Foundation Course on

Air Quality Management in Asia

Modelling

3

Edited by
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Foundation Course on Air Quality Management in Asia

The Foundation Course on Air Quality Management in Asia is for adult learners studying the issue without the support of a class room teacher. It is aimed at students with some basic knowledge of environment and air pollution issues, acquired in a variety of ways ranging from conventional study, working in an environmental related field or informal experience of air pollution issues.

The course provides you with an opportunity to develop your understanding of the key components required to develop a programme to manage urban air pollution and to achieve better air quality. By working through the six modules you will gradually achieve a higher level of understanding of urban air pollution and the measures taken to monitor air quality and to prevent and control urban air pollution.

Urban Air Pollution in Asia

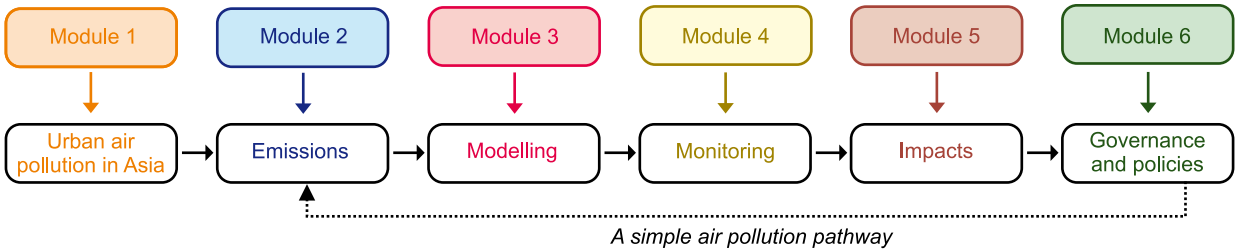
Urban air pollution affects the health, well-being and life chances of hundreds of million men, women and children in Asia every day. It is responsible for an estimated 537,000 premature deaths annually with indoor air being responsible for over double this number of deaths. It is often the poor and socially marginalized who tend to suffer disproportionately from the effects of deteriorating air quality due to living near sources of pollution.

Clean air is recognised as a key component of a sustainable urban environment in international agreements and increasingly in regional environmental declarations in Asia. National and local governments have begun to develop air quality management strategies to address the deterioration in urban air quality. However, the scope and effectiveness of such strategies vary widely between countries and cities.

The aim of air quality management is to maintain the quality of the air that protects human health and welfare but also to provide protection for animals, plants (crops, forests and vegetation), ecosystems and material aesthetics, such as natural levels of visibility. In order to achieve this goal, appropriate policies, and strategies to prevent and control air pollution need to be developed and implemented.

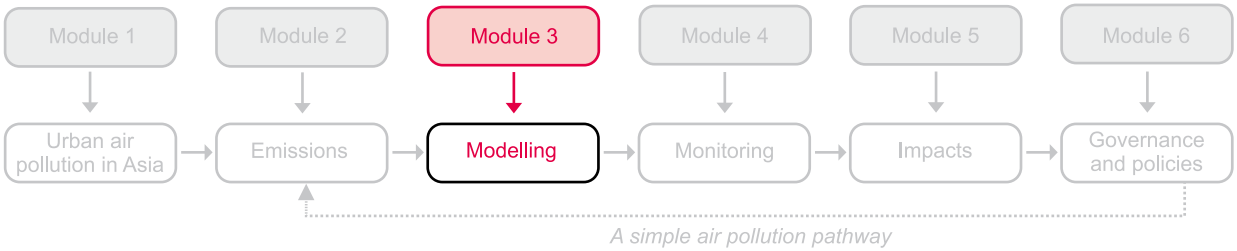
Module Structure

The foundation course consists of six modules which address the key components of air quality management. An international team of air pollution experts have contributed to the development of the course. Each module is divided into a number of sections each devoted to a different aspect of the issue, together with examples and key references.

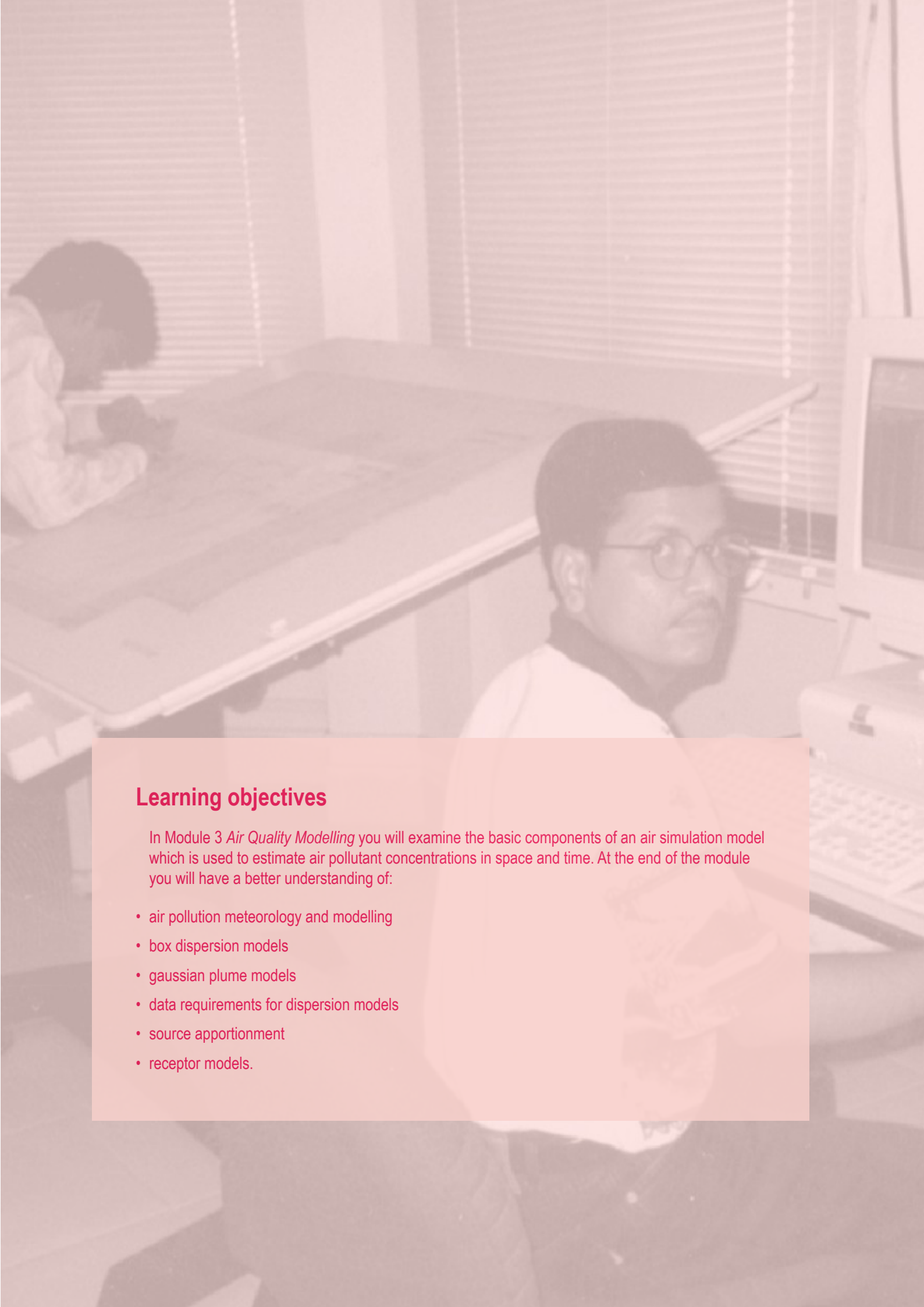


A simple air pollution pathway

Module 3 - Modelling



A simple air pollution pathway



Learning objectives

In Module 3 *Air Quality Modelling* you will examine the basic components of an air simulation model which is used to estimate air pollutant concentrations in space and time. At the end of the module you will have a better understanding of:

- air pollution meteorology and modelling
- box dispersion models
- gaussian plume models
- data requirements for dispersion models
- source apportionment
- receptor models.

List of Acronyms and Abbreviations

ABC	Atmospheric brown cloud
ACFA	Asian Clean Fuels Association
ACS	American Cancer Society
ADAC	Automatic data acquisition system
ADB	Asian Development Bank
ADORC	Acid Deposition and Oxidant Research Center
AirQUIS	Air quality information system
ALAD	Aminolaevulinic acid dehydrase
AMIS	Air quality management information system
APHEA	Air Pollution and Health, A European Approach
API	Air pollution index
APINA	Air Pollution Information Network
APMA	Air pollution in the megacities of Asia project
APNEE	Air Pollution Network for Early warning and on-line information Exchange in Europe
AQG	Air quality guideline
AQM	Air quality management
AQMS	Air quality management system
AQO	Air quality objective
AQSM	Air quality simulation model
As	Arsenic
ASEAN	Association of South East Asian Nations
ASG	Atmospheric Studies Group
ATD	Arizona test dust
AWGESC	ASEAN Working Group on Environmentally Sustainable Cities
AWS	Automatic weather station
BaP	Benzo[a]pyrene
BBC	British Broadcasting Corporation
BMR	Bangkok Metropolitan Area
BRT	Bus rapid transit
BS	Black smoke
BTEX	Benzene, toluene, ethylbenzene and xylenes
CAI-Asia	Clean Air Initiative for Asian Cities
CAIP	Clean air implementation plan
CARB	Californian Air Resources Board
CAS	Chemical Abstract Service
CBA	Cost benefit analysis
Cd	Cadmium
CD	Compact disc
CDM	Clean development mechanism
CEA	Cost-effectiveness analysis
CER	Certified emissions reduction
CMAS	Institute for the Environment, Chapel Hill
CMB	Chemical mass balance
CNG	Compressed natural gas
CO	Carbon monoxide
CO_2	Carbon dioxide
COHb	Carboxyhaemoglobin
COI	Cost of illness
COPD	Chronic obstructive pulmonary disease
CORINAIR	CORe INventory of AIR emissions
CPCB	Central Pollution Control Board
CSIRO	Commonwealth Scientific and Industrial Research Organisation
CVM	Contingent valuation method
DALY	Disability-adjusted life years
DAS	Data acquisition system
DDT	Dichloro-Diphenyl-Trichloroethane
DETR	Department for Transport and the Regions
DQO	Data quality system
DQO	Data quality objective
DWM	Diagnostic wind model
EB	Executive board
EC	European Commission
EEA	European Environment Agency
EGM	Eulerian Grid Module
EIA	Environmental impact assessment
ETS	Environmental tobacco smoke
EU	European Union
FID	Flame ionisation detector
FOE	Friends of the Earth
FST	Foundation for Science and Technology
GBD	Global burden of disease
GDP	Gross domestic product
GHG	Greenhouse gas
GIS	Geographic information system
GTF	Global Technology Forum
HAP	Hazardous air pollutant
HC	Hydrocarbon
HCA	Human capital approach
HCMC	Ho Chi Minh City
HEI	Health Effects Institute
HEPA	Ho Chi Minh City Environmental Protection Agency
Hg	Mercury
HIV/AIDS	Human immunodeficiency virus/ Acquired Immunodeficiency Syndrome
I&M	Inspection and maintenance
IBA	Ion beam analysis
ICCA	International Council of Chemical Associations
IFFN	International Forest Fire News
IPCC	Intergovernmental Panel on Climate Change
IQ	Intelligent quotient
IR	Infrared
ISO	Organization for Standardization
IT	Interim target
IUGR	Intrauterine low growth restriction
IUPAC	International Union of Pure and Applied Chemistry
IVL	Swedish Environmental Research Institute
km	kilometre
LBW	Low birth weight
LCD	Less developed country
LPG	Liquid petroleum gas
LPM	Lagrangian particle module
MAPs	Major air pollutants
MCIP	Meteorology-Chemistry Interface Processor
MMS	Multimedia messaging service
MOEF	Ministry of Environment and Forests
MOPE	Ministry of Population and Environment
MT	Meteo-Technology
MW	Molecular weight
NAA	Neutron activation analysis
NAAQS	National Ambient Air Quality Standards
NASA	National Aeronautics and Space Administration
NDIR	Non-dispersive Infrared
NILU	Norwegian Institute for Air Research
NKBI	Neutral buffered potassium iodide
NMMAPS	National Morbidity and Mortality Air Pollution Study
NO	Nitric oxide
NO_2	Nitrogen dioxide
NO_x	Nitrogen oxides
NYU	New York University
O_2	Oxygen
O_3	Ozone
OECD	Organization for Economic Cooperation and Development
PAH	Polycyclic aromatic hydrocarbons
PAN	Peroxyacetyl nitrate
Pb	Lead
PbB	Level of blood lead
PCB	Polychlorinated biphenyl
PCD	Pollution Control Department
PDR	People's Democractic Republic
PESA	Proton elastic scattering analysis
PID	Photo ionisation detector
PIGE	Particle induced gamma ray emission
PILs	Public interest litigation
PIXE	Particle induced X-ray emission
PM	Particulate matter
PM_{10}	Particulate matter less than 10 microns in diameter
$PM_{2.5}$	Particulate matter less than 2.5 microns in diameter
PMF	Positive matrix factorisation
POP	Persistent organic pollutant
PPM	Parts per million
PRC	People's Republic of China
PSAT	Particulate matter source apportionment technology
PSI	Pollutant standard index
PSU/NCAR	Pennsylvania State University / National Center for Atmospheric Research
PVC	Polyvinyl chloride
QA/QC	Quality assurance/quality control
QEPA	Queensland Environmental Protection Agency
ROS	Reactive oxygen species
RBS	Rutherford backscattering spectrometry
SA	Source apportionment
SACTRA	Standing Advisory Committee on Trunk Road Assessment
SAR	Special Administrative Region
SMC	San Miguel Corporation
SMS	Short message service
SO_2	Sulphur dioxide
SO_x	Sulphur oxides
SPCB	State Pollution Control Board
TAPM	The Air Pollution Model
TEA	Triethanolamine
TEAM	Total Exposure Assessment Methodology
TEOM	Tapered element oscillating microbalance
TSP	Total suspended particulate
UAM	Urban airshed model
UCB	University of California at Berkeley
UF	Ultra fine
UK	United Kingdom
UNDESA	United Nations Department of Economic and Social Affairs
UNDP	United Nations Development Programme
UNECE	United Nations Economic Commission for Europe
UNEP	United Nations Environment Programme
UNFCCC	United Nations framework on climate change
UN-Habitat	United Nations Habitat
US	United States
USEPA	United States Environmental Protection Agency
UV	Ultra violet
UVF	Ultra violet fluorescence
VOC	Volatile organic compound
VOSL	Value of statistical life
VSI	Visibility Standard Index
WAP	Wireless Application Service WHO World Health Organization
WMO	World Meteorological Organization
WRAC	Wide ranging aerosol collector
WTP	Willingness to pay
XRF	X-ray fluorescence
YLD	Years of life with disability
YLL	Years of life lost

List of Tables, Figures and Boxes

Introduction

An air quality simulation model system (AQSM) is a numerical technique or methodology for estimating air pollutant concentrations in space and time. It is a function of the distribution of emissions and the existing meteorological and geophysical conditions. An alternative name is dispersion model. Air pollution concentrations are mostly used as an indicator for human exposure, which is a main component for risk assessment of air pollutants on human health. An AQSM addresses the problem of how to allocate available resources to produce a cost-effective control plan. In this context, an AQSM can respond to the following types of questions:

- What are the relative contributions to concentrations of air pollutants from mobile and stationary sources?
- What emission reductions are needed for outdoor concentrations to meet air quality standards?
- Where should a planned source of emissions be sited?
- What will be the change in ozone (O_3) concentrations if the emissions of precursor air pollutants (e.g. nitrogen oxides (NO_x) or hydrocarbons (HC)) are reduced by a certain percentage?
- What will be the future state of air quality under certain emission reduction scenarios?

