DEPARTMENT OF ENVIRONMENTAL AFFAIRS AND TOURISM

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NATIONAL AIR QUALITY MANAGEMENT PROGRAMME PHASE II TRANSITION PROJECT

PUBLICATION SERIES B: BOOK 3 ATMOSPHERIC MODELLING

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ACRONYMS

ABL	Atmospheric Boundary Layer
CFC	Chlorofluorocarbons
CIT	California Institute of Technology
CH_4	Methane
CO	Carbon Monoxide
CTM	Chemical Transport Model
ECMWF	European Centre for Medium-Range Weather Forecasting
GCM	Global Circulation Models
H_2O_2	Hydrogen Peroxide
HCFC	Hydrochlorofluorocarbons
HFC	Hydrofluorocarbons
MM5	Fifth Generation Mesoscale Model
NO_x	Oxides of Nitrogen
NMHC	Non-methane Hydrocarbons
NWP	Numerical Weather Prediction
O_3	Ozone
OH	Hydroxyl
PM	Particulate Matter
POP	Persistent Organic Pollutant
SAWS	South African Weather Service
SO_2	Sulphur Dioxide
VOCs	Volatile Organic Pollutants

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1 INTRODUCTION

The atmosphere is dynamic and a number of physical and chemical processes are ongoing. Through these processes atmospheric pollutants are transported or dispersed from their source region, they are mixed and diluted, chemically transformed and removed through deposition. Air quality modelling is a technique used to approximate all these processes and to estimate the resultant concentration of pollutants in the ambient air. Modelling can be undertaken for a range of scales from global to local and a wide variety of air quality models have been developed to meet the different needs of end-users. With the emphasis of the National Environmental Management: Air Quality Act on air quality management, this booklet provides an overview of air quality modelling which is a key tool in the management of air quality.

1.1 Purpose of Modelling

Many countries face an urgent need to reduce emissions to the atmosphere due to the high ambient concentration and deposition levels of harmful pollutants such as sulphur dioxide (SO_2), oxides of nitrogen (NO_x), particulate matter (PM) and volatile organic compounds (VOCs). The concentrations and depositions of these pollutants depend on the distribution of pollution sources, the amount of pollutants released to the atmosphere, dispersion and transformation characteristics of the atmosphere and deposition processes. Strategies to reduce emissions need to take all these factors into consideration. Due to the complexity of these problems, there is a need for use of advanced dispersion models.

This technique has become a valuable and widely used tool for air quality applications such as scientific investigations and to support emissions-control policy. From an environmental impact assessment and ambient air compliance perspective, modelling has gained recognition as a regulatory tool used to assess impact from sources for a variety of pollutants under various meteorological conditions. At present, air quality models are one of the only tools available that permit the prediction and evaluation of potential impacts of proposed emission reduction strategies. They are also used for visualising the impact of emissions to the atmosphere. Models are also needed where economic aspects and cost effectiveness need to be examined.

Modelling offers a number of advantages over ambient monitoring. Ambient concentrations of specific air pollutants are only measured at specific monitoring locations. Certain chemical species, aerosols and particulates exist in trace amounts rendering measurements often difficult and costly to obtain. Dispersion models can be used to assess air quality in areas where such monitoring data are not available. Models can also be used to make future projections of air pollution levels. Models offer a relatively inexpensive and convenient means of providing this type of information. For example, models can be used to predict the future concentration of a particular pollutant after the implementation of a new pollution control program. In this regard, concentrations can be predicted for the years in which air quality objectives are to be achieved, taking into account emission controls and new or changed source emissions. The modelling results can then used to estimate the effectiveness of a control program and whether it is worth the cost of implementation. Because of their ability to evaluate a variety of options for managing air quality, models are an important planning tool.

Air pollution models are often used during the permitting process to verify that a new source of air pollution will not exceed air quality standards and guidelines which are in place to protect human health and the environment. Models can estimate ambient concentrations from a proposed facility prior to its construction, thereby assessing the potential impact of a development without actually building and operating the facility.

1.2 Model Application

1.2.1 Regulatory Purposes

Most environmental agencies throughout the world use models for regulatory purposes, particularly in issuing emission permits or for environmental impact studies related to, for example, industrial plants and new roads. In these applications, models are required to provide spatial distribution of high episodic concentrations and long-term averaged concentrations which can be evaluated against air quality standard or guidelines. Pollutants frequently modelled are SO_2, NO_x and suspended particles.

1.2.2 Policy Support

On the global scale, environmental policy is presently faced with global scale problems (global warming, ozone depletion). Other important policy issues related to the atmospheric environment are acidification, eutrophication, photo-oxidant formation, urban air pollution and the problem of air toxics. Well co-ordinated, long-term international actions are needed for solving global and regional scale air pollution problems. Regional scale models play an important role in the development of new protocols for the reduction of acidifying compounds created by emissions of NO_x and NH_3 and low level ozone.

Air quality at the local scale can be improved with appropriate site-specific abatement strategies. In these situations, air pollution models may be crucial for optimising such abatement strategies in the direction of supporting local environmental policy making. With regard to policy support, models are required to forecast the effect of abatement measures which may require that the model provide reliable results for future pollution scenarios.

Environmental or meteorological institutions are responsible for the more practical policy oriented applications. Policy oriented models generally have a relatively coarse grid resolution (between 50-150km) and more simplified physical and chemical schemes compared to research oriented models .

1.2.3 Public Information

The role of models is expected to grow in the field of conveying available air quality information to the public. Air quality forecasting and real-time models are one of the most useful communication tool for on-line information on air quality and the possible occurrence of pollution episodes.

1.2.4 Scientific Research

Models employed for scientific research are mainly concerned with the description of dynamic effects in the atmosphere and the simulation of complex chemical processes involving air pollutants. Until very recently, these types of models proved to be unsuitable for most practical applications due to the large computational time needed. Advanced hardware development has recently changed the situation in favour of complex research type models. Research type models are much more advanced and complex than the simpler policy oriented models but have substantially higher computational requirements especially since they contain comprehensive physical and chemical schemes and are run with very fine resolutions. Advances in computing technology will make it possible for the application of these models in policy support in the near future. Models used by Universities are mostly research oriented (Moussiopoulos *et al.*, 1996).

