solution not dependant on grid
Vertical resolution	3 layers	1 layer
Transport scheme	Shasta/Zalesak	2-D trajectories, Sector classification
Dry deposition	Resistance analogy approach with land-use data	Resistance analogy
Wet deposition	Scavenging coefficients	Scavenging ratios
Chemistry	CBM-IV gas-phase, 24 species, 70 reactions, wet chemistry for SO_2 and SO_4	Acid Rain chemistry for sulphur and nitrogen components
Emissions	Point and area sources for SOx, NOx, VOC, CO using CORINAIR and TNO inventory	EMEP and TNO inventory plus other sources
Meteorology	NWP-model of the Norwegian Met. Inst. with 150 km resolution	NWP-model of the Norwegian Met. Inst. with 150 km resolution and/or synoptic observations
Boundary conditions	Global model	Not Applicable
Reference	Builtjes (1992)	van Jaarsveld (1995)

A3 Continued

Model	EURAD	IVL-model
Institution	University of Cologne	Swedish Environmental Research Institute
Application	Research	Research and Swedish policy making
Type of model	3-D Eulerian	Lagrangian
Domain	Europe	Europe
Simulation period	Episodes up to weeks	Episodes
Horizontal resolution	Variable from 5 km up to 60 km	10 km
Vertical resolution	15 layers, terrain following sigma system	2 layers
Transport scheme	Smolarkiewicz or Bott	Trajectories
Dry deposition	Resistance analogy approach with land use data	Deposition velocities applied to PBL concentrations
Wet deposition	Explicit cloud chemical module	Not treated
Chemistry	RADM-2 gas and liquid phase chemistry, 120 reactions	Explicit, 1500 reactions
Emissions	Point and area sources for SOx, NOx, VOC, CO from EMEP, GENEMIS. Fixed VOC-split	Swedish emissions together with CORINAIR
Meteorology	MM4 forecasts	Typical meteorology derived for the model experiment
Boundary conditions	Observations	Observations
Reference	Hass (1991)	Andersson-Skold et al. (1992)

A3 Continued

Model	REM3	UIB-model
Institution	Freie Universität, Berlin	University of Bergen
Application	Research	Research
Type of model	3-D Eulerian	Eulerian
Domain	NW-Europe	Europe/Northern Hemisphere
Simulation period	Episodes (1 week)	Episodes
Horizontal resolution	0.25 degree. latitude 0.5 degree. longitude	150 km
Vertical resolution	3 layers	10 layers, sigma terrain following
Transport scheme	Yamartino Cubic splines	Bott scheme
Dry deposition	Resistance analogy approach with land-use data	Deposition velocity, input modified as a function of stability and time of the year.
Wet deposition	Scavenging coefficients	Scavenging ratios
Chemistry	CBM-IV and HAR-WELL condensed gas-phase only.	Explicit, 55 species,100 reactions
Emissions	Point and area sources for SOx, NOx, VOC, CO from TNO inventory	EMEP 150 km
Meteorology	Diagnostic interpolation of observation, energy budget method for PBL-variables	NWP-model of the Norwegian Met. Inst. with 150 km resolution
Boundary conditions	Observations	Climatological values/Observations
Reference		Flatøy et al. (1995)

A3 Continued

Model	UK Photochemical model
Institution	UK Met. Office, NET-CEN, University of Leeds
Application	Research, UK National Policies
Type of model	Lagrangian
Domain	Europe
Simulation period	Episodes
Horizontal resolution	10 km
Vertical resolution	2 layers
Transport scheme	Trajectories
Dry deposition	Resistance analogy approach with land-use data
Wet deposition	Not treated
Chemistry	Chemical scheme, 386 species and 684 reactions
Emissions	50km SOx, NOx and VOC from the OECD-map inventory, 10 km from NETCEN
Meteorology	Typical meteorology derived for the model experiments
Boundary conditions	Climatological data or zero
Reference	Derwent and Jenkin (1991)