Figure 3.1 shows the main components of an AQSM.

An alternative and complementary model is source apportionment (SA). SA starts from observed

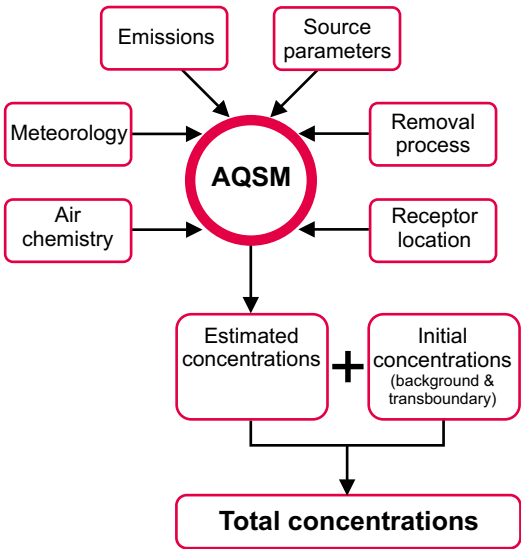


Figure 3.1: Basic components of air quality modelling

concentrations and their chemical composition and estimates the relative contribution of various source types by comparing the composition of sources with the observed composition at the receptors. For this reason SA is also called receptor modelling.

This module provides an understanding of the basic components of an air simulation model which is used to estimate air pollutant concentrations in space and time. It discusses the application of dispersion models and the key data requirements. It examines the use of meteorological data in air quality modelling and the different types of dispersion models available. It presents the different approaches to source apportionment, which are used in determining the contribution of different air pollution sources.

Section 1 Basic Components of an Air Quality Simulation Model

1.1 Emission Estimates

Emission estimates are calculated in a sub-model of the AQSM. In such a model, emission estimates must be developed from basic information such as traffic modal distribution, vehicle fleet age, vehicles types, industrial processes, resource use, power plant loads, and fuel types. As described in Module 2 *Emissions*, empirically derived emission factors are applied to these basic data to estimate emission loads. Pollutant concentrations calculated by AQSM can never be more accurate than the input emissions estimates, unless the model is adapted to monitored pollutant concentrations.

1.2 Applications of Dispersion Models

Starting from reliable emission estimates and using monitored or modelled meteorological data, dispersion models can be applied to simulate air pollutant concentrations at receptor sites at costs much lower than those for air pollutant monitoring. In addition, dispersion models are the only means to estimate concentrations in the following situations. Among many capabilities, dispersion models can:

- estimate spatial distributions of air pollutant concentrations;
- quantify source contributions at receptor locations (e.g. at various points in a residential area);

Table 3.1: Capabilities of air pollution monitoring and modelling in undertaking certain tasks

Task	Monitoring capability	Dispersion modelling capability
to be undertaken	for undertaking the task	
Spatial distributions	Yes, but expensive if a narrow grid network of monitoring sites is needed	Yes
Temporal distributions	Yes, if automatic continuous analysers are employed	Yes, if continuous meteorological and emission data are available
Source apportionment – source-oriented	No	Yes
Source apportionment – receptor-oriented	Yes, if monitoring and modelling are applied simultaneously	
"Exotic" compounds (e.g. gaseous mercury)	No, if monitoring methodology does not exist or is too expensive	Yes
Realisation of planned projects	No	Yes
Hot spot estimation	Yes, if sufficient a-priori knowledge is available	Yes
Forecasting	No	Yes
Estimating outdoor exposures	Yes, if personal monitors are applied	Yes, if time use pattern of human activities are available
Estimating indoor exposures	Yes, if personal monitors are applied	No

- provide concentrations of a compound ("exotic" pollutant) for which measuring methodologies do not exist or are too expensive;
- provide estimates on the impacts of the realisation of a planned manufacturing facility or of process changes in an existing plant;
- estimate the impacts at receptor sites in the vicinity of a planned road or those of envisaged changes in traffic flow;
- support the selection of appropriate monitoring sites (e.g. for "hot spots") when no knowledge on potential concentrations is available;
- forecast air pollution concentrations; and
- help estimate exposures by simulating concentrations and duration of meteorological episodes.

Thus, dispersion modelling is a complementary tool to air pollution monitoring. Table 3.1 summarizes the capabilities of air pollution monitoring and modelling for certain tasks.

Section 2 Air Pollution Meteorology and Modelling

2.1 Parameters of Air Pollution Meteorology

Once pollutants are released into the atmosphere they are transported by air motions which lower the air pollutant concentrations in space over a period of time. Meteorological parameters averaged over one-hour time intervals are usually used to describe this phenomenon. Meteorological parameters include wind speed, wind direction, turbulence, mixing height, atmospheric stability, temperature and inversion.

Wind

Wind is a velocity vector having direction and speed. Usually only the horizontal components of this vector are considered since the vertical component is relatively small. The wind direction is the direction from which the wind comes. Through wind speed, continuous pollutant releases are diluted at the point of release. Concentrations in the plume are inversely proportional to the wind speed.

Wind speed is expressed in the unit metre/second (m/s). At the ground wind speed must be zero. Therefore the wind speed is lower close to the ground than at higher elevations. Figure 3.2 shows typical relationships between wind speed and height during day- and night-time. The wind speed u(z) at a vertical height z above the ground is a function of z and proportional to the power law z^p where p is an exponent which depends primarily on atmospheric stability. The exponent p varies and is approximately 0.07 for unstable conditions and 0.55 for stable conditions (Turner, 1994).

Figure 3.2 also shows examples of the height dependence of temperature during day- and night-time. During the day, while the ground is heated up by solar radiation, temperature decreases linearly with height. During the night, temperature first increases with height and then starts to decrease similarly to that observed during the day.

Objects on the surface over which the wind is flowing will exert friction on the wind near to the surface. Height and spacing of the objects influence the magnitude of friction and the wind speed gradient as a function of height. The effect is described by the roughness length which ranges for urban areas between 1 and 3 m, for suburban areas approximately 0.5 to 1 m and for level areas between 0.001 m and 0.3 m.

Turbulence

Turbulence is the wind fluctuations over time scales smaller than the averaging time used to estimate the mean wind speed. Turbulence consists of eddies (circular movements of air) which may be oriented horizontally, vertically or at all orientations in between. There are two kinds of turbulence: mechanical and buoyant.

Mechanical turbulence is caused by objects on the surface and by wind shear, a slower moving air stream next to a faster moving current. Mechanical turbulence increases with wind speed and the roughness length. The turbulence created by wind shear is due to the increase of wind speed with height.

Buoyant turbulence is caused by heating or cooling of air near the earth's surface. During a sunny day with clear skies and light wind, the heating of the earth's surface creates an upward heat flux which heats the lower layers of the air. The heated air goes upward and thus creates an upward-rising thermal stream – positive buoyant turbulence. At night with light winds, the outgoing infrared radiation cools the ground and the lower layers of the air above while temperature at the higher air layers is unaffected. The cooling near the ground results in a net downward heat flux and

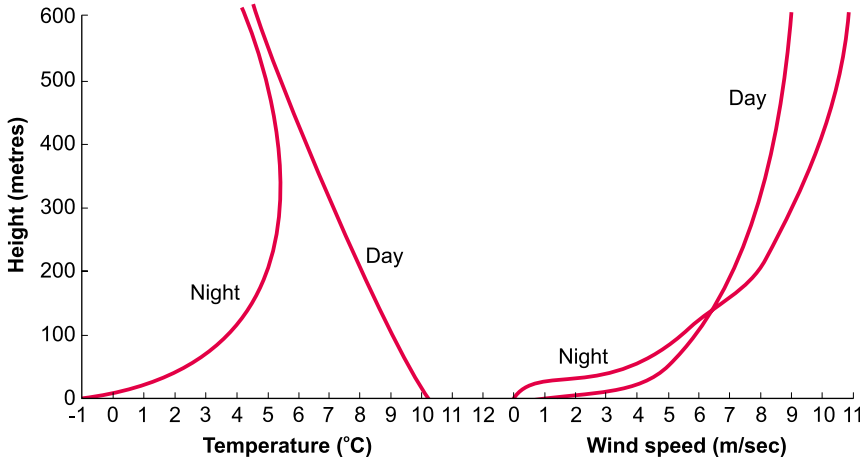


Figure 3.2: Variation of wind speed and temperature with height

Source: Turner (1994)

leads to a temperature inversion (see Figure 3.2) which is a temperature structure inverted from the usual decrease of temperature with height. The temperature inversion causes the atmosphere to become stable and inhibit vertical motion – negative buoyant turbulence.

The generation of mechanical turbulence is always positive but smaller than the positive buoyant turbulence. The negative buoyant turbulence during night-time tends to reduce mechanical turbulence.

Mixing height

During an hourly period on a sunny day upward-rising thermal streams, which characterise unstable atmospheric conditions, will move in the wind direction. A series of upward and compensating downward motions will result in substantial vertical dispersion of the pollutants. Since the eddy structures point to all possible directions there is also substantial horizontal dispersion.

In contrast, at night, with clear skies and light wind, a minimum of buoyant turbulence is extant, characterising stable thermal conditions which also damps out mechanical turbulence.

If the net heat flux at the ground is nearly zero, the condition is characterised as neutral. The vertical thermal structure is a slight decrease of temperature with height, approximately 10°C with each 1000 m height increase (dry adiabatic lapse rate). Atmospherically neutral conditions can be caused by:

- cloudy conditions;
- windy conditions; and
- transitional conditions near sunrise and sunset.

These conditions induce an intermediate level of dispersion.

The mixing height is defined as the upper limit to dispersion of atmospheric pollutants. Under unstable conditions, there is a vigorous vertical mixing from the ground to approximately 1 km and then negligible vertical mixing above that height. For stable conditions the mixing height is much lower.

Stability and plume types

Under unstable conditions a visible continuously emitted plume will appear as large loops (see Figure 3.3). This plume structure is called "looping". Looping is due to the upward motions of the heat flux and the compensating downward motions occurring as the plume is transported downwind.

Considerable vertical and horizontal dispersion of the effluent is taking place during every one-hour period.

Under neutral conditions turbulence is mostly mechanical. As turbulent eddies have many different orientations the resulting vertical and horizontal dispersion is relatively symmetrical. The resulting plume looks like a cone and dispersion under neutral conditions is described as "coning" (see Figure 3.3).

Vertical motion of the plume is inhibited under stable conditions with a temperature inversion and a low mixing height. Horizontal motion is not influenced by temperature and the horizontal extension of the plume may take many appearances. If the horizontal spreading is considerable, the plume is said to be "fanning" (see Figure 3.3).

Inversion, fumigation, stagnation

By definition, an inversion exists when warmer air overlies cooler air. There are four processes to produce an inversion:

- cooling of a layer of air from below (surface inversion);
- heating of a layer of air from above (elevated inversion);

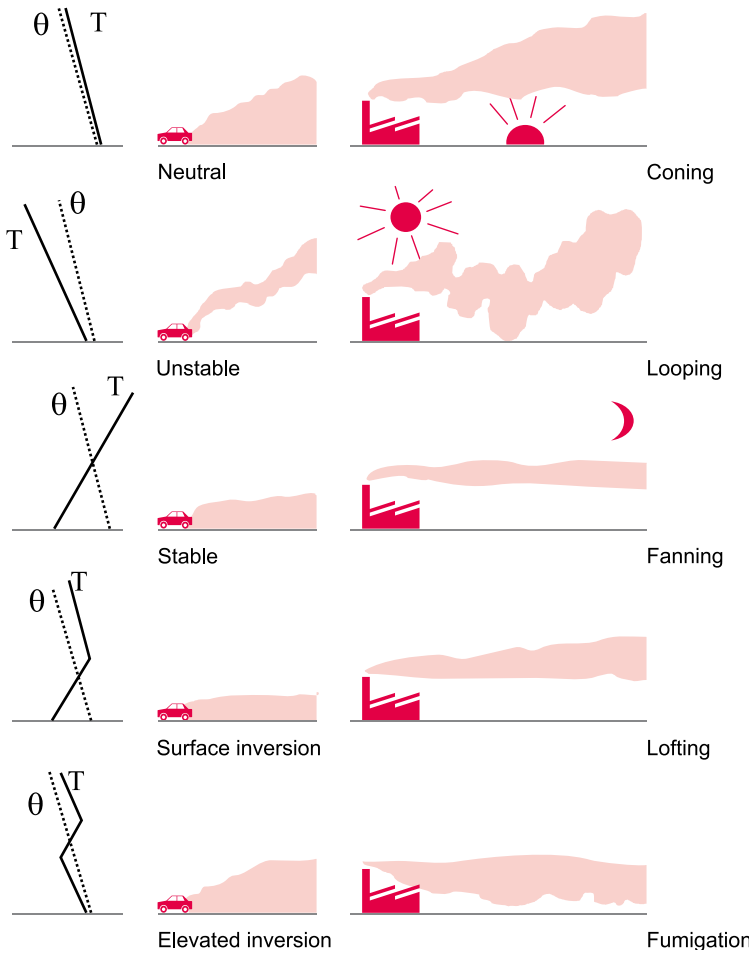


Figure 3.3: Vertical dispersion under various conditions for low and high elevations of the source [T: Temperature, θ: Adiabatic lapse]

Source: Adapted from Liptak (1974)

- flow of a layer of warm air over a layer of cold air (surface inversion); or
- flow of a layer of cold air under a layer of warm air (elevated inversion).