1.3 Limitations and Assumptions using Air Pollution Models

The weather influences the transport and dispersion of pollutants in the atmosphere. The fundamental meteorological properties which drive atmospheric motions and hence air pollution dispersion are the wind (speed and direction) and the temperature profile. Wind acts in the vertical and the horizontal which influences transport, turbulence level and boundary layer mixing depth, while temperature affects plume rise and turbulence level, where turbulence consists of irregular (eddy) motions resulting from atmospheric instability. Wind is mostly responsible for transport, while turbulence results in mixing of chemical constituents. For additional material on air pollution meteorology please refer to Series 3, Book 4 (Air Pollution Dispersion and Effects) and Series 4, Book 2 (Air Pollution Meteorology)

Dispersion studies are frequently required at sites where no routine meteorological datasets exist. In these cases in low-land areas, with broadly flat homogenous terrain, it is normally possible to use a nearby site or interpolate between sites at which a long series of observations have been made. In regions of complex terrain, the simple theories of the boundary layer no longer apply. In such terrain the wind flow patterns may no longer be interpolated directly from the available observational network or from the synoptic wind field. Dispersion in complex terrain is most sensitive to the wind flow, because the wind field determines pollution dispersion.

Although atmospheric models are indispensable in air quality assessment studies, their limitations should always be taken into account. Atmospheric models involve mathematical equations, which result in an estimation of ambient air quality concentrations and deposition. High quality input data is crucial for optimal model output but collecting the necessary input data may be cumbersome. The level of uncertainties in model results is normally a product of uncertainties introduced by the model assumptions and by the input parameters (meteorology and emission data) rendering the output data to be representative to a limited degree. Although output data from most models can be given in the form of a user defined spatial and temporal average this may cause difficulty when making a direct comparison between modelled and measured data for a specific time and location. The following sections highlight some of the key areas which impact on the accuracy of models and modelling.

1.3.1 Meteorological

South Africa's geographical extent is over a million square kilometres. The South African Weather Service (SAWS) currently operates a sparse weather station network of approximately 40 surface observing stations, which provides hourly measurements of temperature, pressure, humidity, rainfall, wind speed and wind direction. These stations are located mainly in the major cities and towns, of which only 10 are found along the coastline. Due to the complexity and continually increasing cost involved, only one of these stations (Irene near Pretoria) conducts systematic measurements of the state of the upper atmosphere.

Due to the scarcity of the network, in particular in the upper air, and the large distance between stations (~100 - 350 km), it is practically impossible to obtain meteorological measurements that are "truly representative" of the regions atmosphere near the surface or at higher (upper) levels.

In South Africa, regionally and temporally representative wind flow statistics (or wind maps) at any point are not readily available and modellers are faced with the challenge of obtaining representative surface wind conditions in data sparse areas. Taking measurements of for example wind speed at a single monitoring site as representative of conditions over hundreds of square kilometres is being over assumptive, but sometimes is the only option and needs to be done.

1.3.2 Emissions Data

The quantification of emissions from sources can be estimated through a number of different methods. These can range from estimates derived from professional engineering judgement to actual measurement. As such the accuracy of the emissions data used to simulate dispersion can range from very low to very high. The quality of the emissions data used in a dispersion simulation can directly affect the confidence in the model outputs.

1.3.3 Type of Model and Model Parameterization

The accuracy of the results of a dispersion simulation can also be influenced by the type of dispersion model that is used. Models range from simple to highly complex, with specific some models specifically developed to address complex situations i.e. complex topography, complex chemistry. Depending on the complexity of the model being used and the nature of output required, models can take between a few seconds to a few days to run. Section 2.9 details some of the common parameters required to establish and run model simulations.

2 TYPES OF ATMOSPHERIC DISPERSION MODELS

Models describing the dispersion and transport of air pollutants in the atmosphere can be distinguished on many grounds, for example

- on the spatial scale (global; regional-to-continental; local-to-regional; local),
- on the temporal scale (episodic models, (statistical long-term models),
- on the treatment of the transport equations (Eulerian, Lagrangian models),
- on the treatment of various processes (chemistry, wet and dry deposition)
- on the complexity of the approach.

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

2.1 Plume-rise Models

A pollutant plume that is released into the atmosphere normally has a higher temperature than the air around it. Pollutants emitted from industries (normally through their stacks) cause the pollutants to have an initial vertical momentum. These factors are referred to as thermal buoyancy and vertical momentum respectively, and play an effective role in plume height above the point of entry into the ambient air. Plume-rise models are therefore used to determine the vertical displacement and to describe the general behaviour of the plume dispersion in the initial stages. Plume-rise models are either semi-empirical or advanced and can include advanced plume-rise formulations.

2.2 Gaussian Models

Gaussian models are based on the assumption that plume concentration, at each downwind distance, has independent Gaussian (normal) distributions both in the horizontal and in the vertical dimensions and many are modified to incorporate special dispersion cases. Figure 2.1 show the classical Gaussian plume dispersion. These models are regarded as the most common type of air pollution models and can be used to calculate long-term averages.

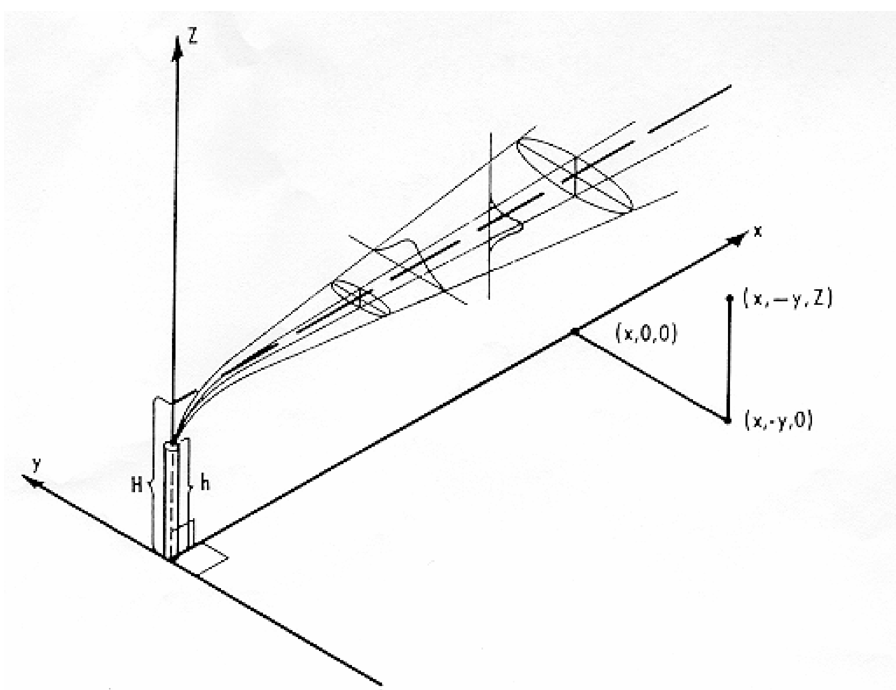

Figure 2.1: Gaussian plume dispersion (Schulze and Turner, 1995)