A4 Local- to-regional scale models

	MEMO	TVM
Institution	Aristotle University Thessaloniki, University of Karlsruhe	CCR ISPRA
Application	Land-sea breezes, mountain/valley breezes, urban boundary layer	Sea-land breezes, Slope and valley winds
Type of model	3-D Eulerian	3-D
Domain	Local-to-regional	Local-to-regional
Simulation period	Episodes (1 day - 1 week)	Episodes (1 day - 1 week)
Typical temporal resolution	Case dependent (below 1 min.)	
Typical horizontal resolution	500 m - 10 km	20-100 km
Typical vertical resolution	Varying between 25 and 35 non-equidistant layers up to 10 km	2-5 km
Transport scheme	TVD scheme	Third order
Dry deposition	Big leaf	
Wet deposition		
Chemistry	inert	
Solution technique		
Emissions	NO_x, CO and VOC	
Meteorology	Prognostic, non-hydrostatic meso-scale model, radiation module included	non-hydrostatic Boussinesq and anelastic atmospheric model
Boundary conditions	Nesting, large scale models, Observations	Open boundaries
Reference	Moussiopoulos 1995, Kunz and Moussiopoulos 1995	Schayes et al. 1995, Thunis 1995

A4 Continued

	MERCURE	RAMS
Institution	EDF	
Application	Wangara Experiment, PYREX, APSIS	
Type of model	3-D	3-D
Domain	Local-to-regional	Local-to-regional
Simulation period	Episodes (1 day - 1 week)	Episodes (1 day - 1 week)
Typical temporal resolution		
Typical horizontal resolution		variable (> 100m), usually 10-30 km
Typical vertical resolution	1 m < Δx < 2 km	stretched grid
Transport scheme	Cubic semi Lagrangian scheme	2^{nd}, 4^{th} and 6^{th} order flux conservation advection
Dry deposition		
Wet deposition		
Chemistry		
Solution technique		Semi-stochastic particle transport and diffusion module
Emissions		
Meteorology	non-hydrostatic anelastic model	Observations
Boundary conditions		Observations
Reference	Elkhalfi and Carissimo 1993	

A4 Continued

	EPISODE	UDM-FMI
Institution	Norwegian Institute for Air Research (NILU), Norway	Finnish Meteorological Institute, Finland
Application	Urban air quality Decision making	Urban air quality
Type of model	3-D Eulerian and segmented plume	3-D
Domain	Local-to-regional	Local-to-regional
Simulation period	Episodes (1 day-1 year)	Episodes (1 hour-1 year)
Typical temporal resolution	1 hour	1 hour
Typical horizontal resolution	Variable, 100m-10,000 km	
Typical vertical resolution	Three layers, variable 10m-1,000 m	
Transport scheme	Bott positive definite 4th degree	
Dry deposition	Resistance model	
Wet deposition	Gas phase wet scavenging	
Chemistry	EMEP photochemistry (70 compounds)	
Solution technique	Operator splitting, segmented Gaussian plume	
Emissions	Industry, traffic, consumption	Industry, traffic
Meteorology	Hourly pre-processed fields	Hourly fields
Boundary conditions	Large scale model or geostrophic observation	
Reference	Grønskei et al., 1993	Härkönen et al., 1994

A4 Continued

	DISPERSION
Institution	Swedish Meteorological Institute (SMHI), Sweden
Application	Urban air quality
Type of model	Line and plume model
Domain	Local-to-regional
Simulation period	Episodes (1 hour-1 year)
Typical temporal resolution	1 hour
Typical horizontal resolution	
Typical vertical resolution	
Transport scheme	
Dry deposition	
Wet deposition	
Chemistry	
Solution technique	
Emissions	Industry, traffic
Meteorology	Hourly meteorological fields
Boundary conditions	
Reference	Omstedt, 1988