All of these occur, although the first process (cooling from below) is the more common.

Inversion due to cooling of air at the surface
Shortly before sunset, the ground surface begins to cool by radiation and cools the air layer nearest to it. By sunset, there will be a strong but shallow inversion close to the ground. All night this inversion will grow in strength and height, until by dawn of the next day, the temperature profile will be practically the same as that shown for dawn. As the temperature of the air adjacent to the ground is below that of the air at some heights above, air pollutants released in this layer are trapped because the air being colder than the layer above it will not rise. This is called "stagnant inversion".

Inversion due to heating from above
Heating an air layer from above can simply occur when a cloud layer absorbs incoming solar radiation. However, it often occurs when there is a high-pressure region (common in summer between storms) in which there is a slow net downward flow of air and light winds. The sinking air mass will increase in temperature at the adiabatic lapse rate (the change in temperature of a mass of air as it changes height). It often becomes warmer than the air below it. The result is an elevated inversion, also called subsidence inversion or inversion aloft. These normally form 500 to 5000 m above the ground, and they inhibit atmospheric mixing. This type of inversions are common in sunny, low-wind situations such as Los Angeles in summer.

Flow of a layer of warm air over a layer of cold air
If a flow of warm air meets a layer of cold air, the warm air mass could simply sweep away the colder air. Under certain circumstances such as trapping the cold air by mountains, a mass of warm air is caused to flow over a cold dome. Even without mountains, atmospheric forces alone can cause a mass of warm air to flow over a cold mass. This is called an "overrunning" effect, when warm air overrides cold air at the surface.

Inversion due to flowing of cool air under warm air
A horizontal flow of cold air into a region lowers the surface temperature. As cold air is denser and flows laterally, it displaces warmer and less dense air upwards. This phenomenon is called 'advection inversion'. It is common where cool maritime air blows into a coastal area and can occur any time of the year. This type of inversion is generally short-lived and shallow.

When cold air flows down a slope from a higher elevation into a valley and displaces warmer air upwards this often leads to inversions at the bottom of the valley. The cold air traps all pollutants released in this layer. The phenomenon is called 'cold-air drainage inversion'. In effect, the valley collects all the ground cooled air from the higher elevations above it. If condensation results and fog is formed, the sun can not get to the ground during the day and the inversion can persist for days.

Fumigation
In air pollution, fumigation is defined as the appearance at ground level of pollutants that were previously:

- in a poorly dispersed smoke plume; or
- trapped in a temperature inversion; or
- trapped between two inversion layers as a result of turbulence (WHO, 1980).

An example is the turbulence arising from early morning heating of the earth's surface by the sun. The subsequent gradual warming of the atmosphere from the ground upwards "burns off" the inversion that builds up during night-time. As the strong convective mixing reaches a fanned plume, it immediately mixes the large pollutant concentrations of the plume towards ground level, "fumigating" that area. This process leads to

high but short-term ground level concentrations. The effect is particular strong if the plume from a shoreline source is carried inland by a stable onshore breeze. As the breeze passes inland, it encounters warmed air, increasing the convectional flow. A strong breeze will prevent the plume from mixing upward; and the convectional flow will drive air pollutants to the ground further inwards (see Figure 3.4).

2.2 Local and Regional Phenomena

Local phenomena such as mountain-valley winds, sea breezes, and other processes occurring at a particular place, all affect the transport of the pollutants. High concentration can accumulate within a city basin due to these phenomena. There are three reasons why the local circulation systems are not good pollution ventilators.

Firstly, the speed of these local circulations is usually rather low. Secondly, they are closed circulation systems. Thirdly, they exhibit a diurnal reversal in direction of flow. The latter two factors mean that there is little true air exchange. Instead of the flow replacing dirty air with 'clean' air, there is a back-and-forth 'slurrying' movement involving a rather limited volume of contaminated air (Oke, 1987).

The city thermal wind system, which is thought to exist with large scale stagnation, is particularly dangerous because the system is totally self-contained over an area of densely packed sources. The low level flow converges upon the city centre from all directions, rises, diverges aloft, and then moves outward to subside on the urban/rural fringe and rejoin the inflow.

On a wider scale, regional phenomena such as dust storms and haze from fires used to clear forests in South East Asia are currently adding to the local air pollution in many countries.

Dust storms contain large amount of mineral dust aerosols in most parts of the Asian region and are referred to as Yellow Sand Events in East Asia. Dust aerosols interact with urban air particulate pollutants. Thus, black carbon particles are becoming mixed with dust during a Yellow Sand Event and are transported across the Pacific Ocean. Figure 3.5 illustrates this phenomenon. Dust storms impair visibility, pose health hazards, and cause a strong perturbation to the atmospheric radiation budget.

In 2001, the United Nations Environment Programme (UNEP) reported the existence of an Atmospheric Brown Cloud (ABC) over parts of South Asia and the Indian Ocean, a visible brown-coloured atmosphere observed by satellites and

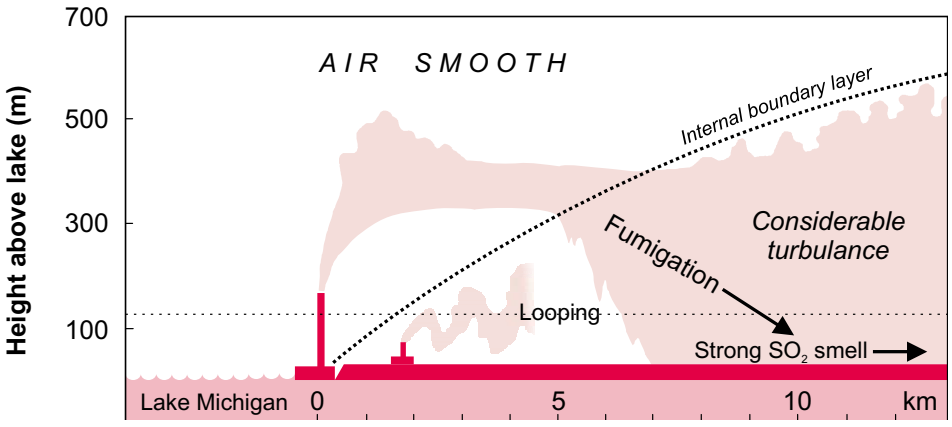


Figure 3.4: Fumigation

Source: Adapted from CGER (1992)

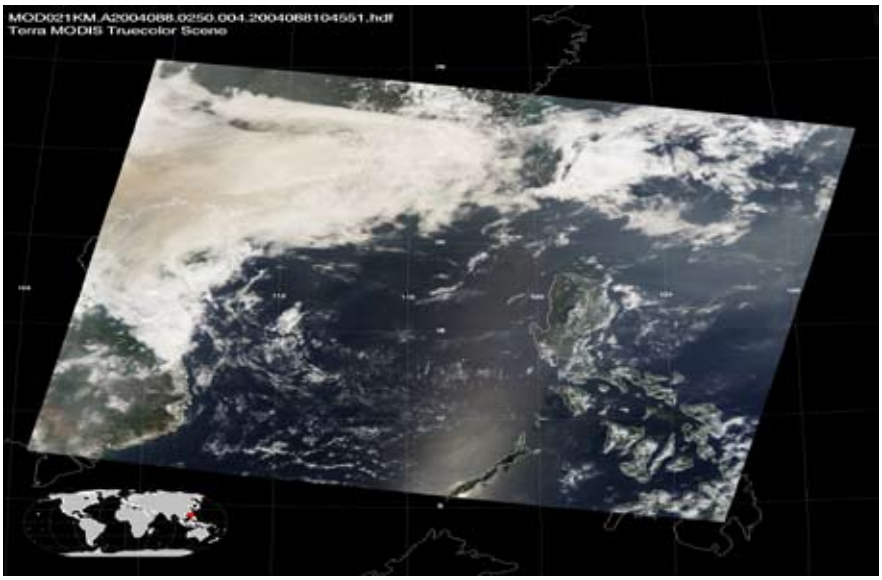


Figure 3.5: Aerosol clouds from dust storms over the Pacific (28 March 2004)

Source: NASA (2007)

aircraft and produced by sunlight absorbed and scattered by particles. The ABC is mostly made up of fine and ultrafine particles which consist of sulphates, nitrates, black carbon, hundreds of organic compounds, and fly ash. The ABC is likely to impair visibility, cause significant impacts on the atmosphere and pose health threats

2.3 Influence of Topography on Wind Speed and Direction

Topographical characteristics such as mountains, valleys, and urban areas all influence the diffusion of stack plumes and releases from low level sources. For a plume, the centreline may become distorted and have directions completely different from the main wind direction above the topographical influences. In mountainous region and valleys wind speed and direction may change substantially from one location to another (see Figure 3.6.).

In urban areas, wind speed and direction may be quite complicated in a street canyon (see Figure 3.7). In addition to the topographical characteristics of the area, atmospheric and surface thermal characteristics influence air motions particularly at low wind velocities.

Local wind velocities may be greater or lesser than would otherwise occur in the absence of heat

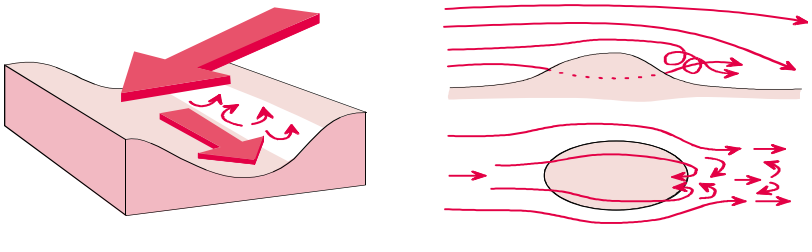


Figure 3.6: Wind flow in a valley and around a hill

Source: Sivertsen (2002).

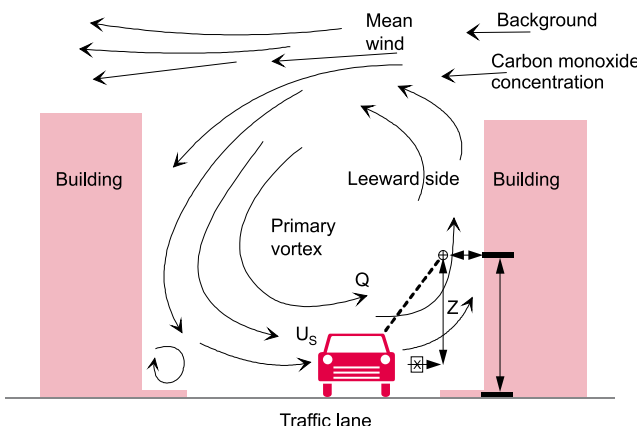


Figure 3.7: Wind pattern in a street canyon

Source: Sivertsen (2002)

emissions from buildings. It can easily be inferred that the airflow around urban structures will be completely different from the airflow in rural areas. Correspondingly, the dispersion of air pollutants is a complex phenomenon and concentrations within a street canyon vary for different wind directions above the urban structure and different shapes of the buildings (Kim *et al*., 2005).

2.4 Meteorological Measurements

In situ meteorological measurements are normally required to provide an input to air quality modelling. The primary directly measured variables include wind speed (three dimensional), wind direction, temperature at two elevations, relative humidity, precipitation, pressure, and solar radiation. Turbulence and mixing height may also be primary variables although they are often estimated by indirect methods of *in situ* or remote temperature sensing. Remote sensing of wind speed and direction and humidity also enhance the meteorological data input to modelling.

Ambient air temperature and relative humidity are the most usual temperature measurements. Ambient air temperature is measured using a thermometer. Humidity is measured with a hygrometer, based on absorption of humidity. As solar radiation easily disturbs such measurements, they are performed in a shielded but at the same time ventilated surrounding (e.g. special housings with louvered screens).

The Automatic Weather Station

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

- wind speed;
- wind direction;
- temperature and/or vertical temperature gradient;
- net radiation;
- wind fluctuations or turbulence;
- relative humidity;
- precipitation; and
- atmospheric pressure.

Some of these data overlap each other. The final selection of parameters will depend on the instruments available and the type of specific data needed for the user.

The Automatic Weather Station (AWS) will collect high-quality, real-time data that is normally used in a variety of weather observation activities ranging from air quality data assessment and industrial accidental release forecasting to long-term modelling for planning purposes.

The weather station designed for air quality studies will have to provide surface data and meteorological information in the surface boundary layer and in the troposphere as a whole. For the purpose of explaining air pollution transport and dispersion most of the sensors may be located along a 10 m high mast.

The basic suite of sensors will measure wind velocity and wind direction, temperature, relative humidity, air pressure, and precipitation. The expanded suite of sensors may offer measurement of solar radiation, net radiation, wind fluctuations (turbulence), vertical temperature gradients and visibility.

To obtain electric power and a data retrieval system with modems and computers, the AWS is often located with one or several of the air quality monitoring stations.

Wind Profiles

Wind speed and direction measurements can be performed using conventional wind vanes. If high frequency measurements are necessary, sonic anemometers are useful. There are low-cost devices.

To measure wind direction and wind speed throughout the atmospheric boundary layer it is useful to use radiosondes and vertical measurements using weather balloons. It is also possible to install a wind profiler or a Doppler Sodar system (DS) at one station in the selected area of interest.