2.3 Semi-empirical Models

Semi-empirical models were mainly designed for practical applications and are made up of a range of different model types. In spite of considerable conceptual differences between individual models, semi-empirical models are characterised by major simplifications and a high degree of empirical parameterisations. This model category includes a variety of box and parametric models.

2.4 Eulerian Models

In an Eulerian model, chemical species are transported in a fixed grid. Eulerian models use numerical terms to solve the atmospheric diffusion equation (i.e. the equation for conservation of mass of the pollutant), and are therefore able to model the transport of inert air pollutants. The numerical solution of the transport term in the Eulerian framework becomes more difficult and often requires substantial computational resources to be accurate enough compared to the Lagrangian approach. The main advantage of the Eulerian models is the well defined three dimensional formulations which are needed for the more complex regional scale air pollution problems. Figure 2.2 shows an example of a basic Eulerian model. Advanced Eulerian models can simulate turbulence and are usually embedded in prognostic meteorological models.

2.5 Lagrangian Models

In a Lagrangian framework a specific parcel of air is followed and the concentrations of a pollutant are assumed to be homogeneously mixed in the parcel. The Lagrangian approach is based on fluid elements that follow instantaneous flow - transport is determined by trajectories of the air flow. They include all models in which plumes are broken up into constituents such as segments, puffs, or particles. Lagrangian models use fictitious particles to simulate the dynamics of a selected physical parameter. In Lagrangian models, transport caused by the average wind and the turbulent terms is taken into account. The main advantage of the Lagrangian approach is the simple numerical treatment of the transport term in the mass balance equation. The main disadvantage is that it is difficult to account for exchange processes between air parcels and windshear, making three dimensional Lagrangian models not very reliable.

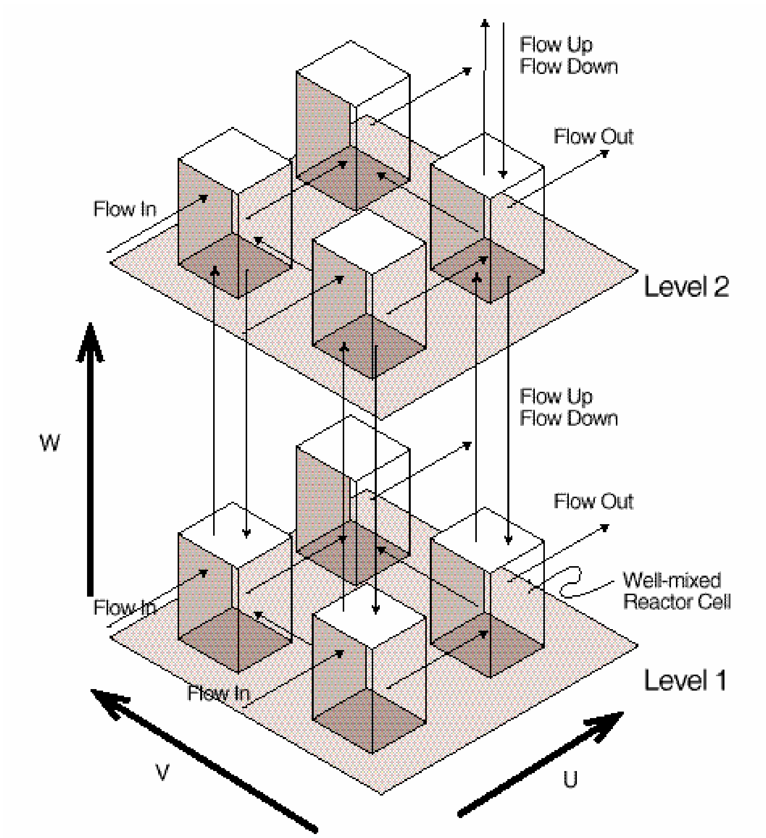

Figure 2.2: Structure of a basic Eulerian model (Environ, 2005)

2.6 Chemical Models

Air pollution models which include a chemical component to simulate chemical transformation in the atmosphere are referred to as chemical models. The type of chemical components used ranges from simple to complex photochemical reactions. Reaction schemes for simulating the dynamics of interacting chemical species have been incorporated into both Lagrangian- and Eulerian-based photochemical models. In Eulerian photochemical models, a three-dimensional grid is superimposed across the entire modelling domain, and all chemical reactions are simulated in each grid cell at successive time steps. In the Langrangian photochemical models, a single cell is advected according to the predominant wind direction, such that any emission encountered along the cell trajectory can be injected into the cell.

2.7 Receptor Models

Receptor models work in a different way to dispersion models in that they start with observed concentration of a pollutant at a receptor point. Receptor models are statistical in nature and are based on mass-balance equations which are used to determine the concentration of a pollutant at its source or at other points within the modelling domain. This is based on the known chemical composition at the source. However, receptor models to not provide a deterministic relationship between emissions and concentration.

2.8 Stochastic Models

Stochastic models are based on statistical or semi-empirical techniques which are used to analyse trends, periodicities, and interrelationships of air quality and atmospheric measurements and to forecast the evolution of pollution episodes. Frequency distribution analysis, time series analysis, and spectral analysis are some of the techniques used to achieve this goal. Stochastic models are limited in the sense that they cannot establish cause-effect relationships but are very useful in situations such as real-time short-term forecasting. Stochastic models generally have the ability to account for uncertainties in model components, in terms of probability frequencies.

