NILU
OPPDRAGSRAPPORT NR 5/75
REFERENCE: 002274
DATE: MARCH 1975

CURRENT AND FUTURE NEEDS FOR AIR QUALITY SIMULATION MODELS

BY

K E GRØNSKEI

THE PAPER WAS PREPARED AS A REPORT ON THE WORK CARRIED OUT UNDER A NATO/CCM FELLOWSHIP STUDY, WHILE THE AUTHOR WAS VISITING THE METEOROLOGY LABORATORY, U.S. ENVIRONMENTAL PROTECTION AGENCY.

NORWEGIAN INSTITUTE FOR AIR RESEARCH
P O BOX 115, 2007 KJELLER
NORWAY

ABSTRACT

The current and future needs for air quality models are clarified by a literature study of their current use and by studying the requirements for information by the law and the administrative system.

The description of the current uses and their requirements for information are given by referring to the required temporal and spatial resolution of the results, and the requirements for source specification. Six different areas of applications have been considered.

1. Environmental Impact Studies
2. Development of Control Strategies
3. Land Use and Transportation Planning
4. Comprehensive Planning
5. Air Pollution Episodes
6. Research on Atmospheric Processes

Three different areas of application that require models on different spatial scales are selected and the development of air quality models are considered in more detail for:

1. Single Stack
2. Street Canyon
3. Multiple Source - Urban Area

The magnitudes of the different terms in the mass-balance equation for the pollution component are compared for two types of meteorological situation:

1. High, steady and homogeneous wind and turbulence conditions.

2. Low horizontal advection velocity and a stable temperature stratification suppressing vertical turbulent transport.

The validation of air quality models is considered and systematic use of the models response to variations in the input parameters is suggested. The parameters that have importance for the specific application should be given attention.

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I INTRODUCTION

1 General

Air quality simulation models are used to describe the cause-effect relationship between emission and ambient air concentration of pollutants. If this relationship can be described in a quantitative way, it provides a powerful tool for making decisions on air pollution problems.

There exist many interrelated aspects of an air pollution problem, e.g. economic, social, technical, environmental, political, local, national and global. Often competing interests have to be considered, and this makes a quantification of the problem particularly important.

The effective solution of air pollution problems requires laws and an administrative system to enforce them. Depending on the specific decision problem, the laws and the administrative system require different kinds of information on the pollution problem. A study of these requirements is useful in the development and the evaluation of air pollution models. However, the state-of-the-art of model development may also indicate modification in the requirements.

2 Systematic Approach

To illustrate the flow of information in a systematic approach towards the improvement of air quality, Figure 1 is presented. The actual events in the atmosphere[1] are shown in the first line in the diagram. The next line indicates the quantification of these different events by measurements and/or registration.

The data on emissions dispersion and ambient air concentrations are synthesized in an air quality model. When a model has been developed it can be used to infer information on one type of data given the other two. For example, if the emissions and the meteorological conditions are given, then the model can provide information on the ambient air concentration. Ambient air concentration and data on the effects are used to provide air quality criteria that constitute the basis for air quality standards.

In the assessment of the total impact of air quality on society, the air quality information has to be given a form that facilitates the consideration of air quality versus priorities and goals in the society. These considerations constitute the basis for decisions on activities producing air pollution.

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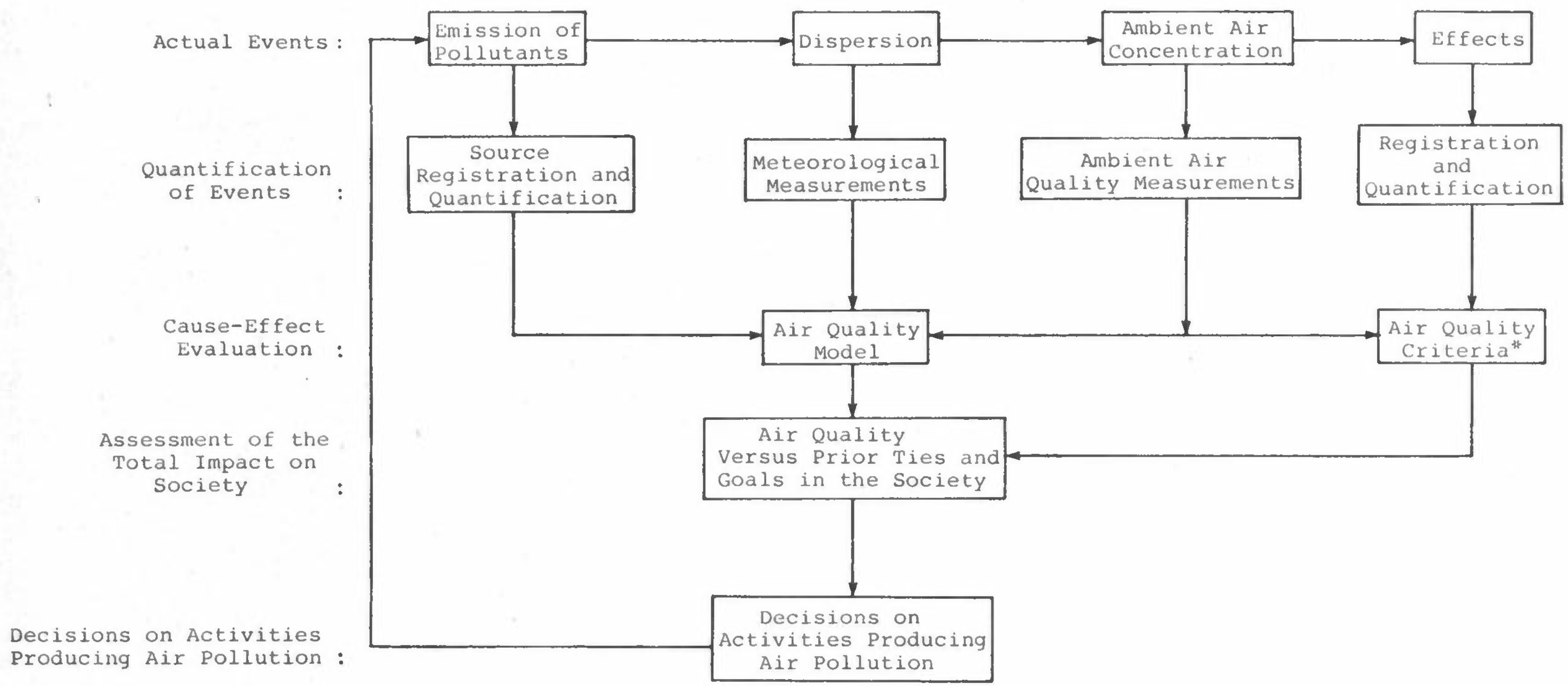
[1] Showing how emission of pollutants cause adverse effects in the surroundings.



*Air quality criteria are scientifically sound statements about effects that have been observed or inferred to have been produced by various exposures to specific pollutants (35).

Figure 1: Flow of Information in a Systematic Approach Towards the Improvement of Air Quality.

3 History

The systematic approach and basis for decisionmaking on air quality has been known for a long time, and was applied to the air pollution situation in some English towns more than one hundred years ago (1). In this study Dr. Angus Smith used a boxmodel to evaluate and interpret his measurements. Dr. Angus Smith complained about the basis for decisions on air quality in 1859:

> "Whilst laws have been made with relation to the impurity of the atmosphere arising from many causes, neither those who made the laws nor those who administer them have ever taken pains to find out what it really was against which they combated, and what crime that was which they have been so anxious to punish.
>
> The same carelessness has been observable on the side of those toward whom the law acted and decisions have in reality been in the hands of those whose fancy or caprice have led them to take advantage of legal enactment; whilst great offenders have frequently escaped because no one has known the points on which they could be most easily assailed."

Much of the theoretical basis for the present air quality models was also developed in England. A presentation of this background from a practical point of view is given by Sutton (3) and Pasquill (4). Building of new factories, the possibility of chemical warfare and the development of peaceful use of atomic energy have all focused attention on the adverse effects of air pollution. A collection of information that is used in the evaluation of specific problems, was edited by Slade (5), and a widely used "Workbook of Atmospheric Dispersion Estimates" has been produced by Turner (6).

A larger concern about environmental problems has been observed after 1960 accompanied by a rapid development of air pollution control legislation (7).

The formulation of the law often represents a compromise between the public health and welfare on the one hand, and technical, economic and political factors on the other. A quantification of the problem is often required so that air pollution considerations will not serve special interests in the society. Several surveys of the development of air pollution models in this period have been presented (19, 20, 21).

Fortak has clearly pointed out the important need for air quality simulation models in the decision process (22). The large variety of the physical processes that influence the dispersion are recognized, and described and classified according to spatial and temporal scales. Fortak (23) has later specified in more detail the importance of different atmospheric processes for urban models for air pollution abatement.

Even if most air pollution problems are local, a tendency is observed towards making the air pollution legislation uniform over larger spatial areas. This minimizes competitive problems in trade and industry due to a non-uniform formulation of environmental constraints. Besides, the transport and dispersion of pollutants does not recognize national and jurisdictional boundaries. When an air pollution problem extends beyond jurisdictional boundaries, special problems occur; since adverse effects may occur in regions outside those where direct control can be enforced. Several nations have developed new or revised Federal legislation on these problems, e.g. U.S.A. in 1970, Canada in 1971, Japan in 1971, The Federal Republic of Germany in 1974. The transfer of responsibility for air quality from a local level to a Federal level, is also an indication of the increasing spatial scales of air quality problems.

4 International Cooperation

As a result of the increasing spatial scales that are of concern international cooperation and agreements are sometimes necessary to solve air pollution problems. As an example, the agreement on the intermittent source control in the Detroit/Windsor area may be mentioned. Detroit is located in Michigan, USA and Windsor is located in Canada. However, both of them are within the same airshed area.

Several international organizations are now concerned with environmental problems that include air pollution. Regarding air quality models, work is going on under the auspices of NATO/CCMS, OECD and in regional groups of the nations.

a. NATO/CCMS:

Under the auspices of NATO/CCMS, air quality assessment studies have been carried out in Ankara, St. Louis and Frankfurt. Similar studies in Oslo, Rotterdam, Milan and Turin have been able to benefit from this initiative (8). Experience on the air quality model studies, that are part of the assessment studies, has been exchanged within the CCMS air pollution modeling panel, and proceedings have been printed for the several meetings. (9, 10, 11, 12). These reports include discussions on the research projects in the participating countries, and also summaries of discussions on specified topics. A part of the meeting at Risø, Denmark, in 1974 was designed to bring together air quality managers and model developers. It is primarily local and regional air pollution problems that have been considered within NATO/CCMS, and emphasis has been given to the development and evaluation of air quality models.

b. OECD

The environmental committee in OECD has supported the development and use of air quality models by:

(1) Sponsoring air quality monitoring and the development of air quality models for long range transport in Europe.

(2) Organizing committees that work with specified problems with relevance to air quality modeling and their application.

Professor James R. Mahoney has prepared an OECD report on the state-of-the-art and application of air quality models (13).

From 1973 and 1974 two groups of rapporteurs have collected information and prepared draft reports on:

(1) Use of techniques in relation to air pollution control and land use planning.

(2) Use of surveillance and control techniques for air pollution alert systems.

Within OECD emphasis is given to the economic and social consequences of the adverse effects and on the development of information that is essential to solve the problems most effectively. In this connection OECD is considering the long range transport of air pollution in Europe. (This involves transport distances of 1000 km.)

c. Regional Groups

Several other groups of countries are also cooperating to develop air quality models. One of these is Scandinavian Council for Applied Research (NORDFORSK), where a group is established to coordinate model development on an urban and regional scale in Scandinavia. Some interest has been focused on the land-sea breeze effect on the regional dispersion of air pollution, since several industrialized areas are located along the coast.

d. World Meteorological Organization

The global aspect of air pollution is considered by the specialized United Nations agency World Meteorological Organization in a worldwide monitoring program.

Scientific evidence has been presented that air pollution produced by human activity influences the atmospheric composition on a global scale, and an evaluation of the climatic effects is urgently needed (14). Models with forecasting capability are required since a modification of the atmospheric circulation condition may have disastrous effects on the living conditions in large areas.