Doppler Sodars are a form of atmospheric echo sounder (or acoustic radar). An audible "beep" is beamed up into the atmosphere and very faint echoes from features within the air itself are detected back at the ground. Reflection (echoing) is caused by unevenness (inhomogeneity) in the structure of the atmosphere. The inhomogeneity results from mainly small, localised differences in air density and humidity due to differences in temperature. This unevenness occurs particularly in regions of turbulent air.

Turbulence

Scintillometers measure the turbulence across a large area (see Box 3.1).

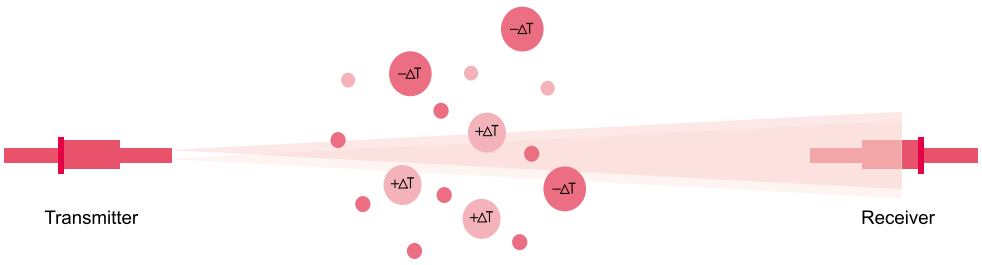
For temperature, humidity or water vapour profiles across the boundary layer radiosondes and tethered balloons can also be considered.

In cold climates, where humidity level is low (mountain, polar, or upper air measurements) the use of a condensation method is preferable. Hygrometers based on this principle are generally called chilled mirror hygrometers.

Precipitation (rain, hail, snow, hoarfrost and fog) is measured using precipitation gauges. The most common types are weighing or tipping buckets. However, the accuracy of these instruments is debatable due to evaporation phenomena. The use of weather sensors might therefore be more advantageous.

Box 3.1

Function of the Scintillometer



Optical scintillation is the observed intensity of a remote light source. It is caused by fluctuations of the refractive index in the air. The fluctuations are caused by changes in temperature, density, pressure and moisture content of the air. A scintillometer uses this effect to measure atmospheric turbulence. Scintillometers are highly sensitive, accurate and reliable instruments without any moving parts. With a beam laser technique scintillometers deliver extensive turbulence information, including the fluxes of heat and momentum.

Source: Scintec (2007), WAU (2002)

[ΔT denotes temperature fluctuations]

One of the most important meteorological radiation parameters is global solar radiation, measured with a pyranometer (see Box 3.2). A pyranometer is suitable for measuring global sun plus sky radiation. Usually, the required measurement is energy flux density of both direct beam and diffuse sky radiation passing through a horizontal plane of known unit area. Solar radiation in locations with a small area varies significantly by region, season and time of day, surrounding terrain elevation, man-made and/or natural obstructions. The pyranometer is standardised according to the international standard ISO 9060:1990, that is also adopted by the WMO. The standard discriminates three classes of devices: "secondary standard", "first class", "second class".

Useful information including recommendations for specific manufacturers on meteorological devices is provided on the Meteo-Technology website (MT, 1999-2007).

The choice of an instrument for a particular meteorological application should be guided by the data quality objectives (DQO) of the application. As a minimum, these DQO should include the accuracy and precision of the data needed for dispersion modelling applications. As for all measurements, a quality assurance/quality control (QA/QC) plan should be developed for meteorological measurements (USEPA, 2006a).

Box 3.2
The Pyranometer

In order to attain the proper directional and spectral characteristics, a pyranometer's main components include an electronic device (thermopile sensor) with a black coating that absorbs the solar radiation, converts it to heat, and generates a voltage output signal that is proportional to the solar radiation. The thermopile sensor has a flat radiation spectrum covering the range of 300 to 50000 nm. A glass dome limits the spectral response from 300 to 2800 nm and shields the thermopile sensor from convection.

One of the most important decisions in preparing for an air quality modelling analysis involves the selection of a site for monitoring, or choosing data from an existent meteorological data base. Data collected either way should be representative of the atmospheric conditions affecting the pollution in a given area of interest as determined by the locations of the sources and receptors

Figure 3.8: Pyranometer showing the glass dome, metal body, black sensor, and radiation screen.

Source: Hukseflux (2007)

for which dispersion modelling is undertaken. In complex terrain, multiple monitoring sites may be required to adequately represent spatial variation in the meteorological conditions.

Meteorological data are mostly collected for climatology and weather prediction purposes and not primarily to support air quality management (AQM) through atmospheric dispersion modelling. Only a limited amount of meteorological information relates to regulatory requirements or national AQM programmes.

2.5 Steady-state, Non Steady-state and Grid Meteorological Modelling

Meteorological models use mathematical formulae to simulate atmospheric processes such as the change of winds and temperature in time over an area of interest. These models are commonly used to develop meteorological inputs for dispersion models and photochemical models. Two types of meteorological modelling are distinguished: steady-state and non steady-state modelling.

In *steady-state modelling* applications start from the assumption that meteorological conditions are constant within the space-time area of the

application. Meteorological parameters determined at a single site in close vicinity of the source(s) are then considered representative of the meteorological variables in the whole area. These models typically focus on the meteorological conditions at the release height of the pollutants (e.g. stack height or the plume height in case of buoyant sources).

Steady state modelling would be applicable in a fairly homogeneous area which can be considered as only mildly changing in topographic parameters such as surface roughness, ground cover, presence or absence of water bodies, mountains, urban structures, etc. In addition, the use of meteorological information from other data sources should be judged by comparing its spatial representativity with respect to the surface characteristics that generally describe the analysis area.

Representativity has an entirely different interpretation for non-steady-state modelling applications, which commonly employs three-dimensional meteorological fields based on measurements at surface and upper air (anything above the height of a tower) sites. The meteorological models which support these applications are designed to appropriately blend available routine weather station data, local site-specific data, and mesoscale data. Because there will not be meteorological sites at every point on the ground and in the upper air, meteorological models must be used to interpolate and extrapolate this 'missing data'.

Two different types of meteorological model provide a three-dimensional grid of meteorological data:

- diagnostic wind models (DWM), which interpolate and/or extrapolate meteorological observations; and
- prognostic or 'mesoscale' models.

The meteorological model outputs can then be used to drive a dispersion model.

Diagnostic meteorological models

Diagnostic meteorological models use data from available locations and assign values to the meteorological variables throughout a three-dimensional grid by interpolation and extrapolation. The conservation of mass principle is applied throughout the process. The term 'diagnostic' is used because the input data and model results are for the same time period. Diagnostic models are not predictive, and their calculated fields for each time interval do not depend on fields at previous times.

An example is CALMET, a diagnostic meteorological model developed as a component of the CALPUFF modelling system (ASG, 2007) for use in air quality applications. CALMET is designed to produce hourly fields of three-dimensional winds and other micro-meteorological variables based on available surface and upper air meteorological observations only. Advantages of CALMET include:

- incorporation of observed data can produce realistic meteorological fields;
- reproduction of small-scale effects due to a resolution of a couple of hundred meters;
- outputs from prognostic meteorological models can be introduced as input into CALMET.

Limitations of CALMET are its complexity of use and the lack of meteorological data in less developed countries.

Prognostic meteorological models

Prognostic models are driven by large-scale synoptic analyses and numerically solve the equations of atmospheric dynamics to determine local meteorological conditions. They do not require local meteorological data to run, although if data are available they should be compared with model results to validate the model. Prognostic models are able to represent all scales, from global down to regional (500-1000 km) to features on scales in the range 1-10 km. The prognostic models describe the three-dimensional fields of temperature, wind speed and direction, and moisture through the region at high spatial resolution.

A three-dimensional prognostic mesoscale model is MM5, developed by Pennsylvania State University/ National Center for Atmospheric Research (PSU/ NCAR, 2006) and available free of charge. MM5 has the following advantages:

- assimilates local meteorological data;
- provides realistic dynamical and physical meteorological fields even in data-sparse areas, suitable for simulations in a complex environment;
- output meteorological fields can be fed into dispersion models.

Disadvantages of the MM5 model include high computational demand and the necessity of expertise of users.

MM5 output can be used with dispersion models such as CALPUFF or the Chemical Transport model (CTM) of the Models-3 Community Multiscale Air Quality (CMAQ) modelling system (Schere, 2002). Figure 3.9 presents an example of the application of the model. Over the next few years it is expected that both real-time and historical meteorological modelling will begin to use the Weather Research and Forecast (WRF) modelling system. This state-of-the-art system will serve as an update to MM5. It is designed to be a flexible, state-of-the-art atmospheric simulation system that is portable and efficient on available parallel computing platforms. WRF is suitable for use in a broad range of applications across scales ranging from metres to thousands of kilometres and will also be community-based (Skamarock *et al.*, 2005). More information on real time prognostic model can be obtained from USEPA (2006b).

2.6 Air Pollution Forecast Models

Air quality forecasts provide the public with air quality information with which they can make daily lifestyle decisions to protect their health. This information allows people to take precautionary measures to avoid or limit their exposure to unhealthy levels of air quality. In addition, many communities use forecasts for initiating air quality action or awareness days, which seek voluntary participation from the public to reduce pollution and improve local air quality. Current air quality forecasting models mostly focus on predicting ozone (O_3) and particulate matter (PM).

Many methods exist for predicting air quality concentrations. Some methods are simple and easy to operate, yet not very accurate. Other methods are more sophisticated and produce more accurate forecasts. Most forecasters use several methods to forecast O_3 and fine PM concentrations. Using several methods can balance one method's strengths with another method's limitations to produce a more reliable forecast. Since fine PM forecasting is new for most agencies, fewer fine particulate forecasting techniques have been tested and used. The success of an air quality forecasting program depends partly on accurate predictions, but also on meeting the needs and objectives of forecast users. Air quality forecasts so far could be used for three major purposes: public health notification, episodic control programmes ("Action Day", "Ozone Alert"), and scheduling specialized monitoring programmes. The questions compiled below assist in identifying forecast users' needs (USEPA, 1999; 2003).

Who will use the forecast?

Forecasters who know their target audience will have more insight into potential ways to adapt the forecast to the users' needs.

For which and how many months are the forecasts needed?

Understanding the time intervals of high O_3 or PM concentrations helps forecasters plan the resources (labour and data) needed for air quality forecasting.

What periods should a forecast cover?

Typically, air quality forecasts are made for the current- and next-day, however, they can be extended to include two- to five-day predictions. Longer-range predictions will likely be less accurate.

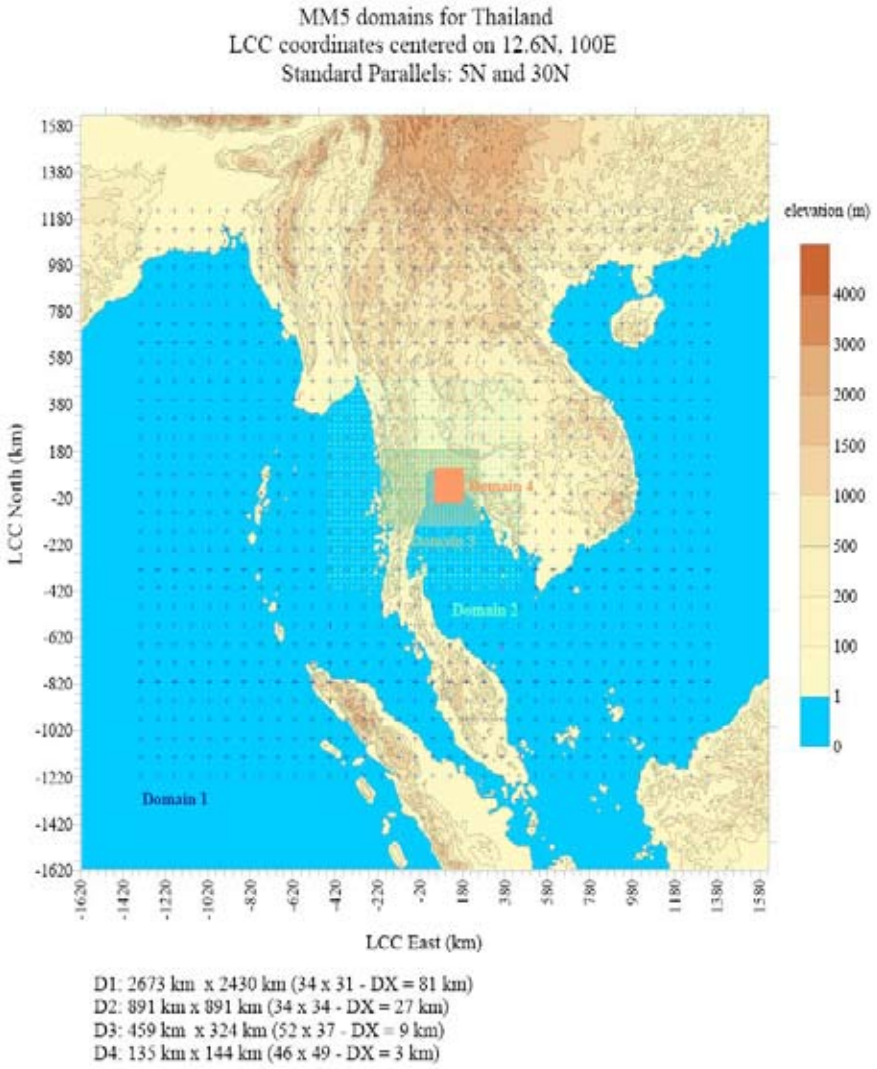


Figure 3.9: MM5 domain for Thailand

Are three-day forecasts needed for weekend/ holiday periods?

During weekends and holidays staff may be unavailable to produce daily forecasts and two- and/or three-day forecasts may be needed. An action plan should be in place to handle a situation with conditions differing appreciably from initial forecasts.

When should forecasts be issued to ensure public outreach deadlines are met?

Preparatory work is needed to communicate forecast information to the public, particularly during air quality episodes. Early issue of forecasts helps ensure effective communication to the public.