2.9 Data Requirements

Generally models are data intensive. Simple screening models require limited inputs whereas more complex models require detailed inputs and parameterisation. The following sections details the typical input requirements for models.

2.9.1 Source Characteristics and Emission Data

The following parameters describe the source of the emission and the physical nature of the emission:

- Geographical location of sources
- Stack diameters
- Height of release of each source

- Exit temperature
- Exit velocities
- Emission rate for each pollutant from each source.

2.9.2 Meteorological Data

The following meteorological parameters are commonly used by models to establish dispersion potential within a modelling domain:

- Atmospheric stability
- Mixing height
- Temperature
- Wind speed
- Wind direction
- Cloud amount and height
- Relative humidity
- Surface pressure
- Sea surface temperature
- Temperature and wind data from upper air soundings

2.9.3 Study Area Characteristics

The following physical characteristics are commonly used in models:

- Surface roughness
- Topography
- Orography

2.9.4 Dispersion and Removal Coefficients

The more complex models use the following parameters when assessing the chemical and physical changes pollutants undergo in the atmosphere:

- Diffusivity
- Solubility (Alpha Star)
- Reactivity
- Geometric Mass Diameter
- Scavenging Co-efficient

2.9.5 Receptor Points

The outputs from models can be presented in a number of different formats. The more common formats are listed below:

- Gridded Receptors
- Discrete Receptors

3 METEOROLOGICAL MODELS

Air quality is strongly governed by meteorology which covers a range of atmospheric processes and spatial scales such as horizontal and vertical transport, turbulent mixing, convection and surface deposition. These processes exert strong control over the physical, chemical and dynamic properties of the atmosphere. Meteorological models provide an understanding of local, regional or global meteorological phenomena and are used to generate meteorological input data required by air pollution dispersion models.

3.1 Diagnostic Models

Diagnostic models such as the California Institute of Technology (CIT) diagnostic wind model (Goodin *et al*., 1980) were specifically designed to resolve the effects of topography. These approaches, however, can still produce unrealistic "residual" vertical velocities at the top of the model domain.

A more advanced and widely used diagnostic model is CALMET (Scire *et al*., 1997a) which has continued to improve and now includes complex terrain, slope-flow algorithms, boundary-layer modules, and a "first-guess field" that can be based on winds fields generated from a dynamical or prognostic model. CALMET can be applied with the CALPUFF dispersion model (Scire *et al*., 1997b). ATMOS1 which uses a 3-D variational analysis technique to analyze wind fields (Davis *et al*., 1984) is another diagnostic model that was designed for calculating fine-scale transport in complex terrain.

Diagnostic models are inexpensive and generally do not involve time consuming integrations of nonlinear equations, making them appealing for use in real-time emergency situations. Another advantage is that, all available observations can be used to perform an analysis. Each analysis is generated with a fresh set of observations, preventing an accumulation of errors at successive time steps.

Diagnostic models interpolate and extrapolate available meteorological measurements. As a result, diagnostic models generally do not capture all the dynamic forces or processes that are operational in the atmosphere and therefore cannot reproduce realistic inter-variable consistency, since they are based on idealised equations. Additionally, diagnostic models often encounter problems when representing flows accurately in data-sparse regions (e.g., mountains or oceans). Routine observations on which diagnostic models are based may lack sufficient temporal and spatial resolution, particularly near the surface and therefore may not be able to resolve certain local-scale and regional-scale features such as sea breezes and low-level jets.

Despite their limitations, diagnostic models are still widely used air quality analysis tools particularly when fine-scale annual or interannual calculations are required.

3.2 Dynamic Models

Dynamic meteorological models are highly complex numerical systems which are based on primitive equations for hydrodynamic flow. A large number of dynamical meteorological models used in air-quality studies were intended originally for weather forecasting and therefore reflects a dominant focus on problems associated with strong dynamical forcing and deep convection (Seaman, 2000).

Non-hydrostatic models have become the dominant framework used in dynamical models due a growing demand for finer-scale numerical models. These models usually have a nested-grid capability, terrain-following vertical coordinates, flexible resolution and a variety of physical parameterization options (deep moist convection, fog, precipitation microphysics, shallow clouds, radiative processes, surface fluxes and turbulence). Non-hydrostatic models most commonly used in the US for air-quality applications are the PSU/NCAR Fifth Generation Mesoscale Model (MM5, Grell *et al.*, 1994) and the Colorado State University Regional Atmospheric Modelling System (CSU-RAMS) (Pielke *et al.*, 1992).

Dynamic models can resolve regional and local-scale atmospheric circulations down to scales of approximately 1km but also require high computational power as their solutions require integrations of non-linear equations over numerous time steps (Seaman, 2000).

One of the most important advantages over diagnostic models is that dynamical models are not reliant on an extensive observation network. Depending on the nature of their grid resolution, dynamic models are able to generate regional and local-scale features not resolved in the data. This type of fine-scale structure is brought about by the models ability to resolve topographical and internal dynamic forcing (Anthes, 1983). The most important disadvantage of traditional dynamical models (without data assimilation capability) is that observations are only considered at the initial time causing a build-up of errors over time. This is due to imperfections in the model's numerics, physics, or initial conditions. Error accumulation in regional and local-scale domains can render a model's solution impractical for air-quality applications after ~48 hours (Seaman *et al.*, 1995).

3.3 Data Assimilating Models

Data assimilation is a technique mainly used for meteorological modelling applications in which observed data are assimilated into the model, thereby improving the model's solutions. It is an effective technique when high-precision meteorological fields are required, but when meteorological models alone cannot resolve important features in these fields.

One type of data assimilation developed for air-quality modelling is the nudging approach (Stauffer and Seaman, 1990). Nudging relaxes the model state toward the observed state by adding an artificial tendency term to one or more of the prognostic equations (Hurley, 2002). It is applied most often to wind, temperature and water vapor, but can be applied for any prognostic variable.

Nudging can be applied either by nudging toward gridded analyses (analysis nudging) or by nudging directly toward individual observations (observation nudging). Analysis nudging is used to assimilate gridded synoptic analyses data that cover most or the entire modelling domain while observation nudging is used to assimilate observation data distributed anywhere in the modelling domain.

The data assimilation approach normally adjusts the solution at each time step throughout the integration period and is particularly valuable for simulations longer than 48 hours as it reduces the accumulation of errors typically inherent in dynamical models (Seaman, 2000).