5 Objective

It is seen that air quality models are needed in a large variety of problems with different temporal and spatial scales. The purpose of this report is to describe the current use of air quality simulation models and then identify some current and future needs. The description is given by referring to the required temporal and spatial resolution. The requirements for source specification and for accuarcy of results are specified where appropriate. Three problems with different spatial scales are selected as examples of how this difference in resolution may influence the model structure and in this way:

a. Provide basic information on performance standards for air quality models.

b. Facilitate the selection and evaluation of an air quality model for a specified problem in a given area.

c. Facilitate the combination of results from modeling of different atmospheric conditions with respect to atmospheric transport, diffusion and reactivity in more comprehensive models.

Considering international cooperation in developing air quality models, only a few countries are able to participate with large resources. However, all countries should participate in order to benefit from existing knowledge. The contributions should be in modeling of conditions that are of significant importance for each countries own pollution problems. Limited efforts, however, are given enhanced significance when presented in a more general framework.

6 Methodology

Much experience has been gained since Angus Smith wrote his article in 1859. However, discussion is still going on as to how to deal effectively with air pollution problems (2). One pollutant control strategy is called "the best practicable means", where all emission of pollutants in the atmosphere is regarded as bad and accordingly controlled to a degree decided by the actual technical possibilities. Another approach may be called the "air quality approach" where it is the ambient air quality and the adverse effects that decide to what extent an air pollution source shall be controlled. A combination of the two approaches is practical policy.

Different countries give different emphasis to these two attitudes. For example, in England more emphasis is given to "the best practicable means" approach while in the USA more emphasis is given to "the air quality standards approach". By definition it is only the air quality approach that requires use of air quality models. Since the USA is a nation where large emphasis is given to the air quality approach, the latter is well illustrated by considering the experience of the Environmental Protection Agency, USA.

The present paper includes a literature study of the current use of air quality simulation models, and by studying the requirements specified by the legislative and administrative system, current and future needs for air quality simulation models will be specified. The specific applications may be classified into the following main classes:

a. Environmental impact studies. The models are used to forecast the impact of air pollution from new sources.

b. Air quality simulation models used to develop control strategies. The requirements here are to differentiate with respect to air quality between different air pollution control strategies.

c. Use of models in land use planning. The requirements here are to present quantified information adaptable to specification of air quality constraints on expected emissions in the land use planning process.

d. Models used as submodels in larger systems considerations. The models have to be adapted to handle emission data provided by the system and to provide air quality data that can be interpreted by the damage function included in the system.

e. Models as a basis for planning emergency actions in air pollution episodes. One of the requirements is to provide a fast answer on source control in order to avoid or lessen an air pollution episode.

f. Models used for research purposes. The requirements here are totally dependent on the purpose of the research.

The author wants further to draw attention to a report prepared for the Committee on Public Works, United States Senate by the Coordinating Committee on Air Quality Studies, National Academy of Sciences and National Academy of Engineering, on the relationship of emissions to ambient air quality. The report provides technical background information on the quantification of atmospheric events as they are shown in Figure 1, and a description is given of the air quality models used for predicting air quality and in application of modeling to air quality strategy. The report describes the models in the current use and their ability to give the information that is required from them (83).

II CURRENT USE IN ENVIRONMENTAL IMPACT STATEMENTS

An air quality impact statement is needed where a new construction emitting air pollution is going to be initiated or where adverse effects on larger areas are going to be considered.

1 Prediction Of Air Quality Where New Sources Are Going To Be Established

In this case the emissions are normally specified and a forecast of future adverse effects is needed. This problem is approached by calculating the ambient air concentration and comparing it with the air quality standards. Air quality standards represent guidelines on tolerable air quality given by political authorities. These standards may be formulated for different averaging times, depending on the effects of the different chemical compounds. The specific values refer to different adverse effects that are regarded as intolerable. In Table 1 the standards used in USA are given:

Pollutant	Type of Standard	Averaging time	Frequency Parameter	Concentration µg/m³	ppm
Carbon monoxide	Primary and secondary	1 hr	Annual maximum[a]	40.000	35
		8 hr	Annual maximum	10.000	9
Hydrocarbons (nonmethane)	Primary and secondary	3 hr (6 to 9 a.m.)	Annual maximum	160[b]	0.24[b]
Nitrogen dioxide	Primary and secondary	1 yr	Arithmetic mean	100	0.05
Photochemical oxidants	Primary and secondary	1 hr	Annual maximum	160	0.08
Particulate matter	Primary	24 hr	Annual maximum	260	-
		1 yr	Annual geometric mean	75	-
	Secondary	24 hr	Annual maximum	150	-
		1 hr	Annual geometric mean	60[c]	-
Sulfur dioxide	Primary	24 hr	Annual maximum	365	0.14
		1 yr	Arithmetic mean	80	0.03
	Secondary	3 hr	Annual maximum	1.300	0.5
		24 hr	Annual maximum	260[d]	0.1[d]
		1 yr	Arithmetic mean	60	0.02

[a] Not to be exceeded more than once per year.

[b] As a guide in devising implementation plans for achieving oxidant standards.

[c] As a guide to be used in assessing implementation plans for achieving the annual maximum 24-hour standard.

[d] As a guide to be used in assessing implementation plans for achieving the annual arithmetic mean standard.

Table 1: Ambient air quality standards.

The standards may also be formulated by referring to the allowable frequency of violations for different averaging times, as is done in Japan and Sweden (15, 16). More complex formulations of the standards may give a better representation of the damage function for the different pollutants. Most standards refer to anticipated adverse health effects. However, an impact statement may also be formulated in economic terms (17).

In the USA the mechanism presently employed for the integration of environmental assessments into the planning process is the Environmental Impact Statement, which is required under Section 102 of the National Environmental Policy Act (NEPA) of 1969. This act requires assessment of environmental effects of proposed highways, airports and other development actions involving Federal funds. According to the Clean Air Act Amendment of 1970 the Administrator of EPA shall review and comment in writing on the environmental impact statements. The Clean Air Act Amendment of 1970 recognizes also the right of persons to bring a citizen's suit

a) against any person (including governmental agencies) violating emission standards or limitation.

b) against the Administrator where there is alleged a failure of the Administrator on any act or duty under this act.

Guidelines for preparation of impact statements are now prepared by EPA. Current use of models to provide information for impact statements as a result of new activities include:

a) Stationary sources (chimneys)
b) Highways
c) Shopping centers, parking lots and airports

a. Stationary Sources

The ambient air concentration in the neighbourhood of a single stack is calculated by using the Gaussian distribution of concentration in the individual plumes. The use of the model is developed and described by Turner (6). This model is now made available in a computerized form on UNAMAP. (Users Network for Applied Modeling of Air Pollution).

When ambient air quality standards are defined, the air quality model is required to justify that a new source will not cause ambient air quality standards to be violated. Three programs, based on the Gaussian point source model, have been connected to the UNAMAP system to provide this information (18).

(1) PTMAX : Performs analysis of the maximum short-term concentration from a point source as a function of stability and wind speed.

Input : Ambient air temperature and characteristics of the source.

Output: Effective height of emission, maximum ground level concentration and distance of maximum concentration for each condition of stability and wind speed.

By comparing this result with the frequency distribution of stability and wind speed classes on a particular site, an impact statement with respect to violation or no violation of short-term ambient air quality standards can be given.

The dispersion parameters given in (6) are applied to estimate the maximum 1-hour concentrations. The model is based upon stationary emission and dispersion of inert gas or aerosol (less then 20 microns diameter), in a homogeneous wind and turbulence field.

The model is applicable where single sources occur in relatively uniform terrain. However, the model needs further justification for distances beyond about 1 km. At this distance the cross-section of the plume has a spatial scale of 15-150 m, depending on the atmospheric transport and diffusion, and this scale represents the effective stack height for which the maximum ground level concentration can be predicted with much confidence according to ref. (6).

(2) PTMTP: This program estimates, for a number of arbitrarily located receptor points at or above ground level, the concentration from a number of point sources. Hourly meteorological data are used.

(3) PTDIS: The program is based on the same basic dispersion model and calculates short-term concentrations directly downwind of a point source at distances specified by the user. An option allows the calculations of isopleth half-widths for specific concentrations at each downwind distance, and provides the opportunity to develop impact statements based on a broader aspect of the damage function, where the concentration in the total area is needed.

The programs are all used to calculate short-term concentrations (1-hr average values). To provide information on longer term averages (3-hr and 24-hr mean values), long time series of 1-hr values are used to calculate non-overlapping average values.

To carry out these calculations, hourly mean values of wind speed and direction, and the horizontal and vertical standard deviations for the Gaussian plume (and their dependence on distance from the source) are needed. Several techniques used to specify these values are given by Slade (5).

As an example of an impact statement for a large stationary source, the analysis for the Edge Moor Thermal Power Plant Unit No. 5 is used (24). The data evaluation that is necessary to develop an impact statement is summarized as follows:

Weather and climatic data from nearby airports are used, together with data on emissions, to make estimates of future concentrations using a Gaussian point source model. The following elements of the basic model are considered :

(a) Effective stack height
(b) Effect of terrain on ground level concentrations
(c) Atmospheric reaction effects
(d) Analysis of background air quality

The ground-level concentrations in the surroundings are considered for annual averages, maximum 3-hour averages and maximum 24-hr averages.

To estimate short-term maximum concentration, Briggs (25) suggests dividing the development of the plume into four phases :

(a) Momentum phase
(b) Building phase
(c) Buoyancy phase
(d) Diffusion phase

Each of the phases has to be considered and different models have to be applied to estimate the effetive plume rise depending on the emission conditions.

Tennessee Valley Authority's experience (26) indicates that as unit sizes are increased and taller stacks are constructed, the plume dispersion model associated with maximum surface concentrations should be changed. The following plume dispersion models were found useful depending on the atmospheric turbulence conditions and the vertical temperature stratification :

(a) Coning
(b) Fanning and Inversion Breakup
(c) Looping
(d) Trapping

Meteorological competence is needed to decide which of the models is needed to estimate maximum concentrations, and their frequency of occurrence, in the surroundings of a single point source. No general rules are formulated in detail.

b. Highways

Impact statements are often required for new highways, and several dispersion models have been developed to predict air quality in relation to motor vehicle transportation (27). In the conclusion of the study it is recommended that further validation, and comparative studies with respect to the models applicabilities, are needed. Until these results are available, it is recommended that models based on a Gaussian diffusion be utilized.

One of these Gaussian models is the EPA model (HIWAY) which is part of the UNAMAP system. This program computes the short-term (hourly) concentration of non-reactive pollutants downwind of roadways. It is applicable when uniform wind conditions and level terrain occur, and is best suited for at-grade highways, but also can be applied to depressed highways (cut sections).

When complex highway configuration are concerned, more complex models may be needed to predict expected air quality. Numerical advection diffusion models are suitable for these purposes. A finite difference scheme suppressing artificial numerical diffusion has been developed by Egan and Mahoney (28). This model is used by Environmental Research and Technology to develop impact statements around complex road segments. The models work fairly well when relatively inert pollutants are concerned, e.g. carbon monoxide, sulphur dioxide and particulates.

For the photochemically reactive pollutants, regional dispersion models that include chemical reaction equations, as well as diffusion equations, are the most applicable. At the present time there are no generally accepted photochemical dispersion models capable of calculating the distribution of the chemically reactive pollutants like hydrocarbons nitrogen oxides and photochemical oxidants. As is discussed by F. Worley (9) :

> "Several problems remain and significant progress in the development of a general photochemical smog model is not to be expected until they are at least partially solved. The critical areas involve prediction of the meteorological variables, distribution functions for emissions, and formulation of chemical reaction mechanisms for multiple hydrocarbon systems."

For evaluation of the impact of a relatively inert pollutant component like carbon monoxide on a regional scale, a model developed by W. Johnson, Stanford Research Institute (29) is sometimes used. This model is included in the UNAMAP system, and computes hourly averages of carbon monoxide concentration for any urban location. The program requires an extensive traffic inventory for the city of interest. The computer program can be operated in any one of the following modes :

(a) Synoptic - real time mode that generates hourly concentrations as a function of time.

(b) Climatological - statistical prediction of frequency of occurrence of cocentrations at various locations in a geographical grid, thus providing detailed horizontal patterns.

As a result of the U.S. legislation on impact statements and the possibilities of citizens' suit, the application of dispersion models to predict future air quality has been considered in several court cases. An example of court consideration on this topic is presented by E. M. Darling et al (30).