A4 Continued

	MARS	UAM/CALGRID
Institution	Aristotle University Thessaloniki, University of Karlsruhe	UBA Berlin
Application	Ozone formation, local air quality, Decision making	Ozone formation
Type of model	3-D Eulerian	3-D
Domain	Local-to-regional	Local-to-regional
Simulation period	Episodes (1 day - 1 week)	Episodes (1 day - 1 week)
Typical temporal resolution	Case dependent (below 1 min.)	
Typical horizontal resolution	500 m - 5 km	2 - 5 km
Typical vertical resolution	Varying between 15 and 20 non-equidistant layers up to 2 km	
Transport scheme	Smolarkiewicz	Smolarkiewicz, Galerkin FEM
Dry deposition	Big leaf	
Wet deposition		
Chemistry	KOREM/RADM2/EMEP	CBM4/SAPRC
Solution technique	Self adaptive predictor-corrector solution algorithm or Gauß-Seidel	QSSA
Emissions	NO_x, CO and VOC	
Meteorology	Non-hydrostatic mesoscale model MEMO	
Boundary conditions	Nesting, large scale models, Observations	
Reference	Moussiopoulos 1995, Moussiopoulos et al. 1995	Reynolds et al. 1979, Stern and Scherer 1984

A4 Continued

	CIT	EKMA-OZIPM4
Institution	CCR ISPRA	Environmental Protection Agency, USA
Application	Ozone formations in alpine regions in Switzerland	Decision making, Urban Air Quality Ozone formation
Type of model	3-D Eulerian	1-D
Domain	Local-to-regional	Local-to-regional
Simulation period	Episodes (1 day - 1 week)	1 day
Typical temporal resolution		1 hour
Typical horizontal resolution	variable, usually 5 km	homogeneous
Typical vertical resolution	Variable (20-2000m)	one vertical column of air
Transport scheme	Galerkin FEM	Lagrangian
Dry deposition	Three resistance model	
Wet deposition	Acid deposition	
Chemistry	LCC model	CBM4 and Dodge mechanisms
Solution technique	Operator splitting: Hybrid exponential, Finite elements	
Emissions		NO_X, NMCO
Meteorology	Observations	Hourly meteorological fields
Boundary conditions	Observations	
Reference	McRae et al. 1982, MacRae and Seinfeld 1983, Russell et al, 1988	EPA, Jeffries and Sexton (1987)

A4 Continued

	DRAIS	MATCH
Institution	KfK	Swedish Meteorological Institute (SMHI), Sweden
Application	Ozone formation	Urban air quality
Type of model	3-D	3-D Eulerian
Domain	Local-to-regional	Local-to-regional
Simulation period	Episodes (1 day - 1 week)	Episodes (1 hour-1 year)
Typical temporal resolution	Case dependent	1 hour
Typical horizontal resolution	Case dependent	5-10 km
Typical vertical resolution	Case dependent	
Transport scheme	FCT	
Dry deposition	Parameterised	
Wet deposition		
Chemistry	RADM/RADM2	
Solution technique	QSSA	Oxidised sulphur and nitrogen
Emissions		
Meteorology	KAMM model	Hourly meteorological fields
Boundary conditions	Observations, coupling to large scale model (EURAD)	
Reference	Tangermann-Dlugi and Fiedler 1983, Nester et al. 1987	Persson et al., 1994

A5 Local scale models

	IFDM	PLUIMPLUS
Institution	VITO Mol, Belgium	Staatsvitgeverij, ‘s Gravenhage, Nederland
Application	Stack emissions	Stack emissions
Type of model	Gaussian	Gaussian in vertical Uniform in 30°-sector horizontal
Domain	Local	Local
Simulation period	Yearly averages, hourly and daily percentiles	Yearly averages, empirical hourly and daily percentiles
Plume rise	Briggs	Briggs
Stability classification	Bultynk-Malet	KNMI-system, surface roughness
Meteorology	Hourly time series	Joint frequency matrix
Reference	R. Cosemans, J. Kretzschmar and G. Maes, 1992	Kleine Commissie Modellen, 1976

A5 Continued

	ISCST 2	AUSTAL 86
Institution	Environmental Protection Agency, USA	TA-LUFT, Germany
Application	Stack emissions	Stack emissions
Type of model	Gaussian	Gaussian
Domain	Local	Local
Simulation period	1 hour to yearly average, n largest concentrations time series	Yearly average, 98-percentiles
Plume rise	Briggs	Briggs
Stability classification	Pasquill Gifford classes, urban and rural modes	TA-LUFT classes (4)
Meteorology	Hourly time series	Joint frequency matrix
Reference	EPA, Trinity Consultants 1992	TA-LUFT, 1986