To prevent unrealistic local forcing or excessive smoothing, assimilated data must be strategically incorporated into a model, taking careful account of the physically realistic weighting strategies and ideal radius of influence as these factors determine the strength by which assimilated data affect the solutions.

Although not mathematically optimised, nudging according to Seaman (2000) has been extensively used with considerable success for a number of studies. When appropriately used, it can be used to support many air-quality studies.

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

4 AIR POLLUTION MODELS USED FOR THE DIFFERENT SCALES OF ATMOSPHERIC PROCESSES

Although atmospheric processes are continuous in space and time, air pollution dispersion is influenced by atmospheric processes which are commonly classified according to their spatial scale. At least four spatial scales of atmospheric phenomena exist: macroscale (also refered to as global or synoptic scale), mesoscale and microscale. Figure 4.1 provides a graphical representation of the scale of atmospheric processes.

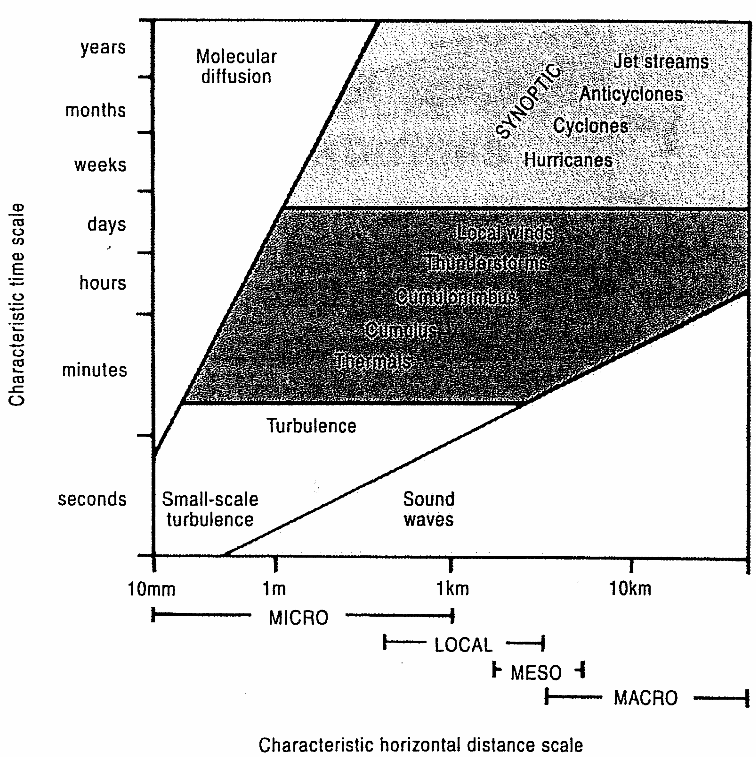

Figure 4.1: Time and space scales of atmospheric disturbances (after Smagorinsky, 1974)

4.1 Macro-scale

The macroscale is the largest of scales and operates on dimensions of more than 1 000 km. Atmospheric flow at this scale is mainly associated with general circulation features, such as trade winds, prevailing westerlies, Rossby waves and jet streams, and include regions of the atmosphere such as the tropics, mid-latitudes, polar regions and the ozone layer. The synoptic or continental, scale is mainly associated with synoptic phenomena, i.e. the geographical distribution of pressure systems and includes elements such as high and low pressure systems, air masses and frontal boundaries. Events characteristic of the synoptic scale are usually from tens to thousands of kilometres in breadth (the area of one continent) and may extend from the surface to the lower stratosphere. Global and regional-to-continental scale dispersion phenomena are generally related to macroscale atmospheric processes.

4.2 Meso-scale

This scale is also known as the local scale. It has a characteristic length ranging from a few kilometres to tens of kilometres in the horizontal dimension and spans from the surface to planetary boundary layer ceiling. Mesoscale flow is mainly dependant on hydrodynamic effects (e.g. flow channelling and roughness effects) and variability of the energy balance (mainly due to the spatial variation of area characteristics e.g. land use, vegetation, and water). Thermal effects are of particular importance at times of weak synoptic forcing, i.e. when ventilation conditions are bad, especially from the air pollution point of view. The mesoscale can be thought of as encompassing an area from the size of towns to that of metropolitan regions. Mesoscale atmospheric processes mainly affect local-to-regional scale dispersion phenomena. The description of such phenomena requires fairly complex mesoscale modelling tools which should at the least be able to simulate local circulation systems such as land and sea breezes.

4.3 Micro-scale

The microscale includes all atmospheric processes less than a few kilometres in size. Air flow at this scale is highly complex and is mainly determined by hydrodynamic effects (e.g. flow channelling, roughness effects). It depends strongly on the detailed surface features (for example the form of buildings and their orientation to the wind direction). Thermal effects play a less significant role in the generation of these flows.

5 DISPERSION MODELS: APPLICATION AT THE DIFFERENT SCALES

In this section, air pollution models are reviewed separately for each scale of dispersion phenomena (global; regional-to-continental; local-to-regional; local).

5.1 Global-Scale Air Pollution Models

Global-scale or hemispheric air pollution models are generally referred to as Chemical/Transport Models (CTMs). These models focus on climate change, for example climatic impacts caused by increased levels of anthropogenic greenhouse gases and aerosols due to the alterations they cause to the radiative balance of the earth-atmosphere system.

These models also simulate changes in the chemical composition of the global atmosphere and can predict future climate. Changes in the chemical composition of the troposphere have a direct impact on biological productivity and human health and climate change. Global models therefore have a strong focus on tropospheric changes and interactions with the stratosphere and deal mainly with pollutants of global concern - methane (CH_4), carbon monoxide (CO), oxides of nitrogen (NO_x), non-methane hydrocarbons (NMHC), chlorofluorocarbons (CFC), hydrofluorocarbons (HFC), hydrochlorofluorocarbons (HCFC) and sulphur compounds (SO_2, aerosols, DMS, H_2S), ozone (O_3) and the oxidising capacity of the atmosphere (defined largely by the concentrations of O_3, hydroxyl (OH) and hydrogen peroxide (H_2O_2)). The output of these models is used to inform activities of the Intergovernmental Panel on Climate Change. Global-scale models provide boundary conditions to regional models which in turn provide boundary conditions to local scale models .