3

Section 3 Air Quality Dispersion Models

3.1 What Can a Dispersion Model Tell?

A dispersion model is a set of mathematical equations used for determining what happens to pollutants emitted in the atmosphere. It simulates the process of atmospheric dispersion, which mixes the pollutant with the existing air. The pollutant is transported by the mean wind and its concentration decreases due to atmospheric turbulence. A dispersion model estimates concentration levels at any point in space and, depending on the availability of meteorological information, for any time.

A dispersion model helps address the following issues:

- assessing compliance of concentrations from emissions of planned facilities with air quality guidelines and/or standards (including existent concentrations due to other sources);
- assessing the impact of emissions of a plant which is to undergo a process change;
- determining appropriate stack heights;
- assessing the contribution of individual plants to the overall concentrations;
- designing ambient air monitoring networks;
- evaluating the impact and efficiency of policy and mitigation strategies (e.g. the effect of emission standards);
- forecasting pollution episodes;
- assessing the risks of and planning for the management of rare events such as accidental hazardous substance releases;
- estimating concentrations of pollutants too difficult or expensive to measure;
- estimating the influence of geophysical factors on dispersion (e.g. terrain elevation, presence of water bodies and land use);
- tracking the originating source of accidental hazardous substance releases.

A dispersion model can replace monitoring and save cost and time.

Not every dispersion model can address the many processes in the atmosphere that occur during the transport of air pollution. Usually, a model considers part of those phenomena and leaves out others. The selection of a specific model depends on the task that has to be addressed.

3.2 Types of Models

All models assume a material balance equation which applies to a specified set of boundaries:

(Accumulation rate) = (Flow-in rate) – (Flow-out rate) + (Emission rate) – (Destruction rate)

The units of all terms in this equation is mass/time unit or g/s.

Box models

Box models (see Figure 3.10) illustrate the simplest kind of material balance.

To estimate the concentration in a city, air pollution in a rectangular box is considered under the following major simplifying assumptions:

- The city is a rectangle with dimensions W (downwind) and L (crosswind), both in units [m]. The box is defined by W·L·H [m^3] where H [m] is called the mixing height;
- The air pollution emission rate of the city is Q [g/s], which is independent of space and time (continuous emission). Q is related to emission rate per unit area, q [g/s·m^2] by:

$$Q = q \cdot (W \cdot L) \quad [g/s]$$

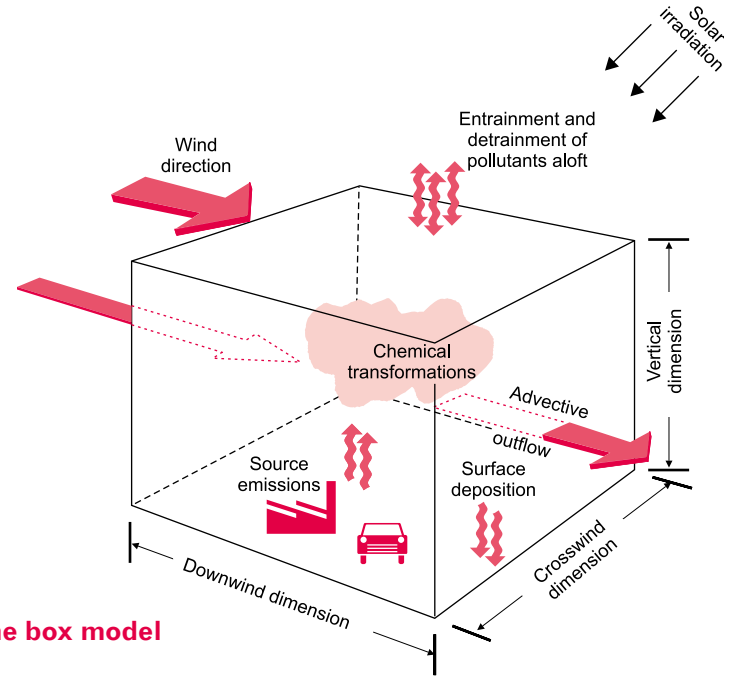


Figure 3.10: The box model

- The mass of pollutant emitted from the source remains in the atmosphere. No pollutant leaves or enters through the top of the box, nor through the sides that are parallel to the wind direction. No deposition, including gravitational settling or turbulent impaction occurs. No material is removed through chemical transformation (destruction rate equals zero).
- Atmospheric turbulence produces complete and spatial uniform mixing of pollutants within the box.
- The turbulence is strong enough in the upwind direction that the pollutant concentrations [mass/volume] from releases of the sources within the box and those due to the pollutant masses entering the box from upwind side are spatially uniform in the box.
- The wind blows with an average (constant) velocity u [m/s].

These assumptions lead to a steady state situation and the accumulation rate is zero. All the terms can then be easily quantified and calculated.

If $\chi(t)$ [g/m^3] denotes the pollutant concentration in the box as a function of time t and χ_{in} the (constant) concentration in the incoming air mass, the:

Flow-in rate = $L \cdot H \cdot u \cdot \chi_{in}$

Flow-out rate = $L \cdot H \cdot u \cdot \chi(t)$

Emission rate = Q

Destruction rate = 0

Accumulation rate= $W \cdot L \cdot H \cdot d\chi(t)/dt$

Then the differential equation emerges:

$$\mathbf{W \cdot L \cdot H \cdot d\chi(t)/dt = Q + L \cdot H \cdot u \cdot \chi_{in} - L \cdot H \cdot u \cdot \chi(t)}$$

which has the solution:

$$\mathbf{\chi(t) = Q/(L \cdot H \cdot u) \cdot (1 - \exp(-u \cdot t/W))}$$

For longer times t the concentration approaches a steady state ($\chi(t) = Q/(L \cdot H \cdot u)$) which corresponds to zero accumulation rate.

There are several drawbacks of box models. Firstly, some of the assumptions are unrealistic (e.g. wind speed independent of height or uniformity of air pollutant concentrations throughout the box). Secondly, the model does not distinguish a source configuration of a large numbers of small sources emitting pollutants at low elevation (cars, houses, small industry, and open burning) from that of a small numbers of large sources emitting larger amounts per source at higher elevation (power plants, smelters, and cement plants). Both types of sources are simply added to estimate a value for the emission rate per unit area (q). Of two sources with the same emission rate, the higher elevated one leads to lower ground level concentrations in reality. As there is no way to deal with this drawback, box models are unlikely to give reliable estimates, except perhaps under very special circumstances.

Gaussian dispersion models

The Gaussian model is based on the following assumptions:

- continuous emissions [mass/time unit, usually g/s];
- conservation of mass;
- steady-state meteorological conditions for the travel time of pollutant from source to receptor;
- concentration profiles in the crosswind direction and in the vertical direction (both perpendicular to the path of transport) are represented by Gaussian or normal distributions (see Figure 3.11).

A Gaussian model is the solution of the basic equations for transport and diffusion in the atmosphere assuming stationarity in time and complete homogeneity in space. A Gaussian dispersion model is normally used for considering a point source such as a factory smoke stack. It attempts to compute the downwind concentration resulting from the point source. The origin of the coordinate system is placed at the base of the stack, with the x axis aligned in the downwind direction. The contaminated gas stream, which is normally called "plume", is shown rising from the smokestack and then levelling off to travel in the x direction and spreading in the y and z directions as it travels.

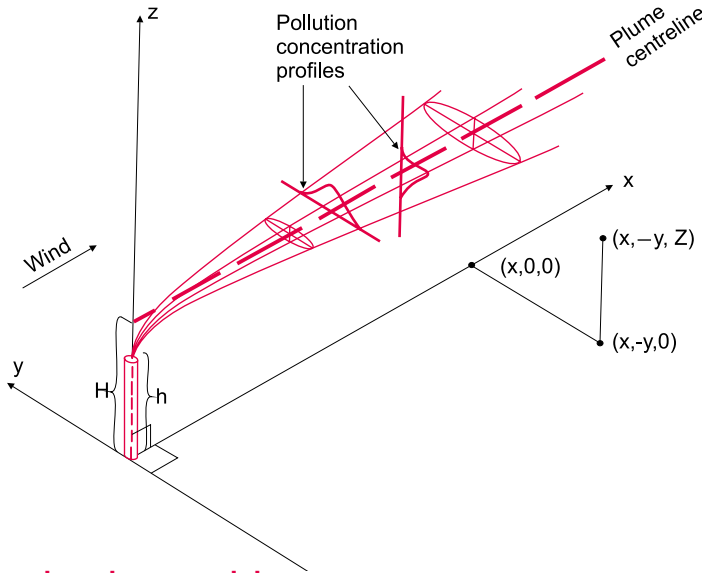


Figure 3.11 The Gaussian plume model

Source: Adapted from Turner (1994)

The plume normally rises to a considerable height above the stack because it is emitted at a temperature higher than that of ambient air and with a vertical velocity component. For Gaussian plume calculation, the plume is assumed to start from a point with coordinates (0,0,H), where H is called the effective stack height and is the sum of physical stack height (h) and the plume rise (dh).

It should be kept in mind that the Gaussian plume approach tries to calculate only the average values without making any statement about instantaneous values. The results obtained by Gaussian plume calculations should be considered only as averages over periods of at least 10 minutes, and preferably one-half to one hour. The Gaussian plume model so far allows one to estimate the concentration at a receptor point due to a single emission source for a specific meteorology. In this form, they are frequently used to estimate maximum concentrations to be expected from single isolated sources:

$$\chi(t) = Q/(2\pi \cdot u \cdot \sigma_y \cdot \sigma_z) \cdot \exp\{-y^2/(2 \cdot \sigma_y^2)\} \cdot [\exp\{-(H-z)^2/(2 \cdot \sigma_z^2)\} + \exp\{-(H+z)^2/(2 \cdot \sigma_z^2)\}]$$

In this equation $\sigma_y = a \cdot x^p$ is the standard deviation of the concentration distribution in the crosswind direction, in [m] at the downwind distance x; and $\sigma_z = b \cdot x^q$ is the standard deviation of the concentration distribution in the vertical direction, in [m], at the downwind distance x. a, b, p and q are constants depending on the stability of the atmosphere (Turner, 1994).

Figure 3.12 presents a typical result of a concentration simulation with the Gaussian model.

Gaussian plume models are also applied to estimate multi-source urban concentrations. The procedure is to estimate the concentration at various locations for each of the point, area and line sources in the city for each meteorological condition and then sum up over all sources, all wind directions, all wind speeds, and all stability classes, weighted by the frequency of their occurrence.

A recent application of the Gaussian plume model is recommended by USEPA under the name AERMOD Modelling System. It is a steady-state plume model that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain (USEPA, 2005). More sophisticated dispersion models are based on two different viewpoints regarding the movement of polluted air parcels:

The Lagrangian viewpoint is the viewpoint of a person riding along with the air. From this viewpoint, the ground appears to be passing below, much as the ground appears to be passing below a person in an airplane. In case of pollution plume or puff, the observer begins riding an air parcel along upwind of the stack from which the pollutant is emitted. As he passes directly over the stack, he reaches into a region of high concentration. The high concentration is localized in a thin thread of contaminated air that passed directly over the stack.

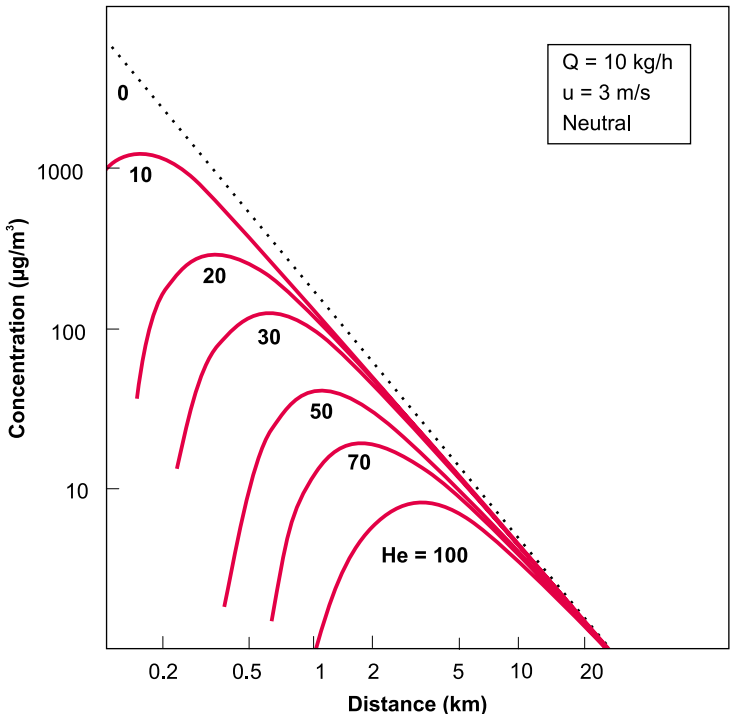


Figure 3.12: Simulated concentrations of a point source at ground level (effective stack height H in metres)

After that the thread of contaminated air expands by turbulent mixing. All the time, reference x is in the middle of the moving cloud. In a Lagrangian model the pollution distribution is described by a set of discrete "particles" (small air volumes) or puffs, which are labelled by their changing location (i.e. their trajectories are followed). Lagrangian particle models represent pollutant releases as a stream of "particles". Since the model "particles" have no physical dimensions, source types may be specified to have any shape and size, and the emitted "particles" may be distributed over an arbitrary line, area or volume (Ministry for the Environment, 2004).

The Eulerian viewpoint is the viewpoint of a person standing on the ground at the base of the emission source. In this case, x represents some fixed distance downwind from the emission point. Mostly, the distances are measured from the base of the stack, not from the centre of a moving cloud. In an Eulerian dispersion model the pollution distribution is described by changing concentrations at discrete points on a fixed grid. In some models, such as The Air Pollution Model (TAPM), a point source can be represented by either the Eulerian Grid Module (EGM), or by a hybrid Lagrangian Particle Module (LPM) for near-source dispersion, converting to EGM mode far from the source (Ministry for the Environment, 2004; CSIRO, 2005).