A5 Continued

	OML	UK-ADMS
Institution	National Environmental Research Institute, Denmark	CERC and UK Meteorological Office, United Kingdom
Application	Stack emissions	Stack emissions
Type of model	Gaussian	Gaussian Non-Gaussian in vertical in convective situations
Domain	Local	Local
Simulation period	Yearly averages, n largest hourly average, 99-percentiles	1 hour to yearly averages, percentiles
Plume rise	Briggs	Equations based on fluxes of mass and heat
Stability classification	Boundary layer scaling parameterisation	Boundary layer parameterisation
Meteorology	Hourly pre-processed time series	Hourly pre-processed time series
Reference	P. Løfstrøm and H.R. Olesen, 1988	Carruthers et al., 1992

A5 Continued

	HPDM	INPUFF
Institution	Sigma Research Corporation, USA	Environmental Protection Agency, USA
Application	Stack emissions	Stack emissions
Type of model	Gaussian	Gaussian, puff trajectory
Domain	Local	Local
Simulation period	1 hour to yearly averages, n largest hourly average, 99-percentiles	1 hour to yearly averages, percentiles
Plume rise	Briggs	Briggs
Stability classification	Boundary layer parameterisation	Pasquill-Gifford
Meteorology	Hourly pre-processed series or on site measurements	Hourly pre-processed time series
Reference	Hanna and Paine, 1989	Petersen and Lavdas, 1986

A5 Continued

	CTDMPLUS	SCALTURB
Institution	Environmental Protection Agency, USA	Norwegian Institute for Air Research (NILU), Norway
Application	Stack emissions	Stack emissions
Type of model	Gaussian	Dispersion regions, Semi-Gaussian
Domain	Local	Local
Simulation period	1 hour to yearly average,	1 hour to yearly averages, percentiles
Plume rise	Briggs	Briggs
Stability classification	Boundary Layer scaling parameterisation	Boundary layer parameterisation
Meteorology	Hourly pre-processed time series	Hourly pre-processed time series
Reference	EPA, Perry et al. 1989	Gryning, Holtslag, Irwin and Sivertsen, 1987

A5 Continued

	CAR	CARSMOG
Institution	RIVM, TNO (The Netherlands)	RIVM, TNO (The Netherlands)
Application	road pollution	real time modelling of road pollution
Type of model	semi-empirical relation based on wind tunnel experiments and field campaigns	semi-empirical relations (see CAR) combined with actual measurements
Domain	various street types (open lanes <==> street canyons)	various street types (open lanes <==> street canyons)
Simulation period	yearly averaged; 98 percentiles	hourly averaged
Chemistry	NO_2 according to photostationary equilibrium	NO_2 according to photostationary equilibrium
Stability classification		
Meteorology	yearly averaged	actual hourly values
Reference	Eerens et al, 1993	den Tonkelaar W.A.M. 1995

A5 Continued

	CAR-FMI	ROADAIR
Institution	Finland Meteorological Institute, Finland	Norwegian Institute for Air Research (NILU), Norway
Application	Road pollution	Road pollution
Type of model	Finite line source, partly analytical Gaussian	Finite line source, Gaussian Emission model based on traffic composition and driving conditions
Domain	Local	Local
Simulation period	1 hour	1 hour
Stability classification	Boundary layer scaling	Pasquill-Gifford stability classes
Chemistry	Discrete parcel method NO_x, O_2, O_3	Conversion of NO to NO_2 by O_3.
Meteorology	Hourly time series	Worst case 1 hour
Reference	Härkönen et al., 1994	Larssen and Torp, 1993

A5 Continued

	CONTILINK
Institution	Norwegian institute for Air Research (NILU), Norway
Application	Road pollution
Type of model	Finite line source Gaussian, semi-stationary
Domain	Local
Simulation period	Hourly concentrations
Plume rise	-
Stability classification	Pasquill Gifford
Meteorology	Wind direction, wind speed, stability
Reference	Larssen et al., 1993