Global-scale models are either one- , two- or three-dimensional (1-D, 2-D or 3-D respectively). 1-D models are rarely in use today because they are regarded as oversimplified. 2-D models describe processes occurring with longitudinally (zonally) and latitudinal averaged rates and concentrations, while 3-D models describe processes in all three dimensions (longitude, latitude, height). 2-D models require lesser computation time, memory and input data than 3-D models but usually contain detailed chemical schemes and can be used for sensitivity studies and analyses. A limitation of 3-D models is that they neglect zonal asymmetries. 3-D models use either daily varying windfields coupled with simplified chemistry or monthly averaged wind fields coupled with detailed chemistry for tracer transport and therefore provide better output than 2-D models. 3-D models offer the best results when dealing with pollutants which have a heterogeneous spatial and temporal distribution.

Apart from Europe and North America there is a general lack of emissions data of pollutants for other parts of the world. Large uncertainties are associated with global scale emission estimates particularly for NO_x and hydrocarbons. Another major drawback is that air pollution models normally use emission data from a range of sources making model comparison a difficult task. CTMs use meteorological information provided by General Circulation Models (GCMs), data assimilation or data from Numerical Weather Prediction (NWP) models.

5.2 Regional-to-Continental-Scale Air Pollution Models

Regional scale models are used to understand the physical and chemical processes that govern the formation, atmospheric fate (transport and deposition) and level of SO_x, NO_x, NH_y and photooxidants (in particular O_3). A large number of regional scale models are also applied to environmental problems caused by heavy metals, Persistent Organic Pollutants (POP), radioactive or hazardous chemical releases, soot, particulate matter and winter smog episodes.

Regional-to-continental scale air pollution models are designed for either policy making or research purposes. Models designed for policy purposes contain less detailed physical and chemical parameterisations in order to model long time periods within realistic time-frames, for example assessment of acidic loads or photochemical exposure need to be modelled over months or years. Models intended for research purposes often contain complicated descriptions and are usually not suitable for long term political applications. Lagrangian and Eulerian dispersion models are commonly used in the regional-to-continental scale.

Regional scale air pollution models rely heavily on meteorological, emission, land-use and orographical data and boundary concentrations. Among these data the meteorological and the emission data are most important and require the largest efforts of preparation. Reliable regional scale meteorological fields are derived from meteorological numerical weather prediction (NWP) models which are used as pre-processors. Uncertainties in the meteorological fields exist in the flow fields around complex terrain, precipitation and cloud fields and the planetary boundary layer. NWP-models can derive parameters such as surface fluxes, turbulent activity, the depth of the planetary boundary layer and cloud parameters, which are not measured regularly in a meteorological network often needed for regional scale air pollution modelling.

Emission data also forms an integral input to regional scale air pollution models. At present, South Africa is still in need of a co-ordinated inventory of atmospheric emissions. An inventory should include SO_2, NO_x, NH_3, VOC, CH_4, CO, CO_2 and N_2O and detailed information on source categories and point sources. In order for modellers to make reliable estimates of the uncertainties involved in the calculated dispersion of regional scale air pollution there is a need for the availability of more emission information (Moussiopoulos, 1996).

5.3 Local-to-Regional-Scale Air Pollution Models

Numerical simulation of air pollutant transport and transformation was first applied on a local-to-regional scale using a mesoscale model. Mesoscale air pollution models are considered most appropriate for large city type or urban scale pollution problems where either a sufficiently large domain is considered or accurate boundary conditions are set up.

A mesoscale air pollution model is usually characterized by either a diagnostic or a prognostic wind field model and a dispersion model. Mesoscale air pollution models require a large amount of meteorological data. Diagnostic or prognostic models provide wind fields and turbulence quantities. The diagnostic approach is a data intensive approach and requires very detailed observed data (which is not always available) to reconstruct an accurate wind field. The prognostic approach which involves the numerical simulation of the wind and turbulence patterns is therefore a preferred method.

Eulerian and Lagrangian dispersion model types are used to model non reactive pollutants but Eulerian types predominate when dealing with reactive pollutants such as ozone and its precursors. The combination of an Eulerian dispersion model and a prognostic wind model is called a "prognostic mesoscale air pollution model". For realistic simulations in the local-to-regional scale, prognostic mesoscale models are required to have reasonable parameterisations that take the dynamics of the atmospheric boundary layer (ABL) into account. The main aim of these models is to show the effect of mesoscale influences (orography and inhomogeneities in the surface energy balance) on air pollutants.

Several types of data sets are required by prognostic mesoscale air pollution models. Geographic data which include the orography (elevations above sea level) and the land use which is distinguished into categories such as arid, agricultural, forested, and urban areas. Accurate information on the land-water distribution for each grid cell is also important. All these data is required in gridded format. Soil parameters for each land use type, including optical properties (albedo, emissivity) and thermophysical parameters (density, heat capacity, thermal conductivity) and soil wetness must be provided. If a diagnostic wind model is used, observed data which is representative for the entire modelling domain is required. At least a few vertical profiles are necessary to sufficiently characterise the three-dimensional wind fields.

If a prognostic wind model is used, radiosonde observations (covering data on height, pressure, temperature, relative humidity, wind speed and direction, preferably at more than one site) are sufficient to calculate wind and turbulence fields. Alternatively, European Centre for Medium Weather Forecasts (ECMWF) meteorological data may be used. Prognostic models usually do not need surface data.

Emission data are usually necessary in hourly intervals, but must be provided in gridded format. Lateral boundary conditions can be improved if emission data are provided for a coarser grid around the modelling domain.

5.4 Local-scale Air Pollution Models

Local-scale air pollution models range from simple (screening type models) to complex types depending on their application and are used to tackle traditional air pollution problems for example those occurring in the surroundings of isolated sources. These models are mainly used for regulatory purposes.

There has been a shift from the use of models based on Gaussian distribution and Pasquill-Gifford classes to those based on boundary layer parameterisation. This progression was made possible by an increased understanding of boundary layer structure and dispersion science.

Air quality guidelines throughout the world are becoming increasingly stringent. More accurate and reliable results are therefore constantly required from these models for regulatory and planning purposes.