Concerning air pollution dispersion models, the following excerpt from the court decision can be presented :

> "The state of the art in the prediction of concentrations of carbon monoxide CO is now at the theoretical stage. There seems to be general acceptance of the "Gaussian plume" theory and the theoretical formulae developed by the General Electric Study of Sept. 1971. There are, however, many variations of the formulae, and no satisfactory evidence was presented to the court that any of them have been empirically validated. The court finds that the air quality calculations contained in the supplemented final Environmental Impact Statement was a reasonably sufficient attempt to deal with the problem, considering the present state of the art."

c. Shopping Centers, Parking Lots and Airports

It is not the establishments themselves, but rather the activity that is connected to them that causes the pollution problems.

To develop impact statements for airports, a methodology is described by Norco et al, Argonne National Laboratory (31). The methodology is developed to integrate the air pollution impact of an airport and its associated ground support activities. Procedures for estimating airport-related air pollutant emissions are defined and the latter can be transformed into air quality estimates through the use of "rollback" analysis or atmospheric dispersion models. The "rollback technique is described and discussed by Morris and Slater (see chapter 12 in ref. 12). An example of the dispersion models referred to in this connection is the Federal Aviation Administration/Argonne Airport Air Pollution Model. One part of the model generates an emission inventory, the second part computes air quality using a modified steady-state Gaussian plume algorithim. The dispersion model uses 1-hr averaging time of meteorological measurements, and makes use of time- and distance-dependent dispersion parameters.

2 Interpolation between Measurements

Impact studies of a basic character for developing air quality standards, include studies of the relation between ambient air pollution concentration and adverse effects like damage to health, vegetation or material, and interpolation between measurements in an air quality monitoring system is often needed. The net of measuring stations is always sparce for estimates of the total pollution impact on a region. These studies may consider different spatial scales, and in that way different models may be required. An example is presented by Benedict, Miller and Smith (17) on the assessment of economic impact of air pollutants on vegetation in the United States.

Studies by Holzworth of air pollution potential (concentration/emission) throughout the country (47), together with a simple rollback model, are used to quantify the pollution concentration throughout the country.

In health studies carried out by Environmental Protection Agency (see chapter 2.1 of ref. (74)) the AQDM model (this is a Gaussian model (40), calculating annual means values), is used to interpolate ambient air concentration between stations in a sparce network. The model results identify the location of gradients in ambient air concentration. This information is used in the dosage estimation for people moving around in the area.

In impact studies for vegetation short-term concentrations that occur in episodes are important in order to specify the damage-function. Episodes with a time scale of 3 hours to 3 days are important.

In impact studies for materials the annual average concentration is frequently important for the damage function.

For health effects both short- and long-term average concentrations are important (see Chapters 9, 10, and 11 in (35)).

In the impact studies for vegetation and materials the following pollutants are considered : SO_2, particulates and oxidants. In the health studies several other compounds are considered, like nitrogen oxide, sulphate and carbon monoxide. In some areas fluorides may be responsible for large damage on vegetation. A large variety of spatial scales may also be involved in these kinds of impact studies.

a. Impact Studies on an Urban Scale

Many countries are engaged in developing models on this spatial scale and several symposiums are arranged each year to present and discuss recent results. The urban models treat spatial scales up to 40 km, and for non-reactive pollutants the principle of superposition of Gaussian plumes is used to construct multiple-source urban-diffusion models.

Such models are based on the assumption of quasi-stationary conditions and homogeneous, wind and turbulence conditions.

These models are highly source-oriented. However, in impact studies on a regional scale the specification of sources is not of vital importance unless the results are to be used to evaluate or develop control strategies.

Several simplified procedures with respect to source resolution have been suggested. Gifford and Hanna (11) have pointed out that models of dispersion from area sources exhibit less sensitivity to horizontal diffusivity and air-trajectory than point-source models. They use this fact to develop a simplified model obeying the steady-state diffusion equation for a horizontally homogeneous wind and turbulence field. The wind and diffusion coefficients are vertically approximated by a power function of the height.

If source specification (point sources) is not required it is possible to apply finite-difference resolution of the sources (area sources) and in that way to include the possibility of modeling the effects of non-homogeneous wind and turbulence conditions.

Impact studies on larger spatial scales are also carried out for research purposes at the present time, and air quality models are applied.

b. A Quantification of the Impact of Air Pollution on an Urban/Regional Scale

In Canada it has been suggested that complete evaluation of the impact on air quality of an urban center must consider effects over distances as great as 200 km and that a three-dimensional air quality model will be required (see Chapter 21 of ref, (12)).

A quantification of the rise of an urban scale plume is of interest in relation to observations from some places like Oslo (see appendix D to ref. (8)).

c. A Quantification of the Impact due to Long-Range Transport

Long-range transport studies are in progress in Europe and the U.S.A. (32, 33). Trajectory statistics are applied to develop air quality models explaining the connection between emissions and ambient air concentrations. A quantification of the impact far away from the source region is needed and the statistics of the large-scale weather elements (cyclones, etc.) becomes important. A typical time scale for the transport is 1-3 days, and chemical reactions and depletion processes become important.

The spatial resolution of pollutant clouds after long-range transport is poorly understood. Measurements presented in ref. (33) indicate that high levels of 24-hr mean concentration have a spatial-scale of several hundred kilometers, due to the vast industrialized areas in Europe.

d. A Quantification of the Impact of Air Pollution on a Global Scale

In recent years a discussion has occurred concerning the impact of high altitude pollution, caused by supersonic aircraft in the lower stratosphere (34).

The models used here recognize the chemical reaction terms. Spatially, they use zonal-average concentrations with a two-dimensional resolution of 1 km vertically, and 5-degree latitude horizontally, (see Chapter 6 by Hesstvedt in ref. (34)). A time scale of 12 hrs becomes important due to the daily variation of solar radiation.

3 Summary

When the important scales for model development are going to be specified from the requirement for information in different application areas, three types of spatial scales have to be considered.

The important time-scales of the effects have been defined in the air quality standards or by studies of effects. When a prediction of air pollution produced by a new source is required, the concentration in the maximum zone is compared with air quality standards. Impact studies carried out to clarify the connection between the ambient air concentration and effects are often based on measurements of air quality. The network of sampling stations need to be supplemented by model calculations in order to specify the spatial representativity of the sampling measurements.

The types of sources, the atmospheric transport and diffusion phases, and their spatial scales are given in Table 1, together with an indication of the present models.

The time-scales that are important for the modeling of different dispersion and chemical reaction phases are dependent on the meteorological conditions. They will be evaluated in more detail later, when a few examples are chosen for a closer examination. A column marked "Chemical Reactions" might also be included in the Table. The reactions are characterized by reaction coefficients. Their importance is determined by the time-scale determined by the type and extension of source and the dispersion phase. The numerical value of the reciprocal of this time scale has to be compared with the appropriate reaction coefficients. Some success has been achieved modeling photochemical reactions in urban areas. However, very little is known about the significant chemical reactions in the actual atmosphere. These become extremely complex when aerosols and water droplets have to be considered in the system.

Type of Source	Dispersion Phase	Spatial Scale	Model Identification
Single Stack	1. Momentum Phase 2. Building Phase 3. Buoyancy Phase 4. Dispersion Phase a. looping b. coning c. fanning	Stack Diameter Building Height L = 10-100 m Transport: 1 km	Plume Rise Formulae (Briggs) Distance Dependent σ_y and σ_z (Turner)
Highway	1. Car Made Turbulence 2. Building Phase 3. Dispersion Phase	Car Dimension Building Height L = 20-100 m Transport: 1 km	Distance Dependent σ_y and σ_z (Turner)
Urban Scale Multiple Sources Reactions in the Atmosphere Producing Oxidants		10-40 km Vertical: 50-100 m	Superposition Principle - Single Stack Complex Photo-Chemical Models
Regional Scale	Mesoscale Processes Long Range Transport	10-1000 km Vertical: 1 km Transport: 1000-5000 km	Knowledge About Weather Systems on a Cyclonic Scale
Global Scale	Atmospheric Structure on a Global Scale	Zonal Average Vertical: 1 km Time scale: 12 hr	Photochemical Models in the High Atmosphere

Table 2: Air Quality Models Developed for Impact Studies.

In order to clarify the present and future needs for air quality models Bruce Turner (Chief, Environmental Applications Branch) developed a questionnaire for the Regional Meteorologists in the US Environmental Protection Agency. The Regional Meteorologists were asked to specify the priority of their present and future needs for air quality models, among the following types :

1) Single source - complicated terrain (Region 3, 8, 9, 10).

2) Complex sources (shopping centers-airports), (Region 5, 9).

3) Stagnation - episodes models (Region 5, 9).

4) Urban short-term estimates including tall stacks (Region 5).

5) Estimate photochemical constituents (Region 1, 2, 6, 9).

6) Single source - uniform terrain (Region 4, 7).

7) Meteorological models to provide meteorological fields.

The types are listed according to the overall priority as deduced from the answers to the questionnaire. The results, however, showed important regional differences. Therefore, the regions are listed in brackets after the type of model to which they give top priority.

As a conclusion it may be said that all kinds of air quality models need further development, and that the different regions are particularly interested in special kinds of models according to their special problems.

In a similar way it may be expected that different countries focus their interest on different kinds of models according to their way of handling air pollution problems and air quality management, and according to their topography and climatology.

III AIR QUALITY SIMULATION MODELS USED TO DEVELOP CONTROL STRATEGIES

Often the development of control-strategies depends on impact studies. However, the relative contribution from the different sources has to be specified by the models to a larger extent than in impact studies. When impact studies detect a problem, there is need to control it in the most effective way possible. Air pollution control may be divided into engineering control and regulatory control (35). The selection of air pollution control methods has en economic impact and a quantification of the effectiveness for improving air quality is needed. The control of air pollution takes place on several administrative levels :

a) Formulation and administration of air quality control legislation.

b) Formulation of emission standards.

c) Formulation of ambient air quality standards.

d) Definition of air quality control regions.

e) Evaluation of air quality programs.

f) Selection of engineering control devices and emission conditions for new installations.

The present use of air quality models is mostly associated with e) and f) above.

1 Formulation of emission standards

In the U.S.A. a simple and modified rollback model has been applied to assess the impact on air quality of the emission standards for automobiles to be enforced in 1975. (See Chapter 8 in (12)). In their critique of the emission standards for CO and for hydrocarbons and oxides of nitrogen (36, 37), the National Academy of Sciences commented on the use of the rollback model. In relation to CO emission standards the critique was based more on the evaluation of the model than on the use of the rollback model itself.

In relation to the HC and NO_x emission standards, it was clearly stated that the linear rollback formulae are particularly inappropriate for hydrocarbons and oxides of nitrogen. However, the panel did not point out any better model alternative. They focused attention on the high concentrations outside the downtown area of Los Angeles, and on the non-linear relationsships between smog effects and the initial concentrations of hydrocarbons and oxides of nitrogen.

2 Evaluation of air quality programs

In the U.S.A. it is required of each State, according to the Federal Clean Air Act of 1970, to adopt a plan which provides for implementation, maintenance and enforcement of primary air quality standards in each air quality control region within such State. The Administrator for the Environmental Protection Agency is given the overall responsibility for the review and submittal of implementation plans. In the Federal Register (38) are given the requirements for preparation, adoption, and submittal of implementation plans. The plans must set forth a control strategy which will provide for the degree of emission reduction necessary for attainment and maintenance of the national standard, including the degree of emission reduction necessary to offset emission increases expected to result form projected growth.

Requirements for control strategies exist for two groups of pollutants :

a) Sulphur oxides and particulate matter.

b) Carbon monoxide, hydrocarbons, photochemical oxidants, and nitrogen dioxide.

In both groups it is required that the adequacy of a control strategy be demonstrated by means of a proportional model (rollback model) or diffusion model, or other procedure which is shown to be adequate and appropriate for the purpose.

In the Federal Register a description is given of the application of the modified rollback model, together with nonspecific requirements to account for topography, spatial distribution of emissions and/or stack height.

If analysis is made by use of a diffusion model, then recommendations are developed (39). A detailed source inventory is used as a basis for source reduction evaluation. The Martin-Tikvart model (40) is used to estimate the spatial distribution of yearly average concentrations. Concentration for short periods (1 hour, 8 hours, etc.) are estimated by a statistical technique developed by R. Larsen (41).