The Gaussian puff model uses the Gaussian equation in three-dimensional and Lagrangian viewpoints. An example of Gaussian puff model which is used as a non-steady-state air quality model is CALPUFF (see Figure 3.13). The model was developed originally by Sigma Research Corporation under funding provided by the Californian Air Resource Board (CARB) (ASG, 2007).

The specifications for the CALPUFF modelling system include:

- capability to treat time-varying point and area sources;
- suitability for modelling domains from tens of metres to hundreds of kilometres from a source;
- predictions for averaging times ranging from one-hour to one year;
- applicability to inert pollutants and those subject to linear removal and chemical conversion mechanisms;
- applicability for rough or complex terrain situations.

The modelling system (Scire *et al*., 1990a, 1990b) developed to meet these objectives consists of three components: (1) a meteorological modelling package with both diagnostic and prognostic wind field generators; (2) a Gaussian puff dispersion model with chemical removal, wet and dry deposition, complex terrain algorithms, building downwash, plume fumigation, and other effects; and (3) post-processing programs for the output fields of meteorological data, concentrations and deposition fluxes.

In April 2003, the USEPA proposed the CALPUFF modelling system as a guideline (Appendix A) model for regulatory applications involving long range transport (FR, 2005; USEPA, 2005). In addition it considered a case-by-case basis for near-field applications where non-steady-state effects (situations where factors such as spatial variability in the meteorological fields, calm winds, fumigation, recirculation or stagnation, and terrain or coastal effects) (see Figure 3.13).

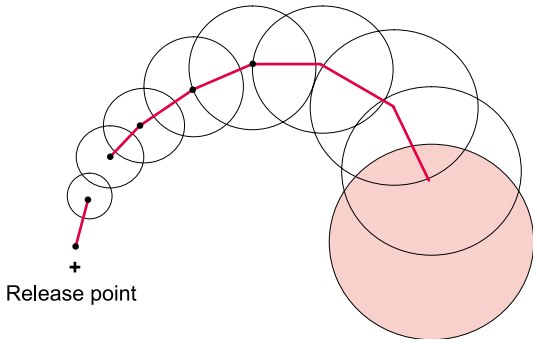


Figure 3.13: Puff modelling

Source: Ministry for the Environment (2004)

Eulerian dispersion models

Most of the models discussed so far deal with pollutants that are assumed to remain in the atmosphere forever. No pollutant really behaves that way but they all rather have natural removal mechanisms. Pollutants such as hydrocarbons (HC), nitrogen oxides (NO_x), and oxidants all undergo reactions in the atmosphere. The reaction times may also be comparable to travel time across a city, therefore, the simple box and Gaussian dispersion model, as presented so far, predict values much higher than the observed values. There are ways to modify the calculations to make correction factors. However, photochemical oxidants are normally complicated and their reaction rates expressions need to be solved simultaneously. Currently the most widely used approach to such problems is a multiple cell or Eulerian model such as the Urban Airshed Model (UAM) (UAM-IV; Isukapalli, 1999) or the Comprehensive Air Quality Model with eXtensions (CAMx, v4.42; Environ, 2005). In these models, the airspace over a city or a region is divided into multiple cells. Each cell is treated separately from the others. Generally the cell division in the x and y directions has uniform grid sizes, normally 2 to 5 km each way for the whole city. In the vertical direction, the layers are specified for more than four levels covering the mixing height. The upper boundaries move up and down with the variation of the mixing height over the day and from location to location within the city.

The basic equation of material balance is retained for each cell. A model simulation for a city and some time period begins with an assumed initial distribution of pollutants and pollutant precursors in all of the cells. Then for a time step of typically 3 to 6 minutes, the program calculates the change in "concentration" of the pollutant of interest and its precursors in each of the cells by numerically integrating the basic equation. This computation requires data or an estimating procedure for the wind velocity and direction at the centre of each cell. This is used for calculating the flows in and out across the boundaries. The computation will also include emission estimates for each of the ground-level cells, a subprogram to compute the chemical transformation during the time step in any cell, and a sub-program for the deposition of the pollutant in the ground-level cells.

Rather than trying to solve all the terms in the basic equation simultaneously, UAM, for example, first computes the changes in concentrations from the end of the previous time step. Then it computes the changes due to chemical reactions in the cell. The results of these two steps are added to estimate the concentration in each cell at the end of the time step.

To simulate a day or a few days in an urban area, this model requires a complete history of the wind pattern, solar inputs, and emissions. If these data are not available, the program has ways of estimating them. A common procedure is to choose a day on which the measured pollutant (usually O_3) concentration was the maximum for the past year or past few years. The model is run using the historical record of the wind speeds and directions, solar inputs, and estimated emissions for that day. The model's adjustable parameters are modified until the calculated concentrations match well with observed ambient concentrations for that day. Then the model is rerun with different emission rates or distributions, corresponding to proposed or anticipated future situations, and the meteorology for that day. In this way, the model performs a prediction of the worst day situation under the proposed future emission pattern.

Many people in the field of air pollution research believe that multiple cell/Eulerian models are the only promising models that give useful guidance on photochemical oxidant problems in places such as Los Angeles. However, this type of model requires an enormous modeller effort. Applications are being tested within an active research community (CMAS, 2007). The model appears to be the latest model of its kind under on-going development supported by USEPA. A number of countries in Asia (e.g. Japan, China,

South Korea, Vietnam and Thailand) have already developed their capacities to run the model. A cooperative effort might benefit a regional study on transboundary pollution control.

3.3 Data Inputs to Dispersion Models

The data inputs to air quality models mainly consist of emission and meteorological data. The modelling parameters include:

- emission sources including their location, rates of emitting and other characteristics;
- receptor locations;
- characteristics such as deposition rates if deposition is also considered;
- meteorological specifications;
- output options that will specify what kind of values are required (e.g. average concentrations in space and time at each grid point); and
- need to be provided in a format adapted to the input interface of the model.

Emissions

Emission data are a crucial input for any dispersion model. They should be accurate, precise and representative for the area to be considered. No dispersion model can compensate for unreliable emission data. Conclusions and control actions derived from simulated concentrations based on unreliable or wrong emission data may be completely misleading and even useless. Module 2 *Emissions* showed how reliable emission data can be achieved from emissions inventories.

Meteorology

Most air quality dispersion models described in the Guideline on Air Quality Models (FR, 2005; USEPA, 2006e) are Gaussian models requiring input data which represents the conditions at the sites of interest. The input data is also required to follow a prescribed data content and format. As a rule, dispersion models such as AERMOD require five meteorological inputs. These are: wind speed and direction, vertical mixing, temperature and atmospheric moisture. Some slightly more detailed models (such as CALPUFF) may also need dew point, cloud cover, cloud layer(s), ceiling height, visibility, and precipitation amount.

For air quality modelling purposes, meteorological grid models are used in conjunction with chemical interaction models to provide gridded output of chemical species or pollutant data. These meteorological parameters are calculated at distinct spatially equidistant points over an area of interest which is called a grid. When these models are applied in a retrospective mode (i.e. modelling a past event) they are able to blend ambient data with model predictions via four-dimensional data assimilation, in order to produce temporal and spatially complete data sets that are grounded by actual observations.

There are several commonly-used meteorological grid models that can develop inputs for air quality models. These grid models differ in their simulation of atmospheric processes but each produce gridded meteorological parameters. There are also several post-processors which are needed to convert the raw meteorological modelling output to suitable air quality model input. A few of the most commonly used meteorological models and post-processors are briefly described below.

The USEPA has developed the Meteorology-Chemistry Interface Processor (MCIP) tool to convert MM5 output into a photochemical model - CMAQ - input. MCIP provides a complete set of meteorological data needed for air quality simulations. Because most meteorological models are not built for air quality modelling purposes, MCIP deals with issues related to data format translation, conversion of units of parameters, diagnostic estimations of parameters not provided, extraction of data for appropriate window domains, and reconstruction of meteorological data on different grid and layer structures (CMAS, 2002).

Maps/GIS information

A geographic information system (GIS) is a system for capturing, storing, analysing and managing data and associated attributes which are spatially referenced to the earth. In the strictest sense, it is a computer system capable of integrating, storing, editing, analysing, sharing, and displaying geographically-referenced information. GIS is a tool that allows users to analyse the spatial information, edit data, maps, and present the results of all these operations. Modern GIS technologies transfer a hard copy map or survey plan into a digital medium. Geographic data is extracted through digitizing the wide imagery both from satellite and aerial sources. In air pollution modelling GIS information may include parameters such as land use type, elevation, surface parameters (surface roughness length, albedo, soil heat flux, and vegetation leaf area index) and anthropogenic heat flux.

3.4 Data Outputs

The output from dispersion models in general is in the form of spatial and time-dependent concentrations which can then be used to generate contour plots of the concentration values or to test compliance with air quality standards with varying averaging periods. Dispersion models may also be expanded to estimate acid deposition with the objective to develop control strategies. A Lagrangian puff model, in combination with an Eulerian grid approach, was used by the Pollution Control Department (PCD) in Thailand to simulate the sulphur deposition in Thailand, caused by the sulphur dioxide (SO_2) and nitrogen oxide (NO_x) concentrations in the Bangkok Metropolitan Region (BMR). Actions for the reduction of SO_2 and NO_x in the BMR were then investigated and a draft control strategy was prepared (see Figure 3.9, above).

3.5 Validation of Models

The accuracy and precision of a dispersion model's results clearly depend on the model equations used to describe dispersion and on the validity of input data. It is crucial to investigate the reliability of a model by comparing simulated with monitored concentrations in well defined source and meteorological configurations. Under the best circumstances a dispersion model simulates concentrations within about a factor of two of actual observations. However, models often overestimate or underestimate concentrations by even a magnitude due to faulty emission or meteorology parameters. It is, therefore, very important to carefully investigate the model's validity. A most recent and comprehensive guideline for dispersion model validation was prepared by FST (2005).

Another approach of validating models is to do model inter-comparison. The aim is to:

- have a common understanding of model performance and uncertainties;
- improve the understanding of the long-range transport of air pollutants.

A model inter-comparison for long-range transport of sulphur in Asia was completed in 2000 (Carmichael *et al*., 2001; 2002). The estimations of eight models for sulphur long range transport were compared in the MICS-Asia Phase-I study. The results showed discrepancies among the models used for the estimation of long-range transport of sulphur which may be due to difference in emission estimates used in the models. Following this study, it was felt that nitrogen compounds, O_3 and aerosols are also critical compounds for effective control of air pollution problems in Asia and the MICS-Asia Phase-II study was initiated (ADORC, 2006).

Section 4 Source Apportionment

4.1 Source Apportionment and Receptor Models

Source apportionment (SA) is the determination of the contribution (fraction, percentage or portion) of air pollution sources at a location of interest. Air pollution originates from sources such as industries, power plants, cars, buses, trucks, boats, windblown dust and open burning. The development of effective control strategies to protect public health and the environment from exposure to air pollution requires knowledge of emission sources that contribute to the pollutant concentrations at the receptor. Pollutant concentrations are obtained from ambient air samples collected at a receptor location.

Table 3.2 gives an overview over the methodologies used in SA.

Two essentially different approaches are used in source apportionment:

- source-oriented approach; and
- receptor-oriented approach.

The *source-oriented approach* starts from an emissions inventory and uses dispersion models in the form of chemical transport models (CTMs) to estimate the contribution of each source at a receptor location. Transport calculations use emission and source characteristics (stack height, exit velocity of stack

Table 3.2: Source apportionment methodology

Approach	Model	Methodology	Reference
Source-oriented	Mechanistic Analysis Techniques	Emissions Inventory Analysis	Kleeman (2003)
		Chemical Transport Models (CTMs), forward estimation	Kleeman (2003)
		Chemical Transport Models (CTMs), backward estimation	Environ (2004)
Receptor-oriented	Unique Chemical Tracer Analysis	Single tracer estimation model	Kleeman (2003)
	Statistical Analysis using Chemical Profiles.	Linear Statistical Models	Kleeman (2003)
		Chemical Mass Balance (CMB) Model	Henry *et al*. (1984); Watson *et al*. (1984); USEPA (2006c); Hildemann (2006s;b)
		Bi-Linear Statistical Models	Henry *et al*. (1984)
		Principal Component Analysis	Henry and Kim (1990); Henry *et al*. (1999); Hildemann (2006a)
		Factor Analysis	Kleeman (2003); USEPA (2006d;2007a)
		Positive Matrix Factorization	Huang *et al*. (1999); Hildemann (2006a;b); USEPA (2006c;d;2007a)
		Empirical Orthogonal Functions	Ashbaugh *et al*. (1984); Gebhart *et al*. (1997)
		Hybrid Statistical Models	Kleeman (2003)
		Chemical Mass Balance with Factor Analysis of Residuals	Kleeman (2003)
		Target Transformation Factor Analysis (TTFA)	Hopke (1988)

Source: Adapted from Kleeman (2003)

gas, pollutant concentrations in exhaust gas) and known meteorological parameters (wind speeds, wind directions, temperature, mixing heights and atmospheric stability classes) to predict pollutant concentrations at specific receptor air monitoring locations. This type of models can be validated by comparison of the predicted spatial and temporal distribution of pollutant concentrations with measured concentrations.

A recent example of a CTM is the Comprehensive Air quality Model with eXtensions (CAMx; ENVIRON, 2004). It is a publicly available model for integrated assessment of gaseous and particulate air pollution. CAMx is designed to:

- simulate air quality over many geographic scales;
- treat a wide variety of inert and chemically active pollutants such as O_3; inorganic and organic PM ($PM_{2.5}$/PM_{10}); mercury and other toxic pollutants; and
- be computationally efficient and easy to use.

CAMx can be used with inputs from any meteorological model and emission inputs from any emissions processor.

CTMs can be applied in both forward and backward directions. In case of backward dispersion modelling, the models start from concentrations at the receptor location and traces back the air parcels that produced these concentrations and the potential sources. This backward approach can be considered as receptor-oriented as it does not use pollutant emissions.