Local-scale models require standard physical data for the stacks, such as stack height and diameter, exit gas velocity and temperature and fixed value or time dependant emission rates. Models which are applied to vehicular emissions require a description of the road network, such as number of cars per day, number of road segments, driving speed, road steepness and land use. Screening type models, which describe a critical meteorological situation use default meteorology as input, while others use meteorological data in the form of wind and stability classes. More advanced models base their simulations on pre-processed meteorological data and require gridded fields of wind and temperature profiles, cloud cover data and surface roughness.

6 PRESENTATION OF RESULTS OF DISPERSION MODELLING

Dispersion modelling generates a large amount of data that must be presented in a meaningful way, depending on the application. The results from dispersion studies are normally presented in a spatial format, with the dispersion patterns indicated in the form of isopleths (lines joins areas of the same concentration). Figure 7.1 shows a standard spatial representation of the results from a dispersion modelling exercise.

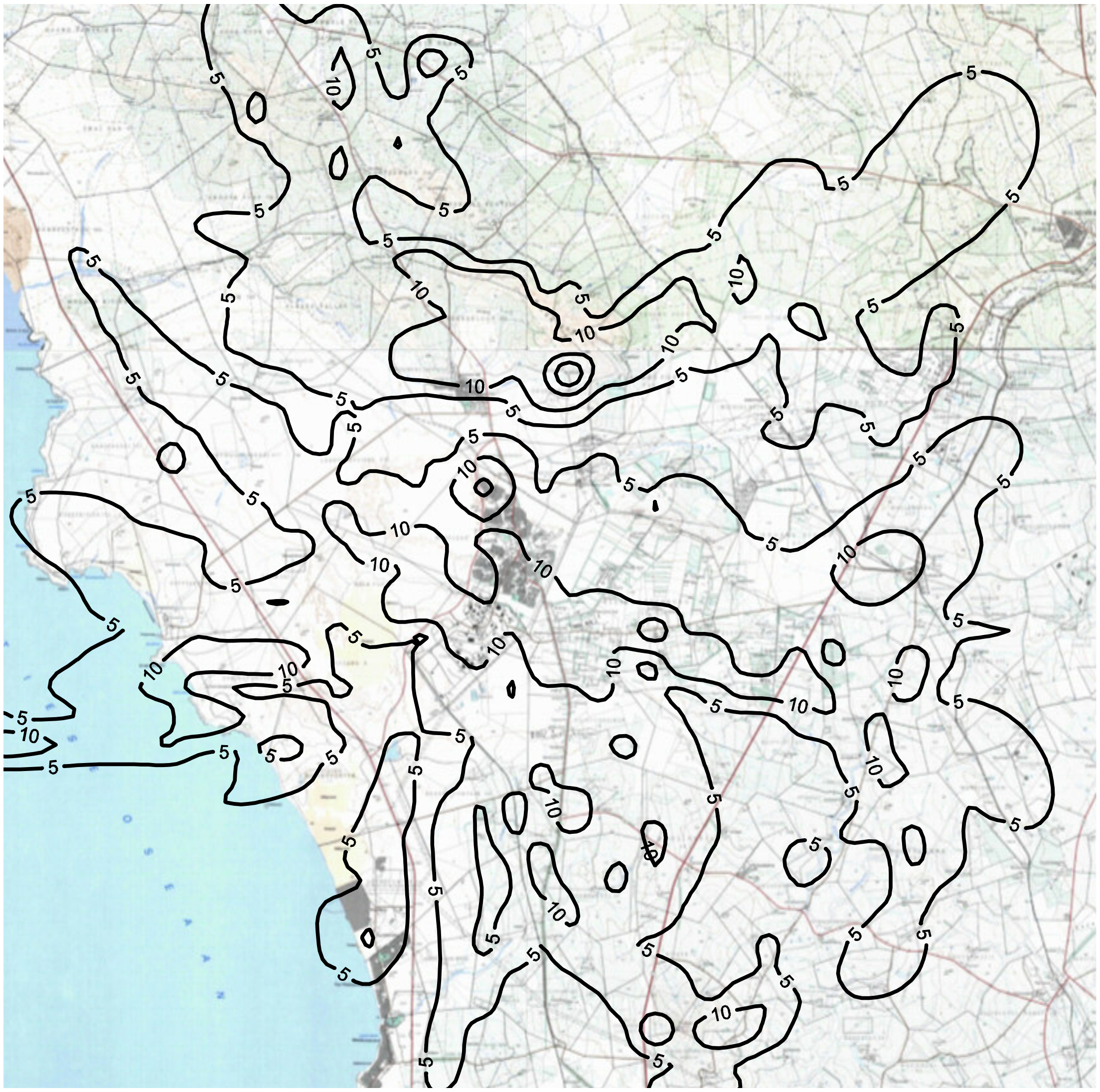

Figure 7.1 Standard presentation of the results of a dispersion modelling study

This format of presenting dispersion modelling results can be confusing. The information presented in the figure

Figure 7.1 highlights one of the benefits of using dispersion modelling as opposed to ambient air quality monitoring, with the dispersion modelling showing pollution concentrations over a wide area, whereas the air quality monitor only shows the pollution concentration at a single point. The results from dispersion modelling can also be shown at a specific point i.e. a sensitive receptor. Figure 7.2 is a time-series plot which shows the variation in modelled concentrations at a specific point. This format of presenting modelled results provides more detailed information and allows for compliance assessment, establishing frequency of exceedence and calculating average exposure.