The statistics on air quality data gives information on the type of standard that has to be used for definition of control. Several States, like Wisconsin, have also developed an episode plan. The use of models in relation to episode planning will be considered in a later chapter.

According to Slater (see section 9 in ref. (12)) "Rollback" is the most popular of these control techniques. Unfortunately, rollback does not allow a detailed consideration of the spatial distribution and height of release of emissions, and is therefore less reliable than the more complex techniques which do consider these factors. The implementation planning program includes a segment that evaluates the control costs, and this is important information together with a quantification of the improvement in air quality for the decision on control strategies.

In the preceding paragraphs two approaches have been presented to solve this problem.

a) The use of rollback, where the contribution from each source is assumed to be proportional to the emission.

b) The use of the Martin-Tikvart model based on a Gaussian plume assumption, and specifying the relative contribution to air quality from the different sources. However, the Gaussian plume assumption is based upon simplified assumptions concerning the wind and turbulence conditions.

3 Selection of engineering control devices and emissions conditions for new installations

In several countries this is an important area for application of air quality models. Knowledge about the first two phases of plume development (the momentum phase and building phase) is used to design the emission conditions in such a way that the plume avoids the turbulence elements produced by the buildings in the neighborhood. The experience serving as guidelines has been developed from field studies and studies with physical models. However, more research is required in this field (see Chapter 31 in ref. (12)).

Further away from the stack, where the lifting and dispersion phase becomes important, a comprehensive plume rise formula and a Gaussian dispersion formula are used to predict the impact on the surroundings, and this information is used to select cleaning equipment and stack height. In several countries specific regulations and models are developed to determine stack height. In Germany new regulations for calculations of stack height, proposed by VDI, take regional differences in dispersion conditions within Germany into consideration (see report by Gilbert in ref. (42)). The same reference includes a comparison between the methods used in different countries to calculate chimney height, and large variations are observed from country to country. The differences in required chimney height are due to differences in ambient air quality standards and in dispersion models. (See report by Strott, Michelmann and Weber in (42) and the report by Bouscareu in (42)).

In Japan wind tunnel results are used to calibrate the dispersion factors (43) in a Gaussian dispersion model, and the dispersion model is used to quantify the air pollution impact on the surroundings of a new factory. The impact studies are further used to suggest modifications in the construction of new plants. This combined use of physical modeling and mathematical/numerical modeling is unique as far as the author knows. It takes advantage of the strong points of the different model approaches in order to develop recommendations for source modification.

In Japan regulations exist that specify the relation between the discharge rate of sulphur oxides (q) and the effective discharge height (H) in the following formula :

$$q = KH^2 \qquad \text{(see ref. 44)}$$

The factor of proportionality K varies between different areas in Japan. The K-value is a comprehensive factor that considers prevailing pollution conditions, degree of industrialization, population density and meteorological conditions, and model calculations may be used to evaluate the factor K. The regulations in Japan provide flexibility between a high degree of stack gas cleaning and the requirements for a high stack.

The methods to modify emission conditions and to recommend stack height are concerned with avoiding a local air pollution problem. The "high stack policy" in Europe has effectively improved air quality locally. However, a large scale problem needs further consideration in the future (55). This fact seems to be appreciated by the Environmental Protection Agency, U.S.A., where stack height is not explicitly included in the difinition of control strategy (38).

The stack heights for new sources are required to be high enough to avoid downwash in the momentum and building phase of the plume development. Possible effects due to topography may also be taken into consideration in the quantification of stack height. The ambient air quality standards and a

Gaussian plume formula are used to determine the amount of emission (or degree of cleaning) in regard to :

a) Maximum short-term concentration.
b) Annual mean concentration.
c) Short-term concentration at critical locations.

4 Summary of current use and an indication of further development of air quality models for control evaluation

In the definition of emission standards overall information is needed on the relative contribution of different sources on air quality. The group of sources as they are specified in Table II, may contribute to problems on different scales.

Today experience exists with control of air pollution on a local, urban and regional scale. Larger scale problems may require control for the future as the air quality impact is evaluated. Table III presents the different scales of air quality problems, different pollutants and the respective sources to be resolved in air quality models to be used to develop air pollution control strategies. It is seen that both on a local and urban scale it is a need to specify the relative contribution from single and multiple elevated point sources. To specify this contribution the different dispersion phases presented in Table II have to be considered. This problem is solved in a comprehensive way by multiple-source urban diffusion models based on superposition of Gaussian plumes. This approach is based on the assumption of wind and turbulence conditions in the atmosphere (homogeneous wind and turbulence conditions) that is not always observed on an urban scale. However, the assumptions are valid up to a certain distance beyond the stack (see previous Chapter). The background concentration due to other sources may be estimated with a cruder spatial resolution. These types of models are under evaluation in Norway (78). Concerning control on the regional scale, further development of models for secondary pollutants is urgently needed.

	Spatial Scale	Pollutant	Source
Local scale	10 - 1000 m	SO_x	Elevated point source Low level area sources
		Particulate Matter	Elevated point sources Area sources
		CO	Nearby auto traffic
Urban scale	10 - 40 km	SO_x	Multiple point sources Low level area sources
		Particulate Matter	Multiple point sources Low level area sources
		Photochemical Oxidants	Auto traffic Industrial processes
Regional scale	100 - 1000 km	SO_x Particulate Matter Secondary Pollutants	Industrial areas Densely populated areas Urban areas Transportation system

Table 3: Scales of Air Pollution Problems Requiring Control.

In the definition of control strategy given in the Federal Register (38), different land use and transportation measures are included, for example

a) Closing or relocation of residential, commercial, or industrial areas,

and

b) Parking restrictions and expansion or promotion of the use of mass transportation facilities.

These control methods are discussed in the next chapter that covers the use of models in relation to land use and transportation planning. The Federal Register (38) also includes emission limitations on a short-term basis made in accordance with standby plans. Work is under development for the EPA on this topic, in order to specify the reliability and effectiveness of such supplementary control systems. These are generally single sources. One of the requirements for supplementary control systems is that of forecasting capability for local dispersion conditions. Empirical knowledge on the connection between large scale meteorological conditions and local dispersion conditions are used for this purpose. Supplementary control systems are in operation on an urban and regional scale in Japan (79). On a local scale the smelter industry and Tennessee Valley Authority are both operating supplementary control systems. Environmental Research & Technology, Inc. has developed the technical capability of handling supplementary control systems (see Chapter 12 in ref. (9)). This technical capability includes :

a) A realtime monitoring system for air quality.

b) An operating model which relates meteorological inputs, emission rates, source data, terrain, and location factors, to ambient air quality.

c) A forecasting capability for meteorological parameters.

IV USE OF MODELS IN LAND-USE AND TRANSPORTATION PLANNING

1 Different Aspects - Administration

In land-use planning, the following aspects of our society have to be considered : industrial and residential development, recreational and agricultural activity, and aesthetic and environmental considerations. In a similar way there exist several aspects to be considered in transportation planning. A developed plan will often be a compromise between different competing interests. In the system of considerations that leads to a plan, there exists social, political and environmental constraints, and air quality represents one of the environmental constraints.

The incorporation of air pollution considerations into the planning process varies from country to country. The legislative and administrative systems for this incorporation may be divided into three groups :

a) A formal legislative process which may or may not specify the models to be used for this incorporation.

b) An administrative procedure specifying consultation between air pollution control authorities and planners.

c) No formal system is specified and the interaction takes place on advisory level, depending on the person responsible for the planning.

2 Administrative Arrangements in the U.S.A.

In 1973 the Administrator of the EPA, U.S.A., published regulations to ensure attainment and maintenance of National Ambient Air Quality Standards. The new regulations require all states to identify those areas within their boundaries that appear likely to exceed any air quality standards during the 1975 - 1985 period. In these areas it is essential to include air pollution considerations and constraints in the plan for the community development. Air quality maintenance areas are specified and special precautions are taken in the planning processes. The projection of the spatial distribution of future air pollutant emissions represents one of the main difficulties in modeling future air quality, and limited experience exists.

3 Model Experiments

An example of the incorporation of air pollution considerations in land use planning is presented by Environmental Research & Technology, Inc., in The Hackensack Meadowlands Air Pollution Study (45). A system is developed that uses the data specified in the land use and transportation plan as input data, transforms these into pollutant emission data, and as a result predicts and displays mean ambient pollutant concentrations within the area of interest. Four different plans are considered and ranked according to an analysis of the air quality contours and the computation of quantitative measures of impact. Five pollutants were considered (CO, HC, O_x susp. part. and NO_x).

The emission data are used to calculate summer, winter and annual mean values by using a modification of the Martin-Tikvart (40) advection - diffusion model.

If air quality does not represent any constraints on the planned development of an area, the air quality should not be decisive in the development of a plan. Several other components to be considered in the land use plan should be quantified. No comprehensive planning tool has yet been developed, although considerable work has been done on many of its major components (46). The use of comprehensive models in the complex decision process will be discussed further in the next chapter.

4 Planning Methods - Air Quality Models

As an alternative approach to comprehensive models, there is a need to include air pollution considerations in the different planning methods. Different planning methods exist where it is easy to incorporate air pollution considerations and models should be developed for this purpose. These are methods by which the same amount of emission may be spatially organized in different ways in order to avoid or minimize adverse effects due to air pollution.

a) Location of Large Stationary Sources

Many of the air pollution problems which exist today are caused by industries that are poorly located from an air pollution point of view. This should be avoided by improved planning which, to a large extent, employs studies of local meteorology, climatology and topography in order to improve spatial arrangements for industrial, residential and commercial areas.

b) Location of Sensitive Receptors

In the planning process, special attention should be given to the old, the sick and to young people. Facilities for their use should be placed in regions with a low pollution level.

c) Small Open Spaces

Small open spaces around low level sources, for instance around a road with heavy traffic, will improve local dispersion and in that way reduce the ambient air concentration locally. The filtration effect of vegetation should also be considered.

d) Transportation Planning

A well-planned transportation system can often substantially reduce the pollution concentration.

e) Organization of a Densely Populated Region

A densely populated region may be organized in different ways, e.g. around one large center, around several smaller centers with open areas in between, in a long corridor, or in several corridors pointing out from one center.

These different forms will lead to different ambient air concentrations of pollution due, among other things, to dispersion conditions and total emission from car traffic.

f) Organization of the Different Utilities Within the Region to be Developed

The spatial arrangement of industrial, commercial and residential areas influence the air quality significantly, for instance by reduction of peak hour traffic in certain residential areas.

Each of these planning methods may influence the future air quality significantly, and models are needed to quantify the difference in air quality as a result of different source distributions. The quantification of ambient air pollution concentrations is dependent on the quantity and conditions of emission, and on the atmospheric dispersion conditions. The different planning methods influence the source distribution on different spatial scales e.g. the large stationary sources often emit most of the pollutants through a stack that may be approximated by a point source. The organization of a densely populated area in different ways influences the source distribution on a regional scale (typical length of several kilometers). The single sources of pollutants are not so important in these considerations and the requirements of A.Q. models are different. Most land-use planning decisions take place on a regional or local scale. However, when large stationary sources must be located, cities in different parts of the country may be considered. To quantify the difference in air quality as a result of site selection, the difference in dispersion conditions is of primary importance. The statistics for the parameters describing these conditions throughout U.S.A. have been developed by Holzworth (47).

In the assessment study of Frankfurt, Germany, the urban planners asked for a quantification of the effect of planned open spaces on air quality (48). Based on monitoring data the conditions in Frankfurt were clarified to a satisfactory degree. However, a more general model is needed.

5 Land-use and Transportation Planning as an Air Pollution Control Method

In the development of the different State Implementation Plans it turned out that for several areas the announced emission reduction from motor vehicles was not sufficient to meet the ambient air quality standards, and additional transportation control strategies had to be developed. These strategies are available as APTD documents from Environmental Protection Agency (49).

It is mainly transportation control methods that are used to improve air quality. These methods include inspection and maintenance, traffic flow controls, restriction on the use of cars, organization of carpools etc., and constitute the basis for calculations of emission. Two types of models are needed and used to predict air quality.

6 Microscale Models

Describing the air quality in the close vicinity of a street or a highway (typical length of 10 m - 1 km). These models must account for air flows around buildings and the effect of heat and turbulence created by vehicles. One objective of this type of model is to clarify the benefits of various roadway configurations.