Receptor-oriented approaches have been termed, by USEPA, "receptor models". They are mathematical or statistical procedures that use and compare the profiles of gases and particles (chemical and physical characteristics) at sources and receptors in a given area to estimate the presence and fraction of source contributions at receptor locations. Unlike CTMs, receptor models do not use pollutant emissions, meteorological data and chemical transformation and deposition mechanisms to estimate the contribution of sources to receptor concentrations (USEPA, 2007a). Receptor models cannot identify the contribution of individual sources if several sources of the same type and emission characteristics are located in the area considered.

The receptor-oriented approach infers source contributions by determining the best fit linear combination of emission source chemical composition profiles needed to reconstruct the measured chemical composition of ambient samples (Watson *et al*., 1984). This is particularly advantageous for sources which are very difficult to assess (e.g. fugitive dust). Receptor models that are widely used are Chemical Mass Balance (CMB) models and factor analyses.

ENVIRON (2005) has developed a reactive tracer method for PM source apportionment called Particulate Matter Source Apportionment Technology (PSAT). PSAT has been implemented in CAMx to provide source apportionment for primary and secondary PM species to geographic source regions, emissions source categories, and individual sources (ENVIRON, 2005). PM source apportionment information from PSAT can be used for assessments to identify what sources contribute significantly to PM and visibility problems.

The USEPA has until now developed three models; the:

- CMB model, based on source emission profiles;
- UNMIX model, generating source profiles from ambient concentrations; and
- positive matrix factorization (PMF) model, also generating source profiles from ambient concentrations (USEPA 2007a).

The USEPA-CMB model (version 8.2) quantifies the contributions from chemically distinct source-types (i.e. sources with similar chemical and physical properties cannot be distinguished from each other by CMB). CMB requires speciated profiles of potentially contributing sources and the corresponding ambient data from analysed samples collected at receptor sites (USEPA, 2006c).

The USEPA UNMIX model estimates the number of sources, source compositions, and source contributions to each given sample of PM concentrations of chemical species measured in the ambient air of a receptor location. Chemical profiles of the sources are generated internally from the ambient data, using a form of factor analysis (USEPA, 2006d; 2007a).

The USEPA PMF technique is a form of factor analysis. The many co-varying variables of samples are described by a small set of factors (e.g. PM sources) related to the original variables. The structure of PMF permits maximum use of available data and better treatment of missing and below-detection-limit values (USEPA, 2007a). A file of concentrations where each column contains a different species and each row contains a different time. Typically an hour or a day is subjected to a constrained weighted least squares approach to decompose the file into a set of profiles and time series of contributions for each profile. The latest version of USEPA PMF is available for download together with a user's guide (USEPA, 2007b). A document which discusses the PMF methodology is also available (USEPA, 2007a; 2007c).

Challenges of source-oriented approaches:

- emission rates are difficult to estimate;
- fugitive sources may elude quantitative estimation;
- transport phenomena may be complicated (e.g O_3, VOCs);
- chemical transformation (secondary air pollutants), deposition, boundary and initial conditions must be known;
- meteorological parameters must be adequate.

Challenges of receptor-oriented approaches:

- sources with similar emission profiles cannot be distinguished;
- if in CMB the emission profiles of all sources in an area are not included, the assessment of CMB models may be misleading;
- profiles might change between source and receptor due to production chemical transformation (secondary pollutants), deposition and interaction with transboundary pollutants;
- consequences of emission reduction cannot be predicted.

4.2 PM Nuclear Analysis in Source Apportionment

For the purpose of source apportionment, airborne PM retained on the filter may be examined or analysed chemically by a variety of methods. Nuclear Analytical Techniques (NATs) are considered here because of their advantages in analysing many elements in air PM non-destructively and simultaneously. The key three NATs for analysis of PM in air are:

- Neutron activation analysis (NAA)
- X-ray fluorescence (XRF)
- Ion beam analysis (IBA).

In the South Asian and Western Pacific regions, NATs exist in thirteen countries (see Table 3.3). In addition, IBA facilities exist in Australia and New Zealand.

Neutron Activation Analysis

In typical NAA, a sample of PM on a filter is exposed to a high flux of thermal neutrons in a nuclear reactor or accelerator. Stable nuclides in the sample (target nucleus) undergo neutron capture reactions. The radioactive nuclides (compound nucleus) produced in this activation process will, in most cases, decay through the emission of a beta particle (ß-) and gamma ray(s) with a unique half-life. After the sample has been removed

from the reactor it continues to emit radiation as the radioactive isotopes decay. A high-resolution gamma-ray spectrometer is used to detect these "delayed" gamma rays from the artificially induced radioactivity in the sample for both qualitative and quantitative analysis. Figure 3.14 illustrate the principle of the method.

Standard materials of known composition are irradiated at the same time for calibration. The spectrum of energy of the gamma rays determines the specific isotopes present in the sample. The intensity of the gamma rays is proportional to the amounts of elements present. Typically five counting regimes are required to detect these elements. The counting regimes are applied after 300 s, 1 hour, 10 hours, 4 days and 15 days. It is highly sensitive (ppb range for many elements), though it does not quantify elements such as silicon, nickel, cobalt, and lead. Typical elemental detection limits range from 0.01 to 10 ng m^{-3}. Individual elemental detection limits can be found in USEPA (1999a). For more detailed information on NAA analysis of PM analysis see Weizhi (2000).

NAA is a simultaneous, multi-element method that can be used to measure more than 40 elements and does not generally require significant sample preparation. It is a non-destructive technique and does not require the addition of any foreign

Table 3.3: Key Nuclear Analytical Technique Facilities in Asian Countries

Country	City	Key NAT facility
Bangladesh	Dhaka	IBA/PIXE
China	Beijing	IBA/PIXE
India	Mumbai	NAA
Indonesia	Bandung	NAA
Korea, Republic of	Daejon	NAA
Malaysia	Kuala Lumpur	NAA
Mongolia	Ulaanbaatar	XRF
Pakistan	Islamabad	NAA
Philippines	Manila	XRF
Singapore	Singapore	IBA/PIXE
Sri Lanka	Colombo	XRF
Thailand	Bangkok	XRF
Vietnam	Hanoi	NAA

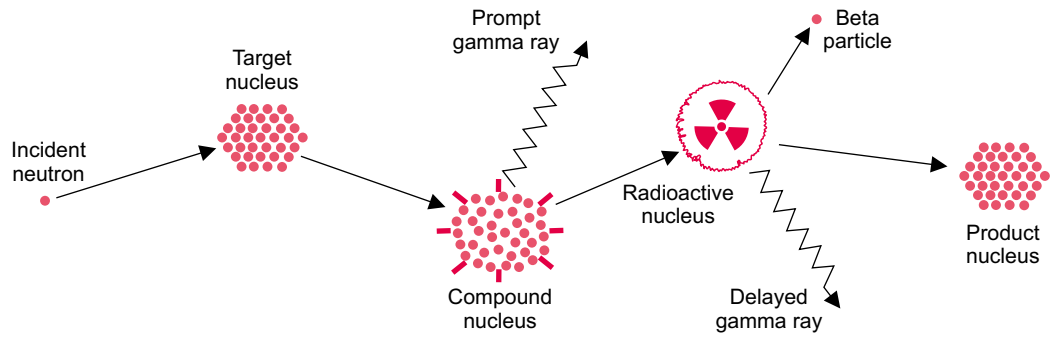


Figure 3.14: Sequence of events that occur during the most common type of nuclear reaction used for neutron activation analysis

Source: Glascock (2004).

materials to the sample for analysis; thus, the problem of reagent-introduced contaminates does not occur. Analysis by NAA is compatible with sampling by high-volume (TSP; PM_{10}) and dichotomous samplers.

X-ray fluorescence spectroscopy

When a primary X-ray from an X-ray tube or a radioactive source hits a sample of PM collected on a filter, the X-ray can either be absorbed by a PM atom or scattered through the material. The process in which an X-ray is absorbed by an atom by transferring all of its energy to an innermost electron is called the "photoelectric effect." If the primary X-ray had sufficient energy, electrons are ejected from the inner shells, creating an excited atom with vacancies on inner shells. These vacancies present an unstable condition for the atom. As the atom returns to its stable condition, electrons from the outer shells are transferred to the inner shells and in the process emit a characteristic X-ray whose energy is the difference between the two binding energies of the corresponding shells. Because each element has a unique set of energy levels, each element produces X-rays at a unique spectrum of energies, allowing one to identify the element and to measure the elemental composition of a PM sample (AmpTek, 2002). Figure 3.15 illustrates the measuring of compounds in samples by XRF.

In XRF spectroscopy, many elements can be measured simultaneously. XRF is non-destructive and requires minimal (or no) sample preparation - the filter is inserted directly into the instrument for analysis. This technology is relatively inexpensive. Because quartz filters used in high-volume samplers cause high background in XRF analysis, filters used in the dichotomous samplers are preferable.

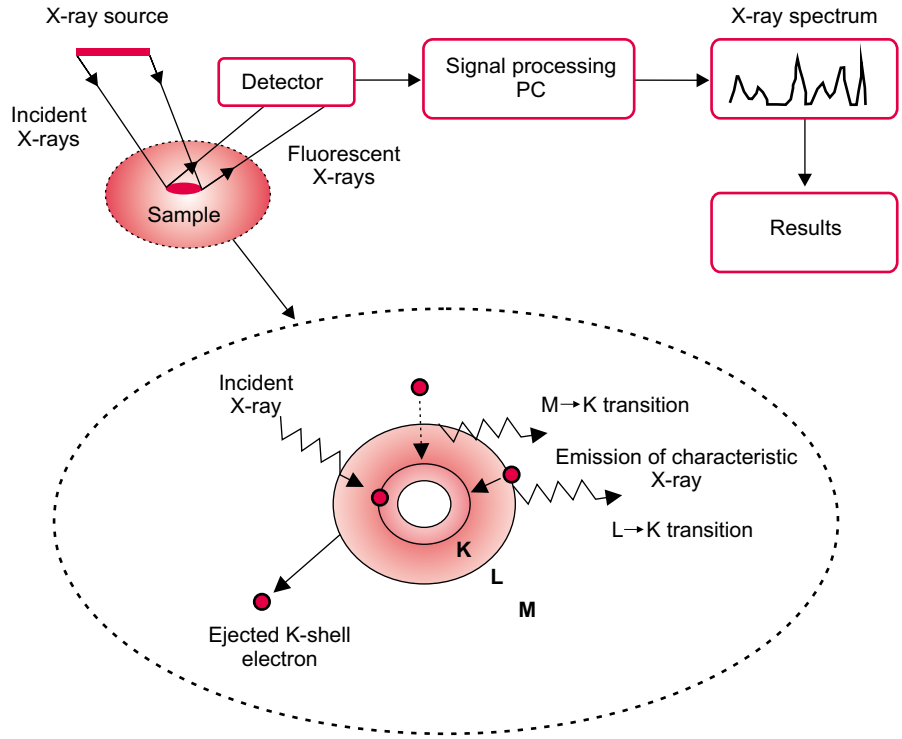


Figure 3.15: The principle of XRF and the typical XRF detection arrangement

Source: Papachristodoulou (2002)

X-ray fluorescence spectrometry can be used for all elements with atomic numbers from 11 (sodium) to 92 (uranium). Typical elemental detection limits for this method range between 2 and 2000 ng m^{-3} (USEPA, 1999b). XRF depends on the availability of PM standards. Two laboratories are currently main suppliers for PM standards:

- National Institute of Standards and Technology (NIST, 2004);
- Institute for Reference Materials and Measurements (IRMM, 2004).

These PM standards are well suited to solve many problems. More details on XRF may be found in Jenkins (1999), Kalnicky and Singhvi (2001), and Van Grieken and Markowicz (2002).

Ion beam analysis

IBA is based on the interaction, at both the atomic and the nuclear level, between accelerated charged particles and the bombarded material, e.g. PM on a filter (see Figure 3.16). When a charged particle moving at high speed strikes a material, it interacts with the electrons and nuclei of the material atoms, slows down and possibly deviates from its initial trajectory. Electrons in the inner shells of the atom (predominantly the K and L shells) are given enough energy to cause them to be ejected, resulting in an unstable electron atomic configuration. Electrons from higher shells in the atom then 'drop down' to fill these vacancies, and in so doing, give off excess energy in the form of X-rays. The energies of these X-rays are characteristic of the element and therefore can be used to identify the elements which constitute the sample material. IBA comprises a suite of four techniques:

- particle induced X-ray emission (PIXE);
- particle induced gamma ray emission (PIGE);
- proton elastic scattering analysis (PESA); and
- Rutherford backscattering spectrometry (RBS).

These techniques are used simultaneously as key analytical tools to assess PM pollution on a regular basis. Most importantly, the choice of analytical method depends on the inorganic compounds of interest and the detection limits desired. Using the four different analysis techniques, IBA can measure more than 40 elements (H – U).

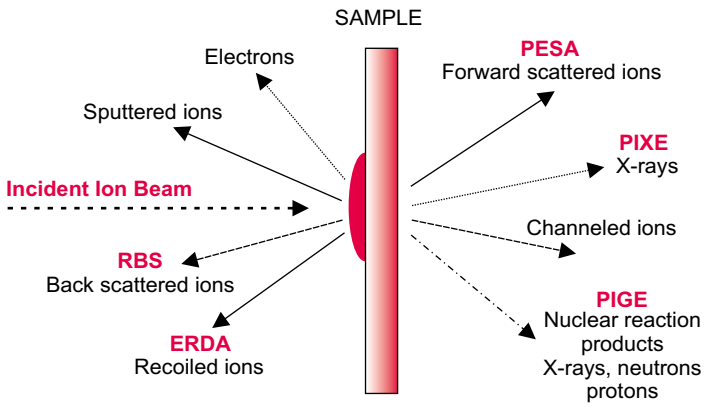


Figure 3.16: Ion beam analysis methods

Source: Garnir and Strivay (1997)

PIXE Particle (Proton) Induced X-ray Emission Analysis

PIXE is a powerful and relatively simple analytical technique that can be used to identify and quantify trace elements typically ranging from sodium (Na) to uranium (U). Sample irradiation is usually performed by means of 2-3 MeV protons produced by an accelerator. X-ray detection is usually done by energy dispersive semi-conductor detectors such as Silicium (Lithium) or High Purity Germanium detectors. This multi-elemental analysis technique can measure more than 30 elements in a short time due to higher cross-sections as compared to XRF. Analysis by PIXE typically involves collecting $PM_{2.5}$ by dichotomous samplers. With the addition of PIGE and PESA, IBA allows for the detection of light elements that is useful for finger printing, source apportionment and estimation of organic carbon. Specific experimental set-ups are used to measure air filters semi-automatically (Cohen *et al*., 1996; Cohen, 1996; Cohen *et al*., 2000; Cohen, 2000; Trompetter *et al*. (2000a; b). Typical detection limits range from 1 to 50 ng m^{-3}. For detailed information on PIXE and PIGE in PM analysis see Cohen *et al*. (2000) and Cohen (2000).