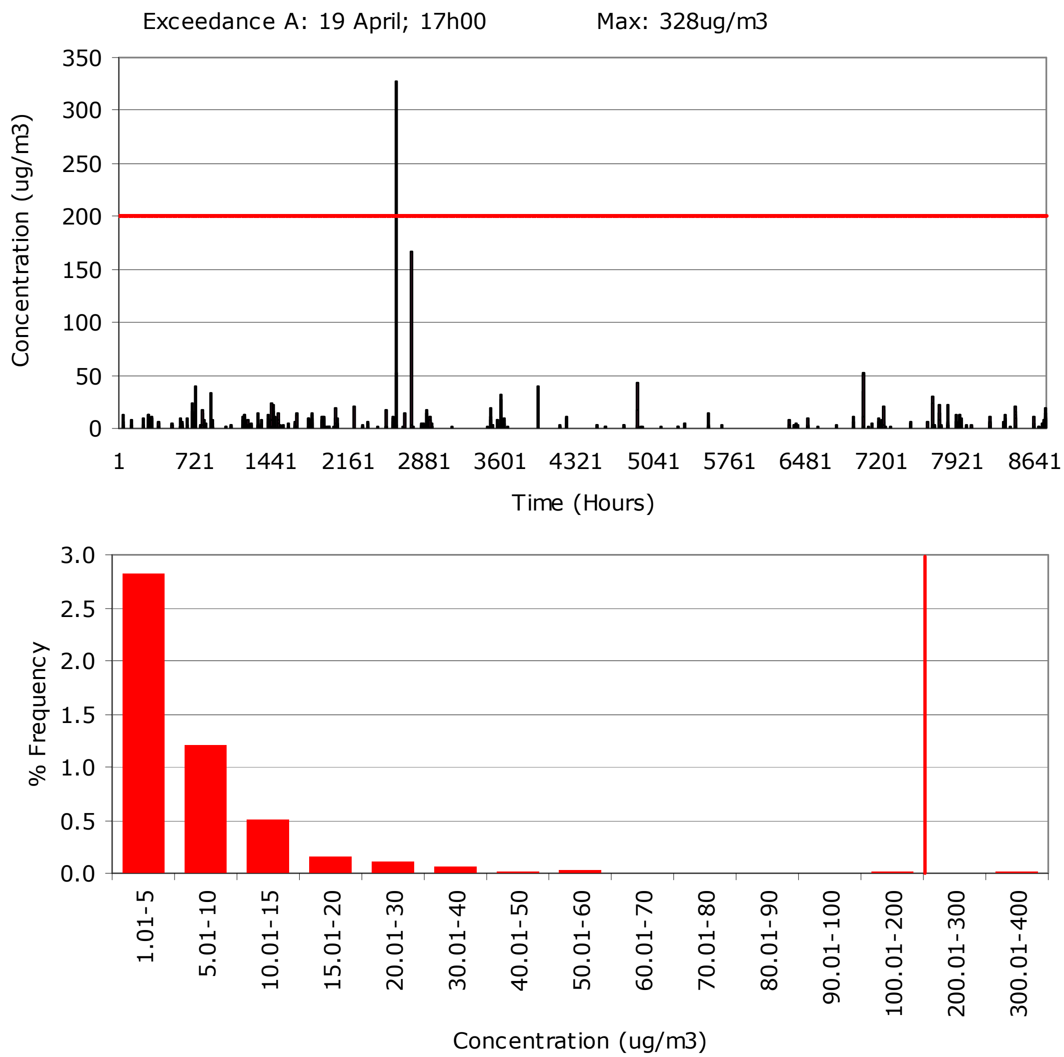

Figure 7.2 Time-series and frequency presentation of the results of a dispersion modelling study

Results can also be presented in tabular form, providing a summary of the pollutants modelled and temporal variation (maximum and average concentrations).

7 QUALITY ASSURANCE OF AIR POLLUTION MODELS/IMPORTANCE OF MODEL VALIDATION AND EVALUATION

A vast number of different air pollution modelling tools available for the analysis of air pollutant transport and transformation are described in scientific journals or technical reports in terms of the mathematical and numerical methods used for formulating the model and descriptions of the parameterisations. Limited information is provided on how to actually use the modelling system, descriptions of the model input and output, model formulation, area of application, model evaluation and validation and the accuracy in the modelled quantities. Improper use can easily lead to misinterpretations of their results. As a consequence, better model descriptions describing the items above and model validation studies are therefore needed to improve this situation.

The quality of an air pollution model can be judged in terms of model consistency and model accuracy using appropriate model evaluation procedures. In general, models are evaluated by comparing predictions against observed measurements. Statistical analysis of deviations between model results and observations is then quantified to reveal model uncertainties. Deviations between model results and observations may be a product of limitation in model assumptions and parameterisations, level of accuracy regarding input data (for example emission and observed meteorological data) and uncertainties in the representativeness of both observed and modelled data etc.

8 TRENDS IN AIR POLLUTION MODELLING

Global air pollution modelling is directed towards refining 3-D chemical transport models and combining them with climate models in the quest to improve environmental and socio-economic impact assessment of atmospheric and climate change. Some areas of improvement include better simulation of sub-grid processes, convective transport, aerosols deposition, measurement techniques. The use of high-quality global emission inventories and meteorological information is also necessary to improve model output.

Although Long Range Transport Air Pollution Models currently have advanced features that enable them to accurately simulate complicated physical and chemical processes, they can be further developed to account fully for the three-dimensional structure of atmospheric dispersion. Source attribution techniques and the linkage of acid rain chemistry and photochemistry to address future multi-pollutant protocols also have potential for further development. Better informed environmental decisions can be based on complex models which are simplified in areas that are not very sensitive to the results.

Appropriate nesting techniques have proved to be important features of air pollution models in the local-to-regional scale since they account for larger scale processes. Future research activities will focus on improving the nesting capabilities of models. The inclusion of nudging as an option is another useful mechanism which influences model results to adapt to observed data. This option is valuable in prognostic meteorological modelling or where an air pollution model relies only on analysed data (Moussiopoulos, 1996).

Another line of thinking stems around linking prognostic mesoscale models to three-dimensional microscale models. This will allow for representation of detailed flow dynamics (for example in street canyons or around obstacles) while taking account of prevailing mesoscale conditions. Further model development concentrates on improving treatment of turbulent transport and developing a more accurate representation of chemical transformation processes in mesoscale air pollution models.

Research indicates that model results vary significantly from model to model. These differences may be attributed to the differences in stability classification schemes, dispersion parameters, meteorological and emission data, and the mathematical equations which govern the model. Model development is geared towards designing more complex but practical regulatory models which will improve the physical processes in the atmosphere.

9 CONCLUSION

Despite their limitations, air pollution models remain important tools for assessing emission reduction strategies, estimating ambient concentration and for gaining a better understanding of the economical aspects of air pollution. Air pollution models also play a vital role in the decision- making process

In order to conduct in-depth model evaluation, there is a need for appropriate experimental data. South Africa may need to create adequate experimental databases on primary pollutants by co-ordinating experimental campaigns at suitable locations in complex terrain.

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