The microscale models in current use are presented in the Chapter II on impact studies. They include :

a) The HIWAY Model (EPA)
b) The street canyon model developed by Stanford Research Institute
c) Model calculations based on a finite difference approximation of the conservation of mass equation.

The method marked c) is used by Environmental Research and Technology (51). Physical models (wind tunnels and water channels) may be used to clarify complex air flow patterns. However, numerical models seem to be more applicable to quantify air quality (43).

The "rollback model" is used to a large extent in connection with transportation planning and especially when local CO concentrations have to be reduced.

7 Larger Scale Models

The objective of mesoscale modeling is to relate pollutant emission over large areas to average air quality and a minimum average-time results for this coarse spatial resolution of about 1 hr.

In problems related to land-use planning and air quality maintenance planning, the source specification is not so important as the development of control strategies. Models describing area-mean concentrations may be applied. The Miller-Holzworth model (52) is used to estimate the city-wide average concentration for the sampling time of interest (53). The Hanna-Gifford model (54) is sometimes used as justification for using the rollback model locally to quantify the effectiveness of strategies within an urban area.

On the urban scale several models are recommended for use in relation to land-use planning. For a relatively inert pollutant like carbon monoxide, Stanford Research Institute has developed a model that is presented in Chapter II (see Johnson et al. ref. (29)). This model may be used for transportation planning on an urban scale, and uses the street canyon model as a submodel. In connection with transportation planning the "rollback" model is also widely used on an urban scale.

In order to control photochemical oxidants by transportation planning, regional-scale photochemical models are needed. Two types of complex photochemical models have been developed (trajectory models and grid models). Worley has presented the state-of-the-art of photochemical modeling on the 2nd CCMS meeting on air quality modeling (see Chapter 13 in ref. (9)). In the conclusion it was pointed out that many problems remain including evaluation of the meteorological variables, distribution functions for emissions, and formulation of chemical reaction mechanisms for multiple hydrocarbon systems.

The Environmental Protection Agency still encourages the use of rollback models to evaluate control strategies for oxidants, pending the development of better models. The more complex models are still applied on an advisory level by the local communities. For example, General Research Corporation used their photochemical model to predict air quality for the city of Santa Barbara and its surrounding area, for the year 2000 (50). Two types of average rate of growth between 1970 and 2000 were used.

8 Summary and Recommendation for Future Development

Land use, transportation and air quality planning are all sectors of comprehensive planning, and each sector can be used to obtain goals in other sector plans. On the one hand air quality models are required to specify air quality constraints in land use and transportation plans, and on the other hand model information is needed in order to quantify the effectiveness when land use and transportation planning are used to obtain air quality goals. Little experience exist on including air quality considerations in land use and transportation planning. In practice the developed plan is reviewed from an air quality point of view, and an impact statement is required.

When improved air quality is considered to be the primary goal of planning, models have been used to describe quantitatively the effectiveness of different planning methods on air quality.

Table IV summarizes the different application of air quality models in relation to different planning methods. In several methods used for transportation planning, "Rollback models" are used as an alternative to the highway transportation model. It should further be remarked that :

a) All models in current use are developed to handle relatively inert pollutants.

b) Models for photochemical reactions are needed to quantify the effect on the oxidant level of different transportation and land use planning methods.

c) There is a need to develop models for the effectiveness on air quality of small open spaces, for the organization of densely populated regions in different ways and for the organization of public industries in different ways. The possible improvements in air quality need to be quantified.

Planning Method	Source Scale	Existing Models
1. Large Point Source	Stack Diameter	Gaussian Plume Models
2. Sensitive Receptors	100 m x 100 m	Multiple Source Models to Define Pollution Gradients
3. Small Open Spaces	100 m x 100 m	
4. Transportation Planning		
a) Street Canyon	10 m x 50 m	Empirical Models
b) Highway	100 m	Highway
c) Intersection	100 m x 100 m	Highway-superposition
d) Parking Lot	100 m x 100 m	Highway-superposition
e) Shopping Center	100 m x 100 m	Highway-superposition
f) Transportation System on an Urban Scale	5 km x 5 km	Rollback SRI Model
5. Organization of Densely Populated Regions	5 km x 5 km	—
6. Organization of Different Utilities	5 km x 5 km	—

Table 4: Current use of Models in Relation to Different Land Use and Transportation Planning Systems.

V MODELS USED AS SUBMODELS IN LARGER SYSTEMS-CONSIDERATIONS (COMPREHENSIVE PLANNING)

It is required of the air quality models that the input from a larger model are accepted and that emission data are transformed to ambient air concentrations. The output data must be presented in a form that other parts of the system can handle. However, air pollution must to a large extent be controlled at its source and a proportional model is applied to describe the connection between emission and its adverse effects. In general, air quality is only one part of an environmental aspect to be taken into consideration by planners along with several other aspects (social, economic, and political). Little experience exists, and few attempts have been worked out to specify a least cost regulatory strategy. (See Gustafson, Chapter 27 in ref. (12)).

From an economic aspect a larger systems consideration might require that the economic cost of air pollution exposures be quantified. These cost functions are poorly defined, and assumptions about their form have been necessary, Shephard (56). Knowledge about the use of the cost-exposure curve requires the concentrations distribution to be known in space and time. Shephard uses a modification of the Martin-Tikvart model for this purpose. The cost-exposure curves are poorly defined, and in most countries an ambient air quality standard is accepted as a political decision on the air quality constraint in development. For most pollutants adverse effects accumulate gradually with ambient air concentration and a standard may be 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 defined, further development of models for larger systems considerations will be developed.

VI MODELS AS A BASIS FOR PLANNING EMERGENCY ACTIONS IN AIR POLLUTION EPISODES/INCIDENTS

1 Air Pollution Episodes/Incidents

An air pollution episode may occur under unfavorable meteorological conditions in (see ref. (57)):

a) Large, heavily industrialized areas, like the Ruhr area in Germany, with a spatial scale of 500 - 1000 km. Such an area would require a regional dispersion model.

b) Individual metropolitan areas with a spatial scale 20 - 25 km, requiring an urban dispersion model.

c) Areas often with relatively small populations, but special topographic and/or climatic features, with very high emissions from a few specific sources. Such an area has a spatial scale of a few kilometer (2-5 km).

An air pollution incident may arise from an accident where a substantial amount of poisonous gas is released into the atmosphere. Accidents can occur under a large variety of circumstances. The decisions on degree of evacuation and other emergency actions have to be made fast, and taking these local circumstances into consideration.

2 Different Types of Pollution Problems May require an Alert System and an Episode Control Plan and Three Main Groups are Identified (57)

a) The build-up of unacceptably high concentrations of primary pollutants such as sulphur oxides and particulate matter, nitrogen oxides and carbon monoxide, which may cause adverse health effect. The chemical reaction products may not be of primary importance.

b) The build-up of secondary pollutant conditions, e.g. photochemical oxidant air pollution, which may be a source of nuisance and cause adverse effects both in the region itself and at some distance from the primary pollutant emission sources. Knowledge about the chemical reactions has to be included in the model.

c) General public complaint about nuisance, particularly with respect to odor. Modeling of an odor problem is extremely difficult and may have to contain a stochastic element regarding the perception of odor (see Chapter 15 in ref. (10) and ref. (64)).

3 Requirements for Information

The needs for information in relation to episode planning have been summarized by Niemeyer (see Chapter 19 in ref. (12)). One of the requirements was a means to assess the impact of different control strategies.

The effectiveness of different control strategies may be assessed in two ways :

a) A pre-assessment based on experience from earlier air pollution episodes.

b) A real time assessment and a possibility to change the strategy depending on the meteorological conditions characterizing the different episodes.

Air pollution episodes occur under unfavorable meteorological conditions. These conditions, causing the pollutants to accumulate, are often associated with a stagnant anticyclonic synoptic weather situation that leads to poor large-scale ventilation. Local and mesoscale circulations become important, and the manifestation of these circulations may differ from one area to another and intensive local case studies are required to evaluate air quality models.

In some areas, like in the Rijnmond area around Rotterdam, fumigation conditions are responsible for the peak concentrations (see Veld's paper [14] in ref. (10)). In other areas the highest concentration may occur during periods with ground-based inversions, as it is reported by Santomauro for the episodes in Milan, Italy (57). Under such conditions the ground level air quality is much more dependent on the low-level source. Limited experience exists with validated air quality models for air pollution episodes, and they have not been used to any large extent in developing supplementary control strategies. Several investigations have been carried out in the Chicago area by Argonne National Laboratory (58, 59, 60) on controlling air pollution episodes.

Wangler and Rossin quantifies the effectiveness of a hypothetical control strategy by using an air quality model (60). The Argonne integrated puff model and steady-state plume model are applied. Some of the basic assumptions of the model may be questioned in relationship to the application. However, the model gives numerical results under certain hypothetical emission and dispersion conditions (these conditions are realistic as far as present knowledge and capability of existing models are concerned). The results show that the specific control strategy worked better in one of the episodes than in the other, indicating that a change in strategy depending on the episode may be required for an effective system.

In Japan an alert system is in operation in several areas, where the control strategy is changed from one episode to another.

Several pollutants are measured (SO_x, NO_x, CO, O_3, non-methane HC and particulate matter), and the relative concentrations at the different ground level stations are used to determine what kind of sources are going to be controlled (61).

Possibilities exist for fast accumulation of air pollutants during episodes, and there is a need for a forecasting capability for high air pollution concentration, so that supplementary control actions may be taken to avoid the episode.

In the U.S.A. the National Weather Service has taken action to develop this forecasting capability (63). Alert systems are required to be included in the state implementation plans in polluted areas (Priority I Areas) (See ref. (38)). Forecasting of stagnation takes place on a national basis in U.S.A., and this information is used by local control agencies, who evaluate its significance for local air quality. Environmental Research and Technology, Inc. has also developed a forecasting capability as a part of a supplementary control system (see Chapter 28 in ref. (12)). A supplementary control system developed to meet air quality standards will also be effective during air pollution episodes.

Statistical models based on empirical experience are used in connection with a real time monitoring systen in order to provide the forecast. During recent years the frequency of air pollution episodes has diminished, probably due to the increased concern about permanent control of air pollution.

4 Air Pollution Incidents

An air pollution incident occurs as a result of an accident. The accident may occur within an industrial plant or during transportation of poisonous chemicals (for example chlorine). With air pollution incidents, it is necessary to specify the areas from which people will have to be evacuated. A model that is easy to use is required. The plan developed for dealing with air pollution episodes/incidents in Illinois may be used as an example (62). Based on knowledge about the source strength, the threshold value for the hazardous material, and the measured wind velocity, a k-factor is determined

$$k = \frac{\text{source strength}}{\text{wind speed x threshold value}}$$

A Gaussian dispersion formulae for a ground level source provides concentration isopletts for different stability classes, and the specification of the evacuation zone is read off graphically. Similar models are probably also developed for chemical warfare purposes.

VII MODELS USED IN RESEARCH ON ATMOSPHERIC PROCESSES

In order to further develop existing air quality models, it is necessary to question the assumptions on which these models are based, and a better evaluation and understanding of atmospheric processes are required.

Tracer studies have been used for a long time in field studies on atmospheric advection and diffusion. In a similar fashion, when the emissions of pollutants are well defined, air quality models may be used to study the complex atmospheric processes. Models used for such purposes should be based upon as few assumptions as possible and complex models will frequently result. Several complex dispersion models have been developed. They may be separated in two classes.

1 Models based on a numerical solution of the mass-balance equations for the pollution components alone

The meteorological conditions have to be specified from a detailed monitoring net. Models of this type have been worked out by Randerson (65), Sklarew (66), Lamb and Neiburger (67) and Shir and Shieh (68). These models rely on measurements of horizontal winds, and then deduce the vertical velocity component by considering mass continuity. The vertical wind component becomes critically sensitive to the measurements of horizontal winds. The importance of the vertical ventilation will be considered later in this paper.