The remaining three methods are used simultaneously to achieve additional information on elements that can be insufficiently measured with PIXE.

PIGE Particle (Proton) Induced γ-ray Emission Analysis

When a charged particle (typically protons) approaches the nucleus of a target atom, the Coulomb force usually repels it. However, when the incident particle has enough energy to overcome the repulsive Coulomb force a charged particle then penetrates through the electrostatic barrier into the nucleus, resulting in interactions with the nuclear forces. During that process, a number of interactions occur, depending on the energy of the incident particle and the type of target nucleus. Typically, a nuclear reaction will occur, resulting in the emission of high energy X-rays (X-rays emitted from nucleus are for historical reasons called gamma rays) and other nuclear particles. In the case of PIGE technique, emitted gamma rays are of particular interest as their energies are characteristic of the element and are therefore used to fingerprint elemental composition while yields are used to quantify elemental concentrations. The detection of the emitted gamma rays is usually done by large volume germanium detectors. PIGE is typically run in conjunction with PIXE and RBS and is used to quantify concentrations of elements such as Boron (B), Lithium (Li), Fluorine (F), Sodium (Na), Magnesium (Mg) and Aluminium (Al) in PM samples (Cohen, 1993). Detection limits vary from element to element and are in the range of about a hundred ng m^{-3}, the uncertainty of data is around a few per cent.

PESA Proton elastic scattering analysis

This is similar to Rutherford backscattering analysis (RBS) but in forward direction and is used to measure hydrogen (H) to help to distinguish between elemental and organic carbon in PM samples. H in PM collected on a filter can be measured providing the filter material is free of hydrogen. Hence Teflon filters consisting of only carbon and fluorine are hydrogen free whereas polycarbonate filters contain much more hydrogen on such filter materials. The limit of detection is approximately 20 ng m^{-3}. A technical good description of PESA can be found in Cohen (1993).

RBS Rutherford Backscattering Spectrometry

In RBS backscattered ions are detected, and backscattering can only occur if the target atom's mass is heavier than that of the incident ion. RBS allows the measurement of mainly carbon (C), nitrogen (N) and oxygen (O) in PM samples. Since RBS can measure the total carbon deposited onto filters, it is possible to distinguish between elemental and organic carbon using RBS. Typical limits of detection for the three elements are in the range of 100 – 400 ng m^{-3}; the typical uncertainty of data is a few per cent. Additionally, RBS can

provide extra information on individual particles. Technical descriptions of RBS used in fine particle pollution studies are published in Markwitz *et al*. (1997;1998a; b); Markwitz (2000) and Cohen (1995). Figure 3.17 shows a typical experimental setup (Trompetter and Markwitz, 2002).

Advantages and Disadvantages of Nuclear Analytical Techniques

Table 3.4 summarises the major technical advantages and disadvantages of these analytical techniques (USEPA, 1999a; b; Markowicz *et al*., 2002). While factors such as element specificity and sensitivity are critically important, considerations such as cost and throughput (the number of samples and number of elements to be determined per sample) are also important.

Apart from the technical disadvantages of NATs indicated in Table 3.4, the costs of establishing a dedicated system and the off-line nature of NATs are key disadvantages, which have limited the use of NATs for PM analysis in Asia. In addition, NAA needs access to a research nuclear reactor.

Current manufacturers of particle accelerators are High Voltage Engineering in The Netherlands (HVE, 2008) and National Electrostatics Corporation in the United States (NEC, 2007). Both companies offer 'cheap' bench-top accelerators that require approximately 10 m^2 of floor space in an air-

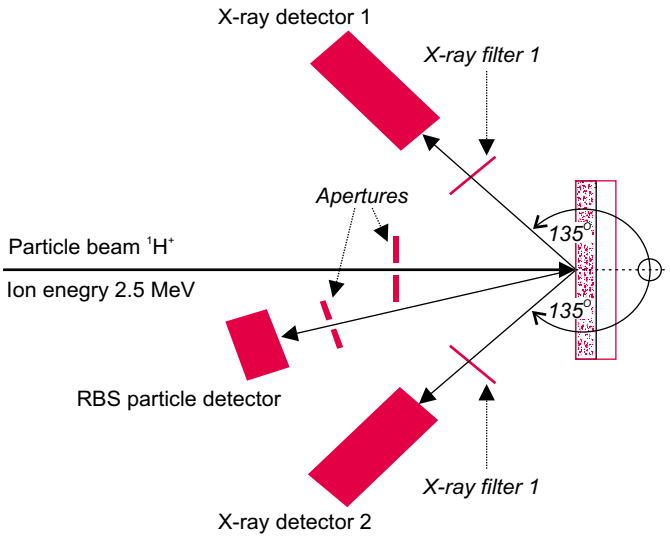


Figure 3.17: Schematic of a typical experimental setup

Source: Trompetter and Markwitz (2002).

Table 3.4 Major technical advantages and disadvantages of selected analytic techniques

NAT	Advantages	Disadvantages
NAA	multi-element non-destructive minimal sample preparation % to ppb range high sample throughput well documented applications	some elemental interferences standard sample matrix corrections required access to research nuclear reactor
XRF	multielement non-destructive minimal sample preparation	standard/sample must match closely (matrix) matrix offsets and background impurities may be a problem
PIXE	multielement non-destructive minimal sample preparation	standard/sample must match closely (matrix) matrix offsets and background impurities may be a problem

Source: USEPA (1999a)

conditioned building and cost approximately US$ 500,000. The dedicated beam line can be homemade, which is normally the case, or purchased from international organisations for approximately US$ 250,000. In summary, for less than US$ 1M, which would exclude the air-conditioned building, a dedicated machine can be purchased. Cost-sharing among countries or commitments from donor agencies may help to overcome the first disadvantage for IBA and XRF.

Application of Nuclear Analytical Techniques in Source Identification

Sources that emit PM can be identified by the elements that are present in the particles or on their surfaces. In order to be able to identify the specific sources unambiguously, key elements have to be measured since many elements originate from many different sources of pollutants. In assisting this task, information is used from large databases on elemental composition generated by NATs for the samples collected. These are available in some individual countries. In the following, examples are given that link key elements to their origin.

In Australia, IBA/PIXE is used to identify the elements for identifying pollution sources (see Table 3.5) (Cohen, 2000).

In Beijing, China, NAA is used to identify major PM pollution sources (see Table 3.6)

PM pollution sources in Vietnam were also identified by NAA (see Table 3.7).

More recently source apportionment using nuclear techniques was performed in Metro Manila (Santos *et al.*, 2004). The coarse particle fraction was determined by a soil-cement mixture and the S-fraction, followed by vehicle emissions and soil tirewear. In contrast, the fine fraction was determined by biomass burning and oil burning, with smaller fractions of aged salt and black carbon (see Figure 3.18). These results give a clear indication of the importance of the various sources and areas where pollution control should be focused (e.g. reduction of biomass and oil burning).

Table 3.5: Sources of PM pollution in Australia as identified by IBA/PIXE

Source	Elements
Motor Vehicles	H, Na, Al, Si, S, Cl, Fe, Zn, Br, Pb, elementary C
Smoke	H, P, Cl, K, Ca, Mn, elementary C
Soil	Al, Si, K, Ca, Ti, Mn, Fe
Seaspray	Na, S, Cl, K, Ca, Br
Industry	H, P, S, V, Cr, Ni, Cu, Zn, Pb, elementary C

Al-aluminium; Br-bromine; C-carbon; Ca-calcium; Cl-chlorine; Cr-chromium; Cu-copper; Fe-iron; H-hydrogen; K-potassium; Mn-manganese; Na-sodium; Ni-nickel; P-phosphorus; Pb-lead; S-sulphur; Si-silicon; Ti-titanium; V-vanadium; Zn-zinc

Source: Cohen *et al*. (2000)

Table 3.6: Sources of PM pollution in Beijing as identified by NAA

Source	Elements
Soil, flying ash	Al, Ba, Ca, Ce, Fe, Ga, Hf, La, Mg, Sc, Sm, Th, Ti, V
Refuse incineration	As, Cs, I, K, Rb, Sb, Se, Zn
Motor Vehicles and Coal Burning	As, Br, Co, Ga, Sb, Se, U, V, W
Seaspray	Cl, Na

Al-aluminium; As-arsenic; Ba-barium; Br-bromine; C-carbon; Ca-calcium; Ce-cerium; Cl-chlorine; Co-cobalt; Fe-iron; Ga-gallium; Hf-hafnium; I-iodine; K-potassium; La-lanthanum; Mg-magnesium; Rb-rubidium; Sb-antimony; Sc-scandium; Se-selenium; Sm-samarium; Th-thorium; Ti-titanium; U-uranium; V-vanadium; W-tungsten; Zn-zinc

Source: Weizhi (2000).

It is important to note that at the different locations the same types of sources are characterised by different elements. For example, Zn is an indicator of vehicle emissions in Vietnam (Hien, 2000) and Australia (Cohen *et al.*, 2000) but not in Beijing (Weizhi, 2000). Therefore harmonisation in the correspondence of elements and source types is necessary.

Table 3.7 Sources of PM pollution in Vietnam as identified by NAA

Source	Elements
Vehicular Emissions	Br, Zn
Coal Burning	Se
Industrial processes	Ce, Co, Cr, Pb, Sb
Road dust	Al, Ti, V
Soil dust	Fe, Th
Biomass burning	K
Marine aerosols	Na, Cl
Mineral fly ash	Sc, La

Al-aluminium; Br-bromine; Ce-cerium; Cl-chlorine; Co-cobalt; Cr-chromium; Fe-iron; K-potassium; La-lanthanum; Sb-antimony; Sc-scandium; Se-selenium; Th-thorium; Ti-titanium; V-vanadium; Zn-zinc

Source: Hien (2000).

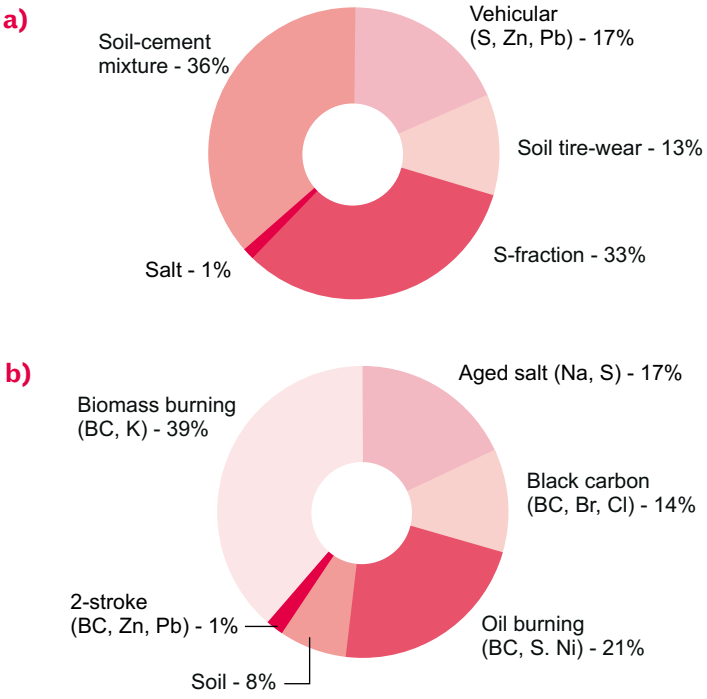


Figure 3.18: Source apportionment of coarse (a. $PM_{10-2.5}$) and fine (b. $PM_{2.5}$) particulate matter in Metro Manila

BC-black carbon; Br-bromine; Cl-chlorine; K-potassium; Na-sodium; Ni-nickel; Pb-lead; S-sulphur; Zn-zinc

Source: Santos *et al.* (2004).

3

Summary

Air quality modelling is an important component of AQM as it allows an understanding of the relative concentration of air pollutants, which can be used to achieve cost-effective pollution control measures. In this module you have learnt how modelling of air pollutants can be used to estimate pollutant concentrations in time and space. You have gained an understanding of the:

- basic components of an air quality simulation module
- role of emission estimates
- applications of dispersion models
- role of monitoring and modelling
- role of wind, turbulence, mixing height and stability
- difference between local and regional phenomena
- influence of topography on meteorological parameters.

You have also learnt about the relevance of air pollution meteorology to modelling (e.g. wind profiles, turbulence and solar radiation) and the different types of air quality dispersion models available, their data requirements and their limitations:

- Steady-state, non steady-state and grid models
- Forecast models
- Gaussian dispersion models
- Puff models
- Eulerian models.

You should now recognise the importance of the quality of input data – both emission and meteorological data and the needs for the validation of the models. Finally, you have learnt about source apportionment, receptor models and analysis methods including using nuclear techniques.

The key messages you should take away from this module on modelling are:

- Dispersion models are a suitable means of estimating air pollutant and greenhouse gas concentrations from stationary and mobile sources, particularly in cases where it is too expensive to monitor or for compounds for which no monitoring methods exist.
- Dispersion models need reliable input data, both from emission inventories and meteorological measurements or models.
- Dispersion models should be validated by means of monitoring data, if available.
- The Gaussian dispersion models and/or Puff models should be used.
- There are several source apportionment approaches which help to determine the contribution of individual source types to air pollution. These approaches do not replace emissions inventories but may be a first step to assess the relevance of different source types.

In Module 4 *Monitoring* you will learn about the role of air quality monitoring in AQM, the factors which need to be considered in the design of an air quality monitoring programme and the different types of monitoring equipment available. You will also examine the issues related to the interpretation and reporting of air quality data.

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