2 Air Quality Models Including Navier-Stokes Equations

Some models use the Navier Stokes equations to specify the three dimensional wind and turbulence fields on local and urban scales, and Alamos Scientific Laboratory has even used their particle in cell method as a quasi-Lagrangian numerical method to solve Navier-Stokes equations in a street canyon. The same method is also used to determine the pollution concentration (see Chapter 32 in ref. (12)). In order to develop air quality models for research purposes on an urban scale, Fox indicates (see Chapter 13 in ref. (11)) that even the hydrostatic balance approximation may not be valid on this scale. This argument is supported by Neumann in his modeling of the land-sea breeze system (70). Accordingly, it may be necessary to include both transcient and stationary modes of motion to model the transport and diffusion over an urban area.

The transient modes on an urban scale will probably have to be treated statistically. In the schemes presented by Fortak (23), the predictability of the transient modes on an urban scale are within the limits of stochastic forecasting procedures, but beyond the present possibilities for deterministic forecasting. The complex models on an urban scale might be used to evaluate the statistics of the transient modes. However, the data requirements for specifying the boundary and initial values are so extensive for the complex models that they may not be applicable on a real time basis.

Pandolfo et al. (69) have proposed a complex model that predicts transport and diffusion in an urban boundary layer. The programs have been developed for the Los Angeles region. However, the model has not been tested with a spatial resolution justifying the use of such a complex model. The stationary mode of motion over an urban area, due to the nonhomogeneous heat source and surface roughness and its variation with large scale meteorological conditions, may be studied by assuming certain balance conditions.

For example, the hydrostatic approximation and the assumption that the first and second local time derivatives of the horizontal divergence may be used as a balance condition (72). In the Oslo-region the stationary mode of motion seems to be of primary importance for describing the ventilation during inversion situations (see Chapter 22 in ref. (10)).

Anthes (71) is developing a model for the regional scale that includes the effect of an inhomogeneous topography. This model includes the hydrostatic approximation.

All modes of motion (for example, the vertical propagation of sound waves), are probably not important for the transport and diffusion of air pollution. Therefore, simplifications may be possible in the complex models for the meteorological parameters, when used in air quality models. The effect on pollution distribution of some of the modes of motion has to be determined by considering air quality model results. In connection with complex model calculations, continuous observations of ambient air concentration under different meteorological situations, may indicate the most important modes for the pollution problems to be considered.

3 Photochemical Models

In the development of models of photochemical smog, there has been a tendency to include more and more hydrocarbon reactions. The most detailed models have to deal with an over three-hundred reactions mechanism (73). Hopefully, it will be possible to simplify the reaction scheme to be used in operational air quality models, when all important reactions are clarified.

VIII A CLOSER EXAMINATION OF AIR POLLUTION MODELING FOR A FEW SELECTED APPLICATIONS

1 Selection of Specific Applications

For a closer examination the application of air quality models in different land use and transportation planning problems is considered.

The different planning methods influence the emission distribution on different scales and the following three examples are selected for specification of requirements of air quality (A.Q.) models :

a) When a location for a large stationary source is to be selected, a quantification of the impact in the form of the distribution of pollution concentration in the surroundings of a single stack is needed.

   Emissions from a single stack may be approximated by a point source. It is well known that under certain meteorological conditions the concentration is approximated well by a Gaussian plume formula.

b) In order to take air quality constraints into consideration in transportation planning, a quantification of changes in the pollution concentration in a street canyon due to changes in the traffic density and to changes in the traffic flow pattern regulated by stop lights is useful.

c) For the organization of a densely populated region, a model to quantify the ambient air concentration on a regional scale due to different emission distributions is needed.
   The emission distribution may be changed by decisions on zoning, definition of emission factors in different areas, spatial arrangement of the different utilities, and transportation planning on a regional scale. Often several different plans are applicable, and a quantification of the difference in air quality between these plans is needed.

2 Requirements for Information

Quantification of ambient air pollution concentrations is dependent on the quantity and conditions of emission, and on the atmospheric dispersion conditions. The different planning methods influence the source distribution on different spatial scales, e.g. the large stationary sources often emit most of the pollutants through a stack that may be approximated by a point source. The organization of a densely populated area in different ways influences the source distribution on a regional scale (typical length of several kilometers). The single sources of pollutants are not so important in these considerations and the requirements of air quality models are different.

Depending on the adverse effects different statistical parameters of the pollutant concentration may be of importance, e.g. the effects may be dependent on the long-term averaged concentration and/or on the sort-term concentrations. Due to the variability in the meteorological processes describing the relation between emissions and ambient air concentrations, different requirements may be given to the air quality models depending on the pollutant under consideration, and on the climatology of the region where the land-use planning takes place.

To specify the requirements of A.Q. models for land-use planning the following elements have to be considered :

a) The spatial scale of the source distribution to be influenced by the planning method.

b) The statistical parameters of the ambient air concentration that have relevance to the adverse effect.

c) The climatology of the area where the land-use plan is developed.

By considering these three elements, requirements may be specified and relevant assumptions may be made for development and/or application of A.Q. models. It is of primary importance that the parameters determining the differences in air quality that result from different land-use plans are included in the air quality models.

Three different applications have been selected to show that different models may be needed on different spatial scales. A simple scale analysis is useful to show this.

In this scale analysis two different classes of meteorological conditions will be considered:

a) The local windfield and turbulence conditions are horizontally homogeneous and determined by large scale air-streams.

b) Mesoscale and/or microscale meteorological processes are important to describe the local wind and turbulence conditions.

The first class of meteorological conditions is often observed in the atmosphere especially in flat areas, and important simplifications may be made in the development of A.Q. models.

The second class include a large spectrum of atmospheric conditions and each of them provides special requirements for A.Q. models. The significance of these requirements have to be determined by considering the points b) and c) on the previous page.

3 Scale analysis to make simplifications in A.Q. models appropriate to the requirements for information.

In the previous section it was specified that the requirements for information from A.Q. models should consider three elements. Three examples of applications of air quality models were selected in order to consider modeling of the impact from air pollution sources with different spatial scales. Two classes of meteorological conditions were selected that may require different air quality models. In order to see how the requirements for information may be used to develop appropriate simplifications for the air quality models, a scale analysis will be made of the terms in the general equation describing the connection between emissions and ambient air concentrations. The continuity equation for the pollution component, taking into account sources and sinks of the pollution component, may be formulated in the following way :

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z} - \frac{\partial T_x}{\partial x} - \frac{\partial T_y}{\partial y} - \frac{\partial T_z}{\partial z} + Q + R \qquad (1)$$

t	=	time coordinate
x, y, z	=	the coordinates in a rectangular coordinate system
c	=	pollution concentration
u, v, w	=	the wind components along the x, y, z axes respectively
T_x, T_y, T_z	=	the turbulent transport of pollutants
Q	=	volume sources of pollution
R	=	reaction rate

Typical non-dimensional (primed) values of the different parameters are defined by :

$$c = \bar{c}\,c', \quad u = \bar{u}\,u', \quad v = \bar{v}\,v', \quad w = \bar{w}\,w'$$

$$T_x = \bar{T}_x\,T_x', \quad T_y = \bar{T}_y\,T_y', \quad T_z = \bar{T}_z\,T_z'$$

$$Q = \bar{Q}\,Q', \quad R = \bar{R}\,R'$$

$$t = \bar{t}\,t', \quad x = \bar{x}\,x', \quad y = \bar{y}\,y', \quad z = \bar{z}\,z'$$

$\bar{c}$, $\bar{u}$, $\bar{v}$, $\bar{w}$, $\bar{T}_x$, $\bar{T}_y$, $\bar{T}_z$, $\bar{Q}$, $\bar{R}$ — The characteristic values of the variables describing the situation are defined so that the corresponding primed, non-dimensional values vary between zero and one within the area under consideration.

$\bar{t}$, $\bar{x}$, $\bar{y}$, $\bar{z}$ — The characteristic values of time, and the horizontal and vertical scales of the problem are defined so that the derivatives of the ambient air concentrations and of the turbulent fluxes of pollutants vary between zero and one within the area under consideration.

By using these typical non-dimensional values Equation (1) may be written :

$$\frac{1}{\bar{t}}\frac{\partial c'}{\partial t'} = -\frac{\bar{u}}{\bar{x}}u'\frac{\partial c'}{\partial x'} - \frac{\bar{v}}{\bar{y}}v'\frac{\partial c'}{\partial y'} - \frac{\bar{w}}{\bar{z}}w'\frac{\partial c'}{\partial z'}$$

$$-\frac{\bar{T}_x}{\bar{x}\,\bar{c}}\frac{\partial T_x'}{\partial x'} - \frac{\bar{T}_y}{\bar{y}\,\bar{c}}\frac{\partial T_y'}{\partial y'} - \frac{\bar{T}_z}{\bar{z}\,\bar{c}}\frac{\partial T_z'}{\partial z'} + \frac{\bar{Q}}{\bar{c}}Q' + \frac{\bar{R}}{\bar{c}}R' \qquad (2)$$

In order to compare the magnitude of the different terms in Equation (2), the following numbers may be compared :

$\frac{1}{\bar{t}}$: the time variation of the pollution concentration.

$\frac{\bar{u}}{\bar{x}}$; $\frac{\bar{v}}{\bar{y}}$; $\frac{\bar{w}}{\bar{z}}$: The magnitude of the horizontal and vertical advection terms.

$\frac{\bar{T}_x}{\bar{x}\,\bar{c}}$; $\frac{\bar{T}_y}{\bar{y}\,\bar{c}}$; $\frac{\bar{T}_z}{\bar{z}\,\bar{c}}$: The magnitude of the horizontal and vertical turbulent transport terms.

$\frac{\bar{Q}}{\bar{c}}$; $\frac{\bar{R}}{\bar{c}}$: The magnitude of the sources and sinks of the pollution component.

The typical values for the turbulence fluxes are often estimated to be proportional to the gradient in the pollution component :

$$T_x = K_x \frac{\partial c}{\partial x} \quad ; \quad T_y = K_y \frac{\partial c}{\partial y} \quad ; \quad T_z = K_z \frac{\partial c}{\partial z}$$

The magnitudes of the turbulent transport terms are :

$$\frac{\bar{T}_x}{\bar{x}\,\bar{c}} = \frac{\bar{K}_x}{\bar{x}^2} \qquad \frac{\bar{T}_y}{\bar{y}\,\bar{c}} = \frac{\bar{K}_y}{\bar{y}^2} \qquad \frac{\bar{T}_z}{\bar{z}\,\bar{c}} = \frac{\bar{K}_z}{\bar{z}^2}$$

The two meteorological situations to be considered are specified as follows:

a) The situation is characterized by stationary and homogeneous wind and turbulence conditions determined by large scale air streams. The temperature stratification is assumed to be neutral. The x-axes of the coordinate system is oriented along the mean air stream.

b) The situation is characterized by low horizontal advection velocity. The wind may be inhonogeneous and the temperature stratification is stable (inversion) suppressing vertical turbulent transport.

4 A.Q. model for a quantification of the pollution concentration in the surroundings of a single stack

The spatial scales $(\bar{x}, \bar{y}, \bar{z})$, as they are defined above, vary substantially with the distance from the stack. In the atmosphere turbulence elements are present at all spatial scales. Elements with spatial scales that move the whole plume when close to the stack may act effectively to dilute the plume further away from the stack. Empirical evidence shows that a Gaussian plume formula describes well an ensemble mean value of the concentration distribution in the surroundings of the stack.

From a theoretical point of view a Gaussian plume formula may be found as a solution of the equation :

$$u \frac{\partial c}{\partial x} = K_y \frac{\partial^2 c}{\partial y^2} + K_z \frac{\partial^2 c}{\partial z^2} \qquad (3)$$

Formulated by typical mean values this means that the numbers $\frac{\bar{u}}{\bar{x}}$ and $\frac{\bar{K}_y}{\bar{y}^2}$ and $\frac{\bar{K}_z}{\bar{z}^2}$ have to be at least one order of magnitude larger than the other numbers expressing the magntitude of the other terms in Equation 2. These requirements are fulfilled in weather conditions belonging to the class of meteorological situations characterized by homogeneous wind and turbulence conditions. When inhomogeneous wind and turbulence conditions occur, for example due to topography ($\frac{\bar{v}}{\bar{y}} \simeq \frac{\bar{u}}{\bar{x}}$ or $\frac{\bar{w}}{\bar{z}} \simeq \frac{\bar{u}}{\bar{x}}$), special considerations have to be made to quantify the ambient air concentration due to a single stack.

5 A.Q. models for quantification of the pollution concentration in a street canyon

The cars moving along a street emit pollutans. A typical spatial scale along the street ($\bar{x}$) becomes very large, and the line of moving cars may be considered as a line source. It is the transport and diffusion perpendicular to the line cource that are important for the ventilation. If mean concentrations within a street canyon are considered, the width of the street and the height of the houses may be used to describe the spatial scales perpendicular to the street canyon ($\bar{y}$, $\bar{z}$). The air streams within the street canyons are very complex, and the ventilation may be described by a diffusion and/or by a transport process. The street canyon submodel developed by W. Johnson et al., at Stanford Research Institute assumes that the flux out of the street canyon is proportional to the locally generated CO emissions in the street, and that a helical circulation (primary vortex) in the street canyon cause the main ventilation (29).

It is difficult to quantify the characteristic values of the variables describing the emission-ventilation conditions. Large variations are likely to be observed with time. To estimate the effectiveness of the ventilation in relation to the emissions, continuous measurements of the CO concentrations were made. The emissions fluctuated in time in accordance with the traffic density controlled by a traffic stop light. From the response in the ambient air concentration in the street canyon, an indication of the typical ventilation parameters is given :

$$\frac{1}{\tau} = \max \left\{ \frac{\bar{v}}{\bar{y}} \; ; \; \frac{\bar{w}}{\bar{z}} \; ; \; \frac{K_y}{\bar{y}^2} \; ; \; \frac{K_z}{\bar{z}^2} \right\}$$

In a street in Drammen, Norway, it was found that :

On September 12, 1972 $\tau = 42$ s
On October 6, 1972 $\tau = 41$ s

A detailed description of the procedure used to find these values is given in Appendix 1.

In order to study the variations in the pollution conditions with meteorological parameters, traffic conditions, etc. some measurements of the variation in pollution concentration within this time scale should be made. The spatial scales involved are assumed to be equal to the width of the street ($\bar{y}$ = 30 m) and to the height of the houses ($\bar{z}$ = 10 m). Measurements used to develop further a street canyon air quality model should resolve the following variations of the parameters :

$$\bar{v} = \frac{\bar{y}}{\tau} \qquad \bar{v} = \frac{30\text{m}}{40\text{s}} = 3/4 \text{ m/s}$$

$$\bar{w} = \frac{\bar{z}}{\tau} \qquad \bar{w} = \frac{10\text{m}}{40\text{s}} = 1/4 \text{ m/s}$$

$$\bar{K}_y = \frac{\bar{y}^2}{\tau} \qquad \bar{K}_y = \frac{900\text{m}^2}{40\text{s}} = 90/4 \text{ m}^2/\text{s}$$

$$\bar{K}_z = \frac{\bar{z}^2}{\tau} \qquad \bar{K}_z = \frac{100\text{m}^2}{40\text{s}} = 10/4 \text{ m}^2/\text{s}$$

If variations with these amplitudes are resolved, the variations that are important for the fluctuations in the ambient air concentration will probably be detected.

6 A.Q. models to quantify air pollution concentration on a regional scale

For the organization of a densely populated region a model to quantify the ambient air concentration on a regional scale, due to different emission distributions, is needed. The source distribution is influenced on a horizontal scale of a few kilometers ($\bar{x}$ and $\bar{y} \simeq 5.10^3$ m). The vertical scale is of the order of 100 m ($\bar{z} \simeq 1.10^2$ m).

To see how different models may be needed in different meteorological situations, the wind and turbulence conditions are specified in the following way :

a) When the wind and turbulence conditions are homogeneous and the temperature stratification is neutral, the wind and turbulence conditions are specified by :

$$\bar{u} = 5 \text{ m/s} \quad ; \quad \bar{K}_z = 5 \text{ m}^2/\text{s}$$

b) When the windspeed $|\bar{v}|$ is low ($|\bar{v}| \simeq 1$ m/s) and the temperature stratification is stable ($K_z \simeq 0.2$ m^2/s), the wind direction is often inhomogeneous.

Where the horizontal windfield is inhomogeneous, the horizontally convergent and/or divergent part will cause vertical motions. It is assumed that the vertical velocity may be found directly from the horizontal divergence and that the vertical velocity is zero at the ground.

$$W_H = - \int_0^H \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) dz$$

During some case studies in Oslo the convergence towards the city center was found to be in the order of 10^{-4} - 10^{-3} s^{-1}. (See Chapter XII in ref. (10)). Some case studies from St. Louis have also shown convergent air streams close to the ground over the urban area. Convergence values up to $10^{-4}\ s^{-1}$ have been ovserved (80).

The horizontal eddy diffusion

The eddy diffusion coefficient (K_x, K_y) are, among other things, dependent on the decomposition of the wind field into an average component and a turbulent component. If a finite difference approximation of the continuity equation is selected for the model development, a certain spatial resolution of the wind field is chosen. The diffusivity of eddies with a spatial scale larger than 2-4 times the grid distance should be described by the time variation of the wind field specified in the grid system. This turbulent effect may in principle be described as a stochastic part superimposed on the mean wind field.

The diffusive effect of eddies with a spatial scale smaller than the grid elements has to be estimated. The K-theory may be used when the spatial scale of the diffusive turbulent elements is restricted in this way. On the other hand the problem is then transferred to a realistic description of the stochastic wind component. In order to compare the different terms in the continuity equation the grid distance is assumed to be 1,000 m, and the horizontal diffusion coefficient is assumed to be $K_x = K_y = K_h = 100\ m^2/s$.

The emission of pollutants

This term represents the forcing term in the modified continuity equation. If the magnitude of this term is known, the magnitude of some other terms has to be of the same order of magnitude. To estimate a typical emission from low level sources in an urban area, data from Oslo on the SO_2 emission (10) are used.

The mean emission rate from an area of about 50 km^2 over the center of the city is used to estimate a typical emission value. The height of the volume source is assumed to be 100 m. Based on these assumptions a typical value of the volume source ($\bar{Q}$) is found to be :

$$\bar{Q} \simeq 0.1 \ \mu g \ SO_2/m^3 s$$

As a summary, Table I specifies the magnitude of the different terms in Equation 2 related to the meteorological situation.

TABLE I

A Quantification of the different terms in the modified continuity equation (Equation 2). Unit: s^{-1}

	Advection		Diffusion	
	$\frac{\bar{u}}{\bar{x}}$; $\frac{\bar{v}}{\bar{y}}$	$\frac{\bar{w}}{\bar{z}}$	$\frac{\bar{K}_x}{\bar{x}^2}$; $\frac{\bar{K}_y}{\bar{y}^2}$	$\frac{\bar{K}_z}{\bar{x}^2}$
Homogeneous advection diffusion situation	10^{-3}	Zero	$4 \cdot 10^{-6}$	$0.5 \cdot 10^{-3}$
Stagnant inversion situation	$2 \cdot 10^{-4}$	10^{-4}	$4 \cdot 10^{-6}$	$2 \cdot 10^{-5}$

The numbers show the relative importance of the horizontal and vertical ventilation terms in an air quality model to be used for land-use planning on a regional scale. In a meteorological situation with homogeneous advection and turbulence, the vertical transport and the horizontal diffusion are small. The numbers describing a stagnant inversion situation, show that a small horizontal velocity (1 m/s) may have an important effect on the ventilation. Empirical observations indicate that systematic vertical motion over an urban area is important. The horizontal diffusion is not important for the description on a regional scale. The vertical turbulent transport may be of importance even in inversion situations. After a time (comparable to the reciprocal values of the numbers in Table I) the ambient air concentration will approach a steady state where the ventilation is equal to the source strength.

Regarding the sinks of air pollution due to chemical reactions, these become important when the reciprocal value of the typical reaction time is comparable with the numbers in Table I. A chemical reaction with a reaction time of a few hours is not very important in situations with advection, but becomes important in stagnant inversion situations.

7 Concluding remarks

It has been identified that in order to specify requirements useful in selection and/or development of A.Q. models, three elements have to be considered :

a) The different land-use planning methods influence the source distribution on different spatial scales and information on air quality is therefore required with different spatial resolutions. This information may be used to develop simplifications for A.Q. models, specifically if the conditions in inhomogeneous meteorological situations have to be described.

b) The statistical parameters describing the ambient air concentrations that are important for the adverse effects, have to be determined for the different pollutants. Often it is the annual mean concentrations that are considered in relation to land-use planning, If peak concentrations are important, in relation to the adverse effects, a model is needed for the stagnant meteorological conditions when the ambient air concentration is ten times higher than in situations with generally stronger advection.

c) The climatology of the area has to be considered in order to determine the frequency and types of meteorological situations in the area where the plan is going to be developed. The frequency of the adverse meteorological situations may be high enough to influence the seasonal mean value.

In this way different A.Q. models may be needed depending on the pollutant component and on the climatology in the area under consideration. When the wind and turbulence conditions are homogeneous, models based on the Gaussian plume formula represent a powerful tool to quantify the air pollution impact due to land-use planning, on different spatial scales. These models apply under specific meteorological situations. The need for other types of A.Q. models is dependent on :

1) The adverse effects of the pollution under consideration.

2) The frequency of situations with non-homogeneous wind and turbulence conditions and the pollution concentration in these situations.

The requirements of A.Q. models are highly dependent on the formulation of the constraints and on the expected air quality. If good air quality is expected in an area (few sources), the air quality considerations will not be given much weight in the planning decision process. However, if a poor air quality is expected, i.e. the forecast ambient air concentrations exceeds air quality standards, the air quality considerations are of decisive importance. The importance of taking air quality into consideration on the planning stage is underlined by the fact that it is very difficult and expensive to correct mistakes once a plan has been developed.

IX THE VALIDATION OF AIR QUALITY SIMULATION MODELS RELATIVE TO THEIR PRACTICAL APPLICATION

1 General

Often large uncertainties are connected to data used as input to air quality simulation models. For example, the point measurements used as validation data for the air pollution model are often influenced by sources on a spatial scale not resolved in the model. The validation tests will in this case show bad results that are not appropriate for the practical application of the model. The validation test ought to insure that the appropriate terms are taken into consideration.

2 Validation methods

W. B. Johnson (see Chapter 6 in ref. (10)) requires a true evaluation and validation program for the individual model elements, i.e. the emissions module, the transport and diffusion module, the transformations and removal module. It is expected that the data from the Regional Air Pollution Study (RAPS) in the St. Louis area will provide a consistent data base to test the different model elements on an urban scale. Several papers have been presented on the validation problem of air quality models (see Chapter 25 in ref. (12) and in ref. (81)). The input data for the different elements are subject to substantial uncertainties that may be considered as stochastic variables. For example, it is not possible to predict and consider all time and spatial variations in the emission field of an urban diffusion model. This makes the interpretation of a validation study difficult. To what degree are the discrepancies between calculation and observation due to noise in the input data, to unrepresentative measurements or to an inappropriate model? Work is sponsored by the Meteorology Laboratory, Environmental Protection Agency to clarify these problems from a statistical point of view.

3 A validation procedure

As seen in the previous chapter different meteorological situations may have a substantial effect on the structure of air quality models, and a structuring of the data according to meteorological situations is necessary. If typical seasonal changes in weather occur, the validation and evaluation data should be collected accordingly.

The separate elements of the model should be tested according to the proposal by W. Johnson (see Chapter 6 in ref. (10)). Often it is a very complicated task to test the true validation of the separate elements, for example, the assumptions about the meteorological conditions. The true evaluation and validation like Johnson suggests would also serve as a basis for further development of the model. A method testing the different elements of the model, and their combination in an air quality model, may be carried out by evaluating the response in the ambient air concentration as a result of variations in the different parameters describing the model. The calculated variations should be validated by comparison with the observed variations. Olsson and Ring (see Chapter 25 in ref. (12)) have called this method a time-series comparison. The time scale used to specify variations should be determined by the magnitude of the different terms as presented in the previous chapter.

This type of validation can be carried out by structuring of observed and calculated concentrations according to initial value and variation. If the ensemble values of the variation behaves according to the model, then the deviation between the observed and calculated values may be regarded as non-predictable variation in the ambient air concentration. If the deviation between the observed and calculated concentration is considered as a stochastic variable with a

Gaussian distribution, the unexplained part of the variance in the concentration (δ_R^2) is connected to the total variance of the observed cocentration (δ_T^2) by the following equation:

$$\delta_R^2 = \delta_T^2 (1 - R^2)$$

R = correlation coefficient

When the total set of data is used to validate existing air quality models, the unexplained variance represents about 50-60% of the total variance, and it is difficult to specify quality differences between the models (82).

To validate air quality models the response in calculated air quality as a result of changes in the input parameters (emission, dispersion) should be compared with observed variations. In order to avoid noice in observed air quality data due to poorly defined input data (e.g. short-term emission values), an ensemble mean value of the observed variation in air quality as a result of a specified change in the emission-dispersion conditions should be used for model validation purposes.

Meteorological situations where the model assumptions do not apply, should be excluded from the validation. For example, when a multiple source model based on a quasi stationary Gaussian plume formula is applied the following situations should be excluded :

a) Situations with wind speeds lower than 2 m/s. The wind conditions over an urban area are not expected to be horizontally homogeneous during these situations.

b) Transient situations when the quasi stationary approximation do not apply. On an urban scale large deviations between observed and calculated hourly mean values may be due to this effect.

Short-term variations in existing emissions can sometimes be used to validate the model for long-term extrapolation purposes. As an example, the study in Oslo may be used (see Appendix D to ref. (8)). A quantification of the improvement in air quality during recent years was required. The previous emissions were not known, and a large variation in the dispersion conditions were observed from year to year. Meteorological data and air quality data were known, and a high correlation was found between ambient air concentration and the vertical temperature gradient. The variation in the regression coefficient was used to quantify the improvement in air quality. This model to consider air quality independent of meteorological variations was tested on the daily variation of emission.

An example of use of ensemble mean values of short-term variation in ambient air concentration as a result of a time variation in the emission is presented in Appendix 1.

Acknowledgements

This paper has been worked out as a result of NATO/CCMS Fellowship study. The author wants further to express his appreciation to the Meteorology Laboratory, U.S. Environmental Protection Agency and to the Norwegian Institute for Air Research for their support. Persons from several groups within the Environmental Protection Agency have contributed with their information and specifically appreciation is expressed to Kenneth L. Calder for his helpful comments during the period of work. As a result of his encouragement a part of this manuscript has been presented at the Fifth Meeting of the Expert Panel of Air Pollution Modeling in Roskilde, Denmark (see Chapter 11 in ref. (12)).

The author wants further to express his gratitude to the following persons providing the information forming the basis for the study: Office for Research and Monitoring :

a) The Meteorology Laboratory: Larry E. Niemayer, Director of the Laboratory, D. Bruce Turner, Charles Hosler, Dr. Douglas Fox, Paul Humphrey, Dr. Ralph Larsen, George Holzworth, Gerald DeMarrais, Dr. Ronald Ruff, Karl Zeller, Dr. Ken Demerjian, John Clark, Dale Coventry, Dr. Jim Peterson, Dr. William L. Snyder, Joseph A. Tikvart, and E. L. Martinez.

b) In the Laboratory of Quality Assurance and Environmental Monitoring : Dr. Donald Gillette.

   In Washington, D.C.: Dr. Robert Papetti and Dr. Peter House provided useful information.

Office of Air Quality Planning and Standards under the Air and Water Programs:

Special acknowledgements is given to Herschel Slater and Dr. Kay Jones for their help in this study, and for useful information from Ronald Venezia and John Robson in the Land Use Planning Branch. George Walsh, Director in the Emission Standards and Engineering Division, Robert Neligan, Director in the Monitoring and Data Analysis Division and Robert Schell in the Standards Implementation Branch of the Control Programs Development Division.

Outside the Environmental Protection Agency the authro wants to express his gratitude to Professor Arthur C. Stern at the University of North Carolina and to Professor James Mahoney and Dr. Bruce Egan, Environmental Research and Technology, Inc., Lexington, MA for their comments on the plan and help in providing information and references for this study.

For the patience and skill in typing the manuscript the author owes acknowledgements to Hazel Hevenor, Lea Prince and Susan Godfrey, all of the Meteorology Laboratory, and to Laila Hope, Norwegian Institute for Air Research, for retyping due to last corrections.

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Appendix 1 : A method to determine the typical ventilation time for a street in Drammen, Norway

A continuous monitoring station for CO (UNOR - 2) was placed downstream (with respect to traffic) of a traffic light in a street in Drammen, Norway. All cars moved in the same direction. The cars had to pass an open space before entering the street canyon where the measuring instrument was placed. The cars arrived in groups determined by the green light period from the traffic stop light. The observed response in the ambient air concentration from two case studies is shown in Figure 1 and 2.

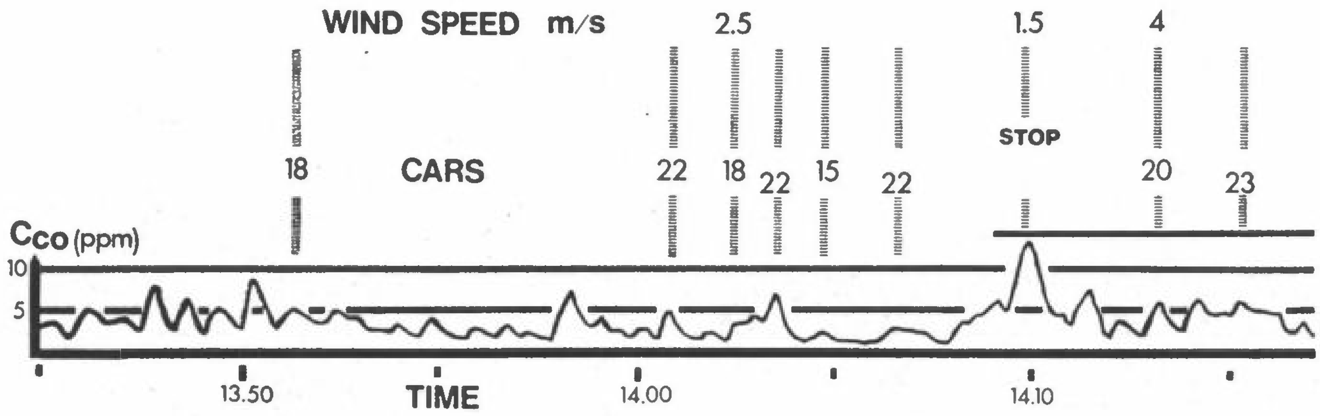

Figure 1 : CO-concentration downstream of a stop light in the city of Drammen, Sept. 12, 1972.

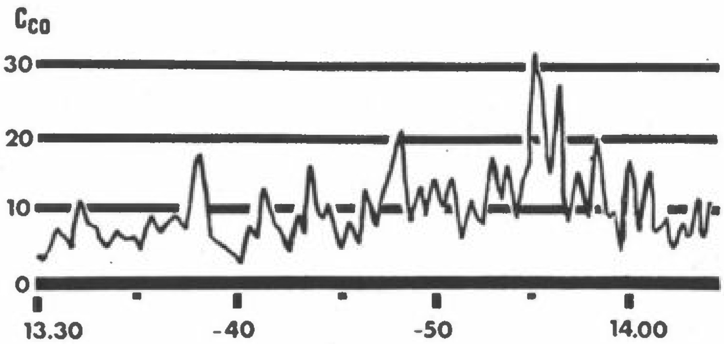

Figure 2 : CO-concentration downstream of a stop light in the city of Drammen, Oct. 6, 1972.

A period of 55 seconds, corresponding to the frequency of the stop light is easily identified. The fluctuations take place above a lower concentration, and a large variation in the amplitude is observed mostly due to differences in the ventilation.

If the ventilation is assumed to be proportional to the concentration, the equation describing the non-stationary process may be formulated in the following way :

$c(t)$: concentration of CO
τ : typical ventilation time
$Q(t)$: volume source of pollutant

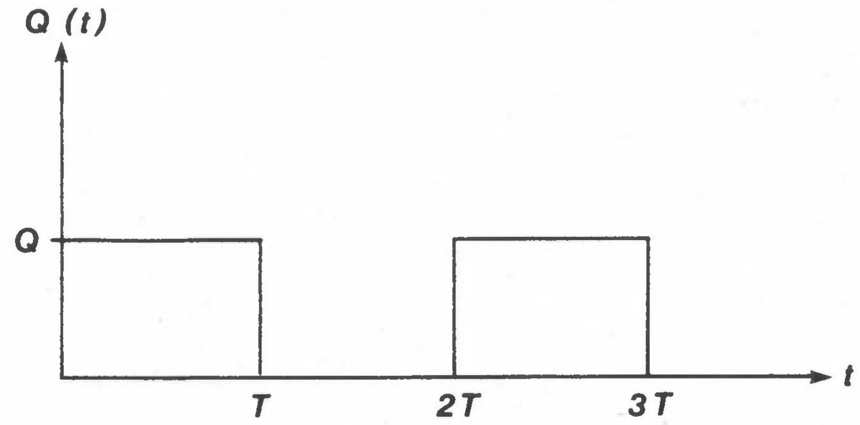

Figure 3 : The emission variation with time.

It is assumed that the volume source has a variation with time presented in Figure 3. The initial conditions are specified by :

$$C\ (O) = C_0 \qquad \text{(A.2)}$$

The solution of Equation A.1, given the specified emission distribution with time and the initial conditions specified in Equation A.2 :

$$C(t) = (Q\,\tau\,(1-e^{-t/\tau}) + C_o\ e^{-t/\tau}), \quad 0 \leq t < T$$

$$\text{(A.3)}$$

$$C(t) = (Q\,\tau\,(1-e^{-T/\tau}) + C_o\ e^{-T/\tau})\ e^{-(t-T)/\tau}, \quad T \leq t < 2T$$

Defining δ as the difference in ambient air concentration over a time period (2T) determined by the frequence of the stop light, δ, is specified in equation (A.4).

Equation (A.3) is used to determine δ_1 :

$$\delta_1 = C(2T) - C(0)$$

$$= (Q\tau + (C_o - Q\tau)\ e^{-T/\tau})\ e^{-T/\tau} - C_o \qquad (A.4)$$

Two dimensionless variables are defined :

$$X \stackrel{def}{=} \frac{T}{\tau}$$

$$A \stackrel{def}{=} \frac{TQ}{C_o} \qquad (A.5)$$

$$\frac{\delta_1}{C_o} = A\left(\frac{e^{-x} - e^{-2x}}{x}\right) + e^{-2x} - 1 \qquad (A.6)$$

If it is assumed that no accumulation takes place from one period to another, $\delta_1 = 0$.

$$A = \frac{(e^{x} - e^{-x})x}{1-e^{-x}} \qquad (A.7)$$

The amplitude of the fluctuation in the ambient air concentration (Δ) due to the variation in the emission is determined using Equation (A.3).

$$\Delta = C(T) - C_o = Q\tau\,(1 - e^{-T/\tau}) + C_o\ e^{-T/\tau} - C_o \qquad (A.9)$$

$$\frac{\Delta}{C_o} = A\,\frac{1 - e^{-x}}{x} + e^{-x} - 1$$

A is determined using Equation (A.7) :

$$\frac{\Delta}{C_o} = e^x - 1$$

$$\tau = T/\ln\left(1 + \frac{\Delta}{C_o}\right) \qquad (A.9)$$

The registration of the carbon monoxide concentration shown in Figures 1 and 2 are used to estimate the mean amplitude of the fluctuations in the ambient air concentrations. The ventilation time (τ) is estimated from (A.9)

$\bar{C}((2n + 1)T)$: The mean value of all maximum concentrations occurring with a period of 2T.

$\bar{C}(2nT)$: The mean value of all minimum concentrations occurring with a period of 2T.

On September 12, 1972 : 2T = 55 s

$\bar{C}((2n + 1)T) = 5.2$ ppm CO

$\bar{C}(2nT) = 2.7$ ppm CO

$\bar{\Delta} = \bar{C}((2n + 1)T) - \bar{C}(2nT) = 2.5$ ppm CO

$\frac{\bar{\Delta}}{\bar{C}(2nT)} = 0.92$; $\underline{\tau = 42 \text{ s}}$

On October 6, 1972 : $2T = 55$ s

$\bar{C}((2n+1)T) = 13.2$ ppm

$\bar{\Delta} = 6.4$ ppm

$\bar{C}(2nT) = 6.8$ ppm

$$\frac{\bar{\Delta}}{\bar{C}(2nT)} = 0.94$$

$\underline{\tau = 41 \text{ s